Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:44 PM GMT

PDB ID	:	1GQO
Title	:	TYPE II DEHYDROQUINASE FROM BACILLUS SUBTILIS
Authors	:	Robinson, D.A.; Roszak, A.W.; Coggins, J.R.; Lapthorn, A.J.
Deposited on	:	2001-11-28
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

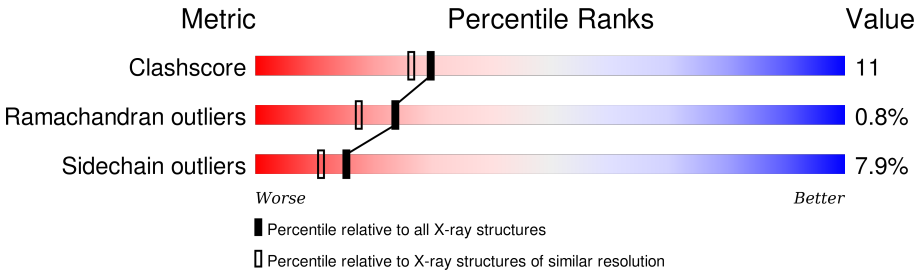
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	64% 27% 9%
1	B	143	65% 29% 6%
1	C	143	78% 17%
1	D	143	71% 24%
1	E	143	71% 19% 8%
1	F	143	78% 19%
1	G	143	71% 24%

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Mol	Chain	Length	Quality of chain
1	H	143	63% 29% 5%
1	I	143	62% 27% 8%
1	J	143	69% 26% 5%
1	K	143	67% 24%
1	L	143	62% 27% 8%
1	M	143	69% 27%
1	N	143	69% 20% 7%
1	O	143	73% 22%
1	P	143	69% 23% 6%
1	Q	143	76% 21%
1	R	143	66% 27% 6%
1	S	143	70% 22% 6%
1	T	143	76% 17% 6%
1	U	143	69% 24% 5%
1	V	143	72% 18% 5%
1	X	143	69% 22% 6%
1	Y	143	67% 26% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	151	-	-	X	-
2	GOL	D	151	-	-	X	-
2	GOL	G	151	-	-	X	-
2	GOL	K	152	-	-	X	-
2	GOL	L	151	-	-	X	-
2	GOL	O	151	-	-	X	-
2	GOL	O	152	-	-	X	-
2	GOL	P	151	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	Q	151	-	-	X	-
2	GOL	R	151	-	-	X	-
2	GOL	S	151	-	-	X	-
2	GOL	S	152	-	-	X	-
2	GOL	U	151	-	-	X	-
2	GOL	Y	151	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28764 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DEHYDROQUINASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	0	0	1
			1094	696	190	208			
1	B	143	Total	C	N	O	0	0	0
			1105	705	191	209			
1	C	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	D	142	Total	C	N	O	0	1	1
			1094	696	191	207			
1	E	142	Total	C	N	O	0	2	1
			1108	707	190	211			
1	F	142	Total	C	N	O	0	3	1
			1107	706	191	210			
1	G	142	Total	C	N	O	0	2	1
			1101	702	191	208			
1	H	142	Total	C	N	O	0	0	1
			1096	700	190	206			
1	I	142	Total	C	N	O	0	0	1
			1090	694	190	206			
1	J	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	K	137	Total	C	N	O	0	0	1
			1051	667	185	199			
1	L	142	Total	C	N	O	0	1	1
			1085	689	191	205			
1	M	142	Total	C	N	O	0	1	1
			1098	698	193	207			
1	N	133	Total	C	N	O	0	0	1
			1028	656	178	194			
1	O	142	Total	C	N	O	0	0	1
			1096	697	193	206			
1	P	142	Total	C	N	O	0	0	1
			1099	703	190	206			

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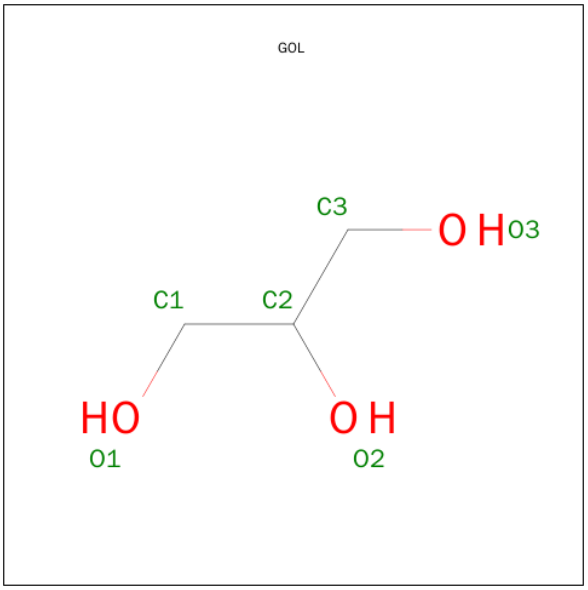
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	0	0	1
			1109	708	193	208			
1	R	142	Total	C	N	O	0	1	1
			1094	696	190	208			
1	S	142	Total	C	N	O	0	0	1
			1108	707	193	208			
1	T	142	Total	C	N	O	0	1	1
			1104	705	190	209			
1	U	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	V	136	Total	C	N	O	0	0	1
			1056	674	184	198			
1	X	134	Total	C	N	O	0	0	1
			1034	659	179	196			
1	Y	142	Total	C	N	O	0	0	1
			1096	700	190	206			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			5	3	2		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			5	3	2		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	X	1	Total C O 6 3 3	0	0
2	X	1	Total C O 6 3 3	0	0
2	X	1	Total C O 6 3 3	0	0
2	Y	1	Total C O 6 3 3	0	0
2	Y	1	Total C O 6 3 3	0	0
2	Y	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	90	Total O 90 90	0	0
3	B	98	Total O 98 98	0	0
3	C	100	Total O 100 100	0	0
3	D	96	Total O 96 96	0	0
3	E	93	Total O 93 93	0	0
3	F	91	Total O 91 91	0	0
3	G	91	Total O 91 91	0	0
3	H	75	Total O 75 75	0	0
3	I	91	Total O 91 91	0	0
3	J	91	Total O 91 91	0	0
3	K	83	Total O 83 83	0	0
3	L	86	Total O 86 86	0	0
3	M	97	Total O 97 97	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	96	Total O 96 96	0	0
3	O	89	Total O 89 89	0	0
3	P	97	Total O 97 97	0	0
3	Q	97	Total O 97 97	0	0
3	R	103	Total O 103 103	0	0
3	S	84	Total O 84 84	0	0
3	T	87	Total O 87 87	0	0
3	U	101	Total O 101 101	0	0
3	V	107	Total O 107 107	0	0
3	X	79	Total O 79 79	0	0
3	Y	80	Total O 80 80	0	0

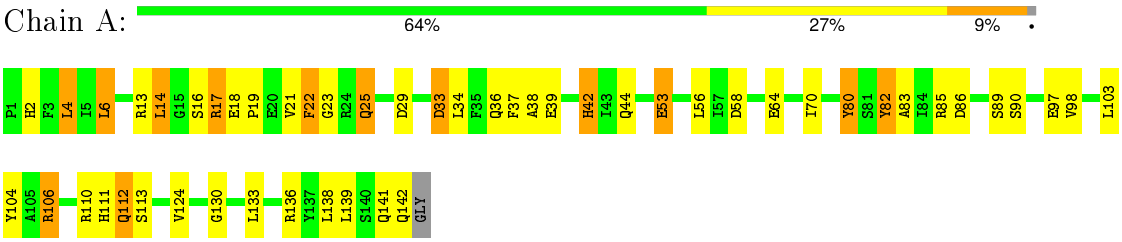
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

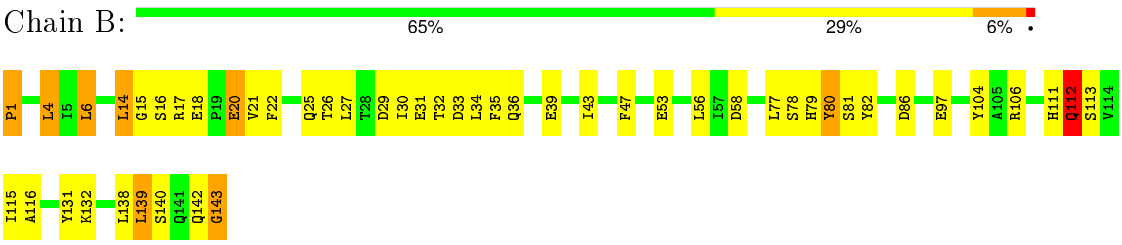
- Molecule 1: DEHYDROQUINASE

Chain A:



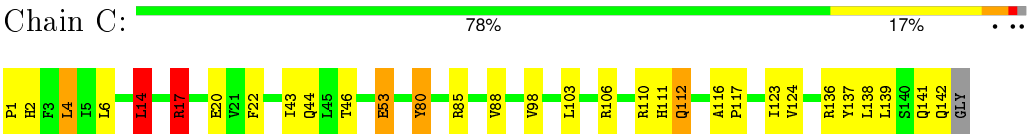
- Molecule 1: DEHYDROQUINASE

Chain B:



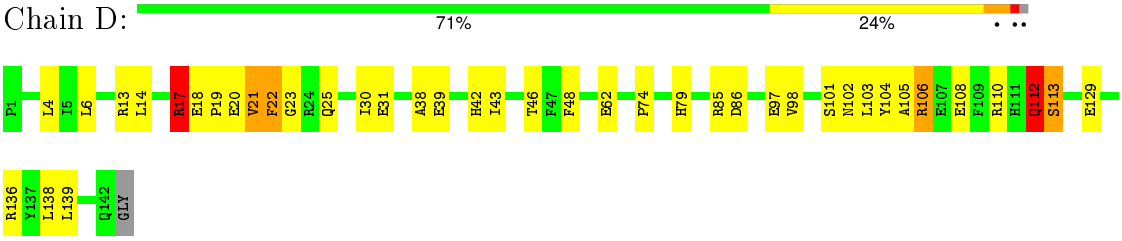
- Molecule 1: DEHYDROQUINASE

Chain C:



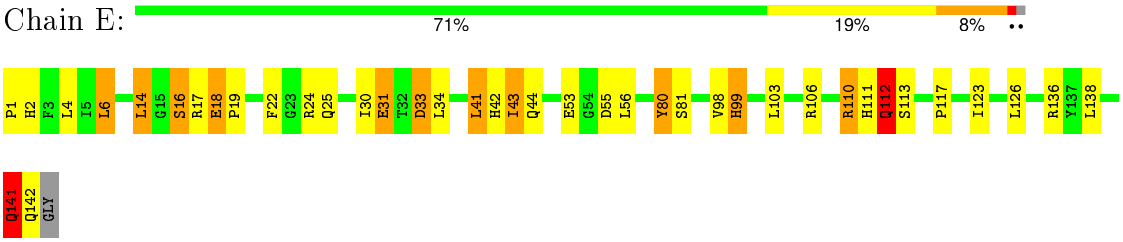
- Molecule 1: DEHYDROQUINASE

Chain D:



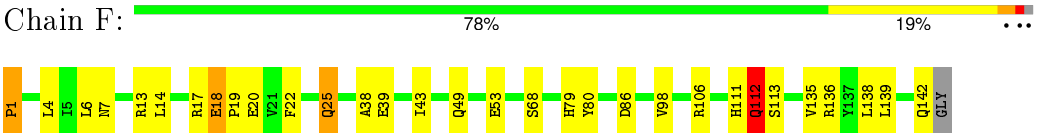
- Molecule 1: DEHYDROQUINASE

Chain E:



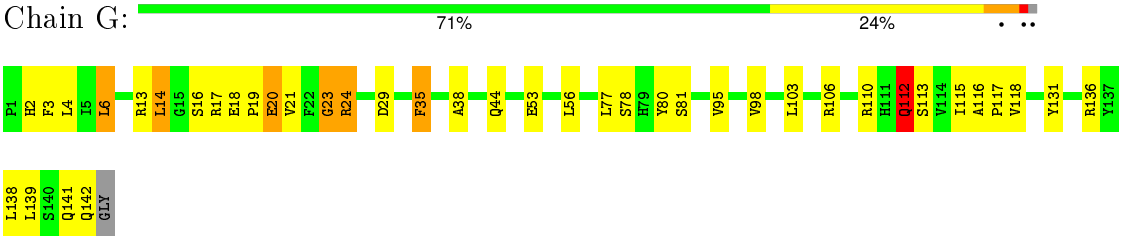
• Molecule 1: DEHYDROQUINASE

Chain F:



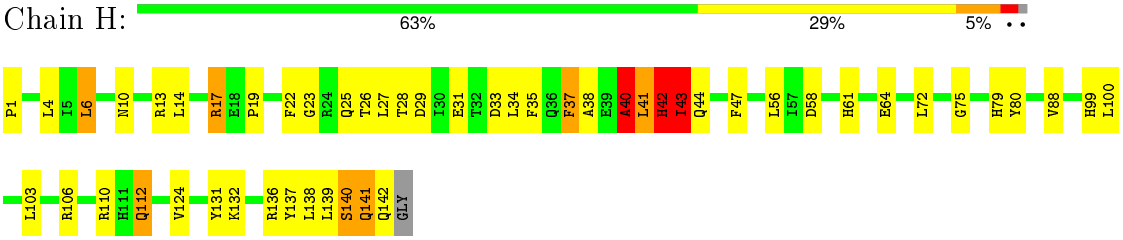
• Molecule 1: DEHYDROQUINASE

Chain G:



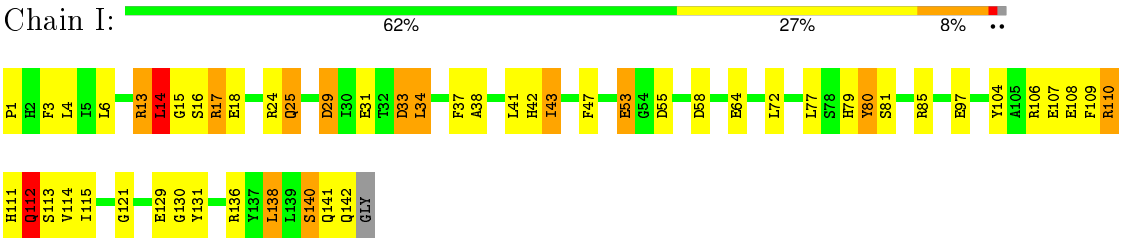
• Molecule 1: DEHYDROQUINASE

Chain H:



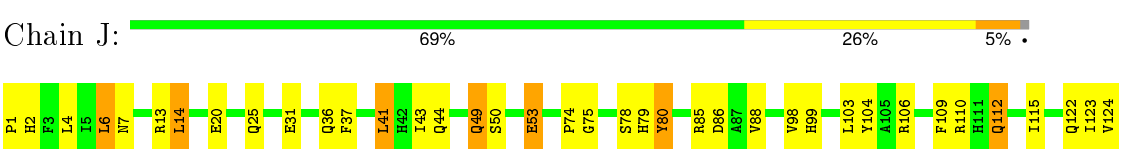
• Molecule 1: DEHYDROQUINASE

Chain I:



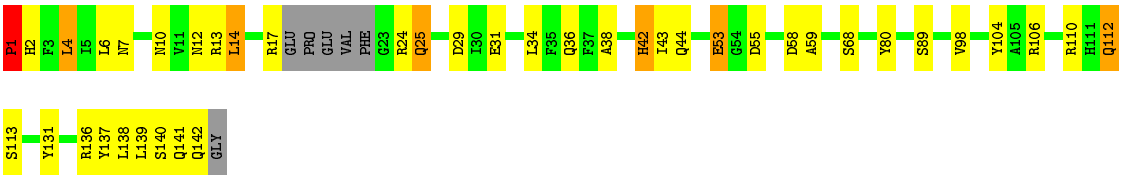
• Molecule 1: DEHYDROQUINASE

Chain J:



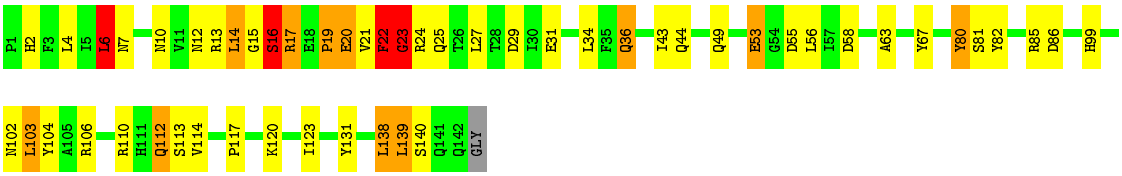
• Molecule 1: DEHYDROQUINASE

Chain K:



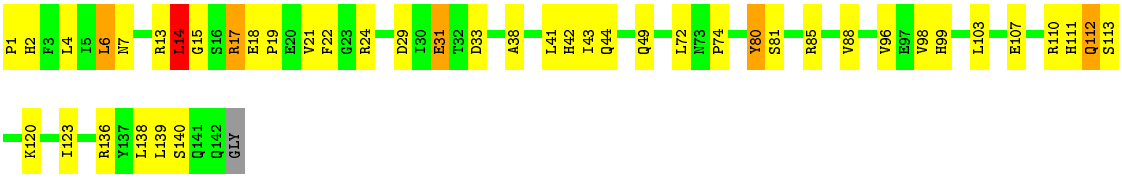
• Molecule 1: DEHYDROQUINASE

Chain L:



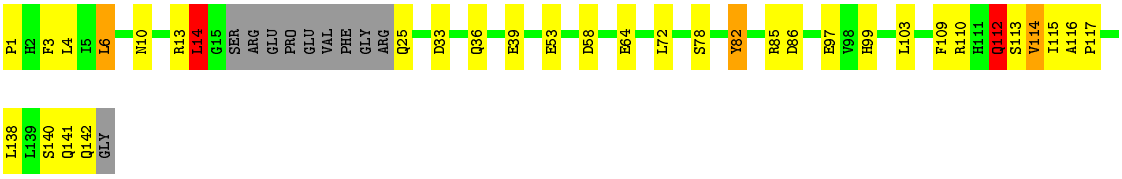
• Molecule 1: DEHYDROQUINASE

Chain M:



• Molecule 1: DEHYDROQUINASE

Chain N:

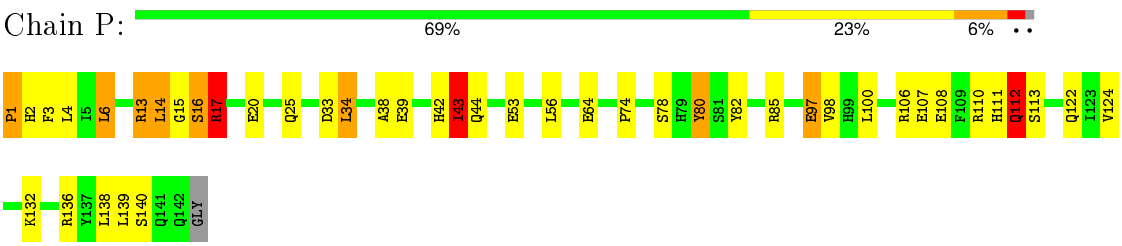


• Molecule 1: DEHYDROQUINASE

Chain O:

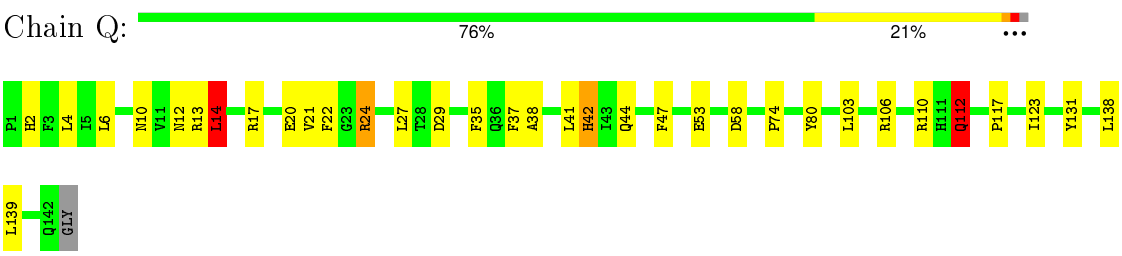
• Molecule 1: DEHYDROQUINASE

Chain P:



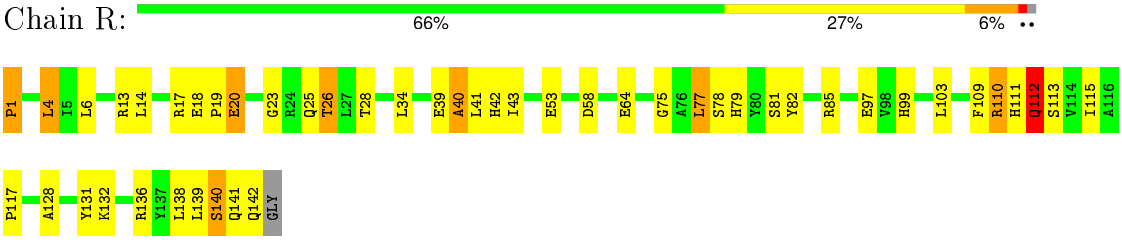
• Molecule 1: DEHYDROQUINASE

Chain Q:



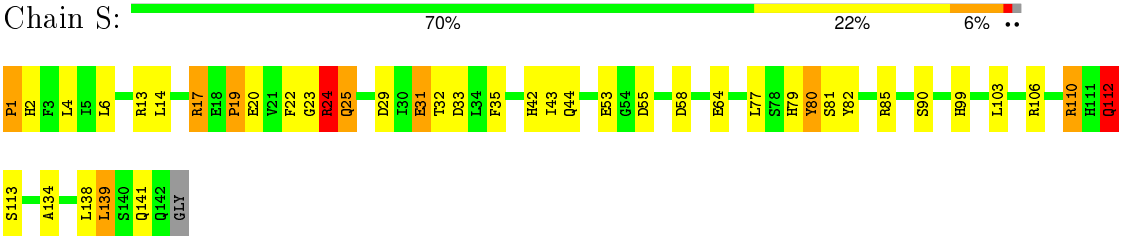
• Molecule 1: DEHYDROQUINASE

Chain R:



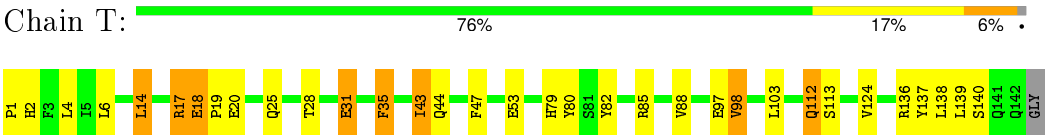
• Molecule 1: DEHYDROQUINASE

Chain S:



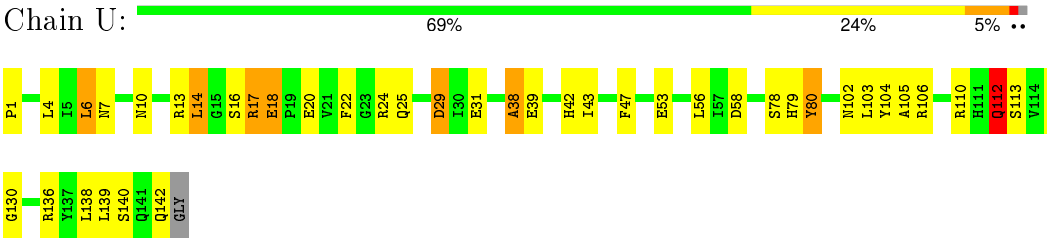
• Molecule 1: DEHYDROQUINASE

Chain T:



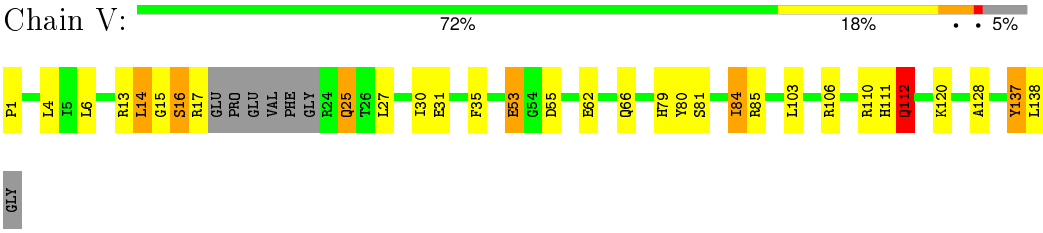
• Molecule 1: DEHYDROQUINASE

Chain U:



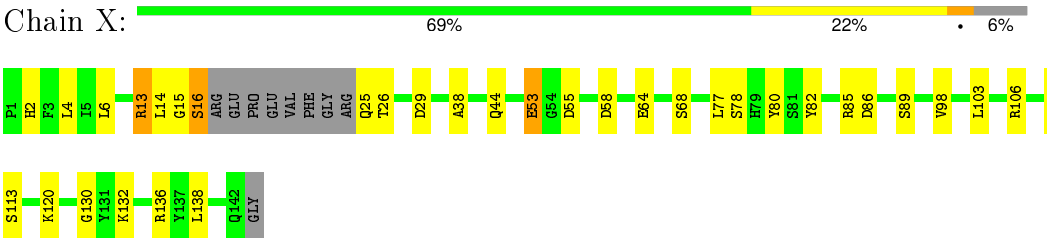
• Molecule 1: DEHYDROQUINASE

Chain V:



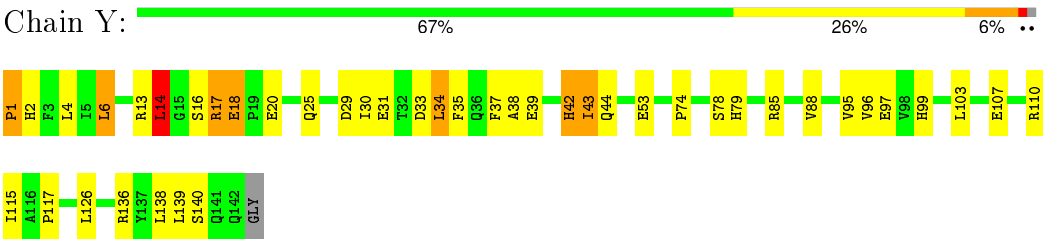
• Molecule 1: DEHYDROQUINASE

Chain X:



• Molecule 1: DEHYDROQUINASE

Chain Y:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.21Å 195.61Å 97.36Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	21.84 – 2.10	Depositor
% Data completeness (in resolution range)	86.0 (21.84-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	0/1117	1.81	27/1519 (1.8%)
1	B	2.48	2/1128 (0.2%)	1.63	16/1529 (1.0%)
1	C	0.92	0/1116	1.63	13/1518 (0.9%)
1	D	0.93	0/1122	1.78	16/1526 (1.0%)
1	E	1.14	1/1143 (0.1%)	2.27	29/1554 (1.9%)
1	F	0.89	1/1146 (0.1%)	1.64	14/1558 (0.9%)
1	G	0.87	0/1135	1.64	16/1543 (1.0%)
1	H	1.14	1/1121 (0.1%)	2.09	28/1525 (1.8%)
1	I	1.02	1/1113 (0.1%)	1.81	29/1514 (1.9%)
1	J	0.88	0/1116	1.68	18/1518 (1.2%)
1	K	0.96	0/1071	1.79	28/1454 (1.9%)
1	L	0.97	0/1112	1.96	41/1513 (2.7%)
1	M	0.94	1/1126 (0.1%)	1.79	18/1530 (1.2%)
1	N	0.94	0/1048	1.89	22/1424 (1.5%)
1	O	0.88	0/1119	1.75	23/1521 (1.5%)
1	P	0.94	1/1123 (0.1%)	1.74	21/1527 (1.4%)
1	Q	0.93	0/1133	1.87	22/1539 (1.4%)
1	R	0.91	0/1122	1.80	27/1526 (1.8%)
1	S	0.91	0/1132	1.75	22/1538 (1.4%)
1	T	0.89	0/1133	1.71	23/1540 (1.5%)
1	U	0.95	0/1116	1.72	11/1518 (0.7%)
1	V	0.88	0/1077	1.62	18/1462 (1.2%)
1	X	0.94	1/1054 (0.1%)	1.84	24/1432 (1.7%)
1	Y	0.94	1/1120 (0.1%)	1.75	17/1523 (1.1%)
All	All	1.06	10/26743 (0.0%)	1.80	523/36351 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	H	0	1
1	I	0	1
1	K	0	1
1	R	0	1
1	X	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLY	C-OXT	76.84	2.69	1.23
1	H	141	GLN	C-N	23.02	1.86	1.34
1	E	141	GLN	C-N	-21.85	0.83	1.34
1	B	39	GLU	CB-CG	-5.93	1.40	1.52
1	F	39	GLU	CB-CG	-5.50	1.41	1.52
1	X	78	SER	CB-OG	5.43	1.49	1.42
1	M	107	GLU	CD-OE2	5.39	1.31	1.25
1	I	107	GLU	CD-OE1	-5.21	1.20	1.25
1	Y	136	ARG	NE-CZ	5.15	1.39	1.33
1	P	39	GLU	CB-CG	-5.13	1.42	1.52

All (523) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	141	GLN	O-C-N	-53.94	36.39	122.70
1	H	141	GLN	O-C-N	-27.34	78.96	122.70
1	H	141	GLN	CA-C-N	-26.95	57.92	117.20
1	Q	24	ARG	CD-NE-CZ	18.41	149.38	123.60
1	N	82	TYR	CB-CG-CD2	17.36	131.42	121.00
1	D	85	ARG	NE-CZ-NH2	15.71	128.16	120.30
1	R	17	ARG	CD-NE-CZ	15.59	145.42	123.60
1	Q	110	ARG	NE-CZ-NH1	15.41	128.00	120.30
1	D	31	GLU	CA-CB-CG	14.80	145.95	113.40
1	H	110	ARG	NE-CZ-NH1	14.77	127.69	120.30
1	Q	24	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	X	86	ASP	CB-CG-OD1	14.50	131.35	118.30
1	L	110	ARG	CD-NE-CZ	14.50	143.90	123.60
1	M	24	ARG	NE-CZ-NH1	14.46	127.53	120.30
1	O	36	GLN	CB-CG-CD	13.67	147.14	111.60
1	E	106	ARG	NE-CZ-NH2	13.11	126.86	120.30
1	L	82	TYR	CB-CG-CD2	13.03	128.82	121.00
1	D	106	ARG	NE-CZ-NH1	12.91	126.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	106	ARG	NE-CZ-NH1	12.90	126.75	120.30
1	Q	24	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	N	82	TYR	CB-CG-CD1	-12.66	113.40	121.00
1	P	106	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	J	13	ARG	NE-CZ-NH1	-12.35	114.13	120.30
1	O	24	ARG	CD-NE-CZ	12.28	140.79	123.60
1	M	110	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	X	53	GLU	OE1-CD-OE2	-12.04	108.86	123.30
1	Y	110	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	M	17	ARG	CG-CD-NE	11.71	136.39	111.80
1	S	106	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	L	106	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	K	136	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	T	85	ARG	NE-CZ-NH1	-11.55	114.53	120.30
1	A	33	ASP	CA-CB-CG	11.51	138.73	113.40
1	N	85	ARG	NE-CZ-NH2	11.51	126.05	120.30
1	H	40	ALA	N-CA-CB	11.45	126.12	110.10
1	N	110	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	R	110	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	L	17	ARG	CD-NE-CZ	11.06	139.09	123.60
1	I	85	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	X	85	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	N	85	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	I	80	TYR	CB-CG-CD1	10.74	127.44	121.00
1	Q	42	HIS	CA-CB-CG	-10.71	95.39	113.60
1	Q	17	ARG	CD-NE-CZ	10.63	138.48	123.60
1	H	17	ARG	CD-NE-CZ	10.57	138.40	123.60
1	E	110	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	E	55	ASP	CB-CG-OD1	10.42	127.68	118.30
1	N	13	ARG	NE-CZ-NH1	-10.41	115.10	120.30
1	Y	53	GLU	OE1-CD-OE2	-10.36	110.88	123.30
1	E	141	GLN	CA-C-N	-10.33	94.48	117.20
1	D	85	ARG	NE-CZ-NH1	-10.31	115.14	120.30
1	M	33	ASP	CB-CG-OD1	10.28	127.55	118.30
1	A	85	ARG	NE-CZ-NH1	-10.24	115.18	120.30
1	X	136	ARG	NE-CZ-NH2	10.23	125.42	120.30
1	E	106	ARG	NH1-CZ-NH2	-10.22	108.15	119.40
1	P	53	GLU	OE1-CD-OE2	-10.20	111.06	123.30
1	N	114	VAL	CA-CB-CG2	10.17	126.15	110.90
1	N	85	ARG	NH1-CZ-NH2	-10.14	108.25	119.40
1	R	53	GLU	OE1-CD-OE2	-10.06	111.23	123.30
1	S	13	ARG	NE-CZ-NH2	10.01	125.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	ARG	NE-CZ-NH2	9.99	125.30	120.30
1	F	136	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	M	85	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	E	136	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	L	17	ARG	NE-CZ-NH2	9.73	125.16	120.30
1	H	41	LEU	C-N-CA	9.71	145.96	121.70
1	J	80	TYR	CB-CG-CD1	9.57	126.74	121.00
1	J	31	GLU	OE1-CD-OE2	9.44	134.63	123.30
1	D	13	ARG	NE-CZ-NH2	9.42	125.01	120.30
1	I	53	GLU	OE1-CD-OE2	-9.41	112.01	123.30
1	O	29	ASP	CB-CG-OD1	9.35	126.71	118.30
1	E	106	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	G	53	GLU	OE1-CD-OE2	-9.27	112.18	123.30
1	H	41	LEU	CA-C-O	9.27	139.56	120.10
1	A	58	ASP	CB-CG-OD1	9.25	126.63	118.30
1	D	17	ARG	CD-NE-CZ	9.20	136.48	123.60
1	A	42	HIS	CA-CB-CG	-9.20	97.97	113.60
1	H	58	ASP	CB-CG-OD1	9.19	126.57	118.30
1	H	41	LEU	O-C-N	-9.18	108.00	122.70
1	S	85	ARG	CD-NE-CZ	9.14	136.39	123.60
1	J	106	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	L	85	ARG	NE-CZ-NH2	9.11	124.85	120.30
1	A	136	ARG	NE-CZ-NH2	9.07	124.83	120.30
1	X	106	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	U	106	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	K	106	ARG	CD-NE-CZ	8.90	136.06	123.60
1	U	112	GLN	CB-CG-CD	8.89	134.71	111.60
1	S	31	GLU	OE1-CD-OE2	8.86	133.94	123.30
1	O	24	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	J	85	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	X	26	THR	CA-CB-CG2	8.82	124.75	112.40
1	L	67	TYR	CB-CG-CD2	-8.81	115.71	121.00
1	O	53	GLU	OE1-CD-OE2	-8.81	112.73	123.30
1	I	106	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	T	17	ARG	CD-NE-CZ	8.78	135.90	123.60
1	P	17	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	L	58	ASP	CB-CG-OD2	8.76	126.18	118.30
1	H	112	GLN	CB-CG-CD	8.68	134.16	111.60
1	U	53	GLU	OE1-CD-OE2	-8.66	112.90	123.30
1	E	136	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	G	110	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Q	106	ARG	NE-CZ-NH1	8.56	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	110	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	M	110	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	N	53	GLU	OE1-CD-OE2	-8.45	113.16	123.30
1	C	112	GLN	CB-CG-CD	8.44	133.54	111.60
1	J	53	GLU	OE1-CD-OE2	-8.42	113.20	123.30
1	T	136	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	104	TYR	CD1-CE1-CZ	8.36	127.32	119.80
1	S	17	ARG	CA-CB-CG	8.34	131.76	113.40
1	B	53	GLU	OE1-CD-OE2	-8.33	113.30	123.30
1	G	136	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	X	86	ASP	OD1-CG-OD2	-8.30	107.53	123.30
1	K	58	ASP	CB-CG-OD1	8.27	125.74	118.30
1	Q	13	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	L	106	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	U	136	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	80	TYR	CA-CB-CG	8.08	128.75	113.40
1	A	80	TYR	CB-CG-CD1	8.06	125.84	121.00
1	V	112	GLN	CB-CG-CD	8.06	132.55	111.60
1	I	80	TYR	CA-CB-CG	8.05	128.70	113.40
1	P	108	GLU	OE1-CD-OE2	8.05	132.96	123.30
1	C	85	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	S	112	GLN	CB-CG-CD	7.98	132.35	111.60
1	A	97	GLU	OE1-CD-OE2	-7.93	113.79	123.30
1	T	35	PHE	CB-CG-CD1	7.91	126.33	120.80
1	Y	17	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	T	137	TYR	CB-CG-CD2	-7.89	116.26	121.00
1	C	80	TYR	CA-CB-CG	7.89	128.39	113.40
1	T	82	TYR	CB-CG-CD1	-7.87	116.28	121.00
1	M	24	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	Q	80	TYR	CB-CG-CD1	7.81	125.69	121.00
1	H	110	ARG	NH1-CZ-NH2	-7.78	110.85	119.40
1	R	112	GLN	CB-CG-CD	7.74	131.72	111.60
1	Y	31	GLU	CA-CB-CG	7.73	130.41	113.40
1	I	110	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	N	110	ARG	CD-NE-CZ	7.73	134.42	123.60
1	I	43	ILE	CA-C-O	7.72	136.31	120.10
1	R	110	ARG	CD-NE-CZ	7.72	134.40	123.60
1	F	17	ARG	CD-NE-CZ	7.68	134.36	123.60
1	S	106	ARG	CD-NE-CZ	7.67	134.34	123.60
1	X	58	ASP	CB-CG-OD1	7.64	125.17	118.30
1	L	67	TYR	CB-CG-CD1	7.62	125.57	121.00
1	K	31	GLU	CA-CB-CG	7.51	129.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	6	LEU	CB-CG-CD2	7.50	123.75	111.00
1	C	80	TYR	CB-CG-CD1	7.50	125.50	121.00
1	Q	112	GLN	CB-CG-CD	7.48	131.06	111.60
1	Q	106	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	N	3	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	A	53	GLU	OE1-CD-OE2	-7.43	114.39	123.30
1	I	29	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	S	33	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	B	80	TYR	CA-CB-CG	7.38	127.42	113.40
1	T	85	ARG	CD-NE-CZ	7.35	133.90	123.60
1	N	86	ASP	CB-CG-OD1	7.33	124.89	118.30
1	C	53	GLU	OE1-CD-OE2	-7.32	114.51	123.30
1	H	43	ILE	CA-C-O	7.28	135.39	120.10
1	R	136	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	T	80	TYR	CG-CD1-CE1	7.26	127.11	121.30
1	F	80	TYR	CA-CB-CG	7.26	127.19	113.40
1	K	80	TYR	CA-CB-CG	7.25	127.18	113.40
1	O	86	ASP	CB-CG-OD2	7.24	124.81	118.30
1	P	17	ARG	CD-NE-CZ	7.24	133.73	123.60
1	I	55	ASP	CB-CG-OD2	7.23	124.81	118.30
1	K	42	HIS	CA-CB-CG	7.23	125.89	113.60
1	L	131	TYR	CB-CG-CD2	7.23	125.34	121.00
1	I	112	GLN	CB-CG-CD	7.20	130.33	111.60
1	K	1	PRO	CA-N-CD	-7.15	101.49	111.50
1	Q	53	GLU	OE1-CD-OE2	-7.12	114.75	123.30
1	P	112	GLN	CB-CG-CD	7.05	129.93	111.60
1	X	29	ASP	CB-CG-OD1	7.04	124.64	118.30
1	S	141	GLN	OE1-CD-NE2	7.03	138.06	121.90
1	A	86	ASP	CB-CG-OD1	7.02	124.62	118.30
1	H	137	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	G	106	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	N	13	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	F	106	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	I	33	ASP	CA-CB-CG	6.96	128.72	113.40
1	K	55	ASP	CB-CG-OD1	6.96	124.56	118.30
1	E	80	TYR	CA-CB-CG	6.95	126.60	113.40
1	E	112	GLN	CB-CG-CD	6.93	129.63	111.60
1	R	97	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	L	53	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	R	85	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	V	106	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	85	ARG	NH1-CZ-NH2	6.86	126.94	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	107	GLU	OE1-CD-OE2	-6.84	115.10	123.30
1	I	85	ARG	CD-NE-CZ	6.83	133.17	123.60
1	P	17	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	I	129	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	P	53	GLU	CG-CD-OE2	6.79	131.87	118.30
1	A	13	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	L	80	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	S	13	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	L	86	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	82	TYR	CB-CG-CD2	6.72	125.03	121.00
1	O	29	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	106	ARG	CD-NE-CZ	6.71	133.00	123.60
1	N	3	PHE	CB-CG-CD2	6.71	125.50	120.80
1	X	55	ASP	CB-CG-OD1	6.70	124.33	118.30
1	P	110	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	E	41	LEU	CA-C-O	6.69	134.15	120.10
1	U	13	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	R	17	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	M	112	GLN	CB-CG-CD	6.67	128.95	111.60
1	O	112	GLN	CB-CG-CD	6.66	128.92	111.60
1	L	139	LEU	CA-CB-CG	6.65	130.60	115.30
1	J	112	GLN	CB-CG-CD	6.64	128.87	111.60
1	L	22	PHE	C-N-CA	6.63	136.23	122.30
1	P	85	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	I	109	PHE	O-C-N	-6.63	112.09	122.70
1	X	106	ARG	CD-NE-CZ	6.63	132.88	123.60
1	F	17	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	Q	80	TYR	CA-CB-CG	6.62	125.98	113.40
1	Q	29	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	U	29	ASP	CB-CG-OD2	6.59	124.23	118.30
1	P	124	VAL	CG1-CB-CG2	-6.54	100.43	110.90
1	K	53	GLU	OE1-CD-OE2	-6.52	115.48	123.30
1	E	33	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	I	17	ARG	C-N-CA	6.48	137.91	121.70
1	L	29	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	Y	85	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	V	1	PRO	CA-N-CD	-6.46	102.46	111.50
1	K	80	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	136	ARG	CD-NE-CZ	6.45	132.62	123.60
1	G	112[A]	GLN	CB-CG-CD	6.44	128.34	111.60
1	G	112[B]	GLN	CB-CG-CD	6.44	128.34	111.60
1	A	110	ARG	CD-NE-CZ	6.43	132.61	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	82	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	R	39	GLU	CA-C-N	6.40	131.28	117.20
1	B	106	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	N	14	LEU	CA-CB-CG	6.39	129.99	115.30
1	V	13	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	V	80	TYR	CA-CB-CG	6.35	125.46	113.40
1	R	40	ALA	CA-C-N	6.34	131.15	117.20
1	L	34	LEU	N-CA-CB	6.33	123.06	110.40
1	T	136	ARG	NH1-CZ-NH2	6.33	126.36	119.40
1	S	139	LEU	CB-CA-C	-6.32	98.19	110.20
1	T	112	GLN	CB-CG-CD	6.32	128.03	111.60
1	U	80	TYR	CA-CB-CG	6.32	125.40	113.40
1	K	13	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	I	13	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	112	GLN	CB-CG-CD	6.28	127.94	111.60
1	A	29	ASP	CB-CG-OD1	6.28	123.95	118.30
1	F	112[A]	GLN	CB-CG-CD	6.26	127.87	111.60
1	F	112[B]	GLN	CB-CG-CD	6.26	127.87	111.60
1	A	17	ARG	CD-NE-CZ	6.24	132.34	123.60
1	E	6	LEU	CA-CB-CG	6.24	129.65	115.30
1	J	137	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	J	50	SER	N-CA-CB	6.20	119.79	110.50
1	Y	110	ARG	NH1-CZ-NH2	-6.19	112.59	119.40
1	R	41	LEU	C-N-CA	6.19	137.18	121.70
1	P	43	ILE	CA-C-O	6.19	133.10	120.10
1	N	97	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	B	33	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	112	GLN	CB-CG-CD	6.17	127.66	111.60
1	L	22	PHE	O-C-N	-6.17	112.71	123.20
1	V	110	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	Y	1	PRO	N-CA-CB	-6.17	95.81	102.60
1	L	13	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	I	17	ARG	CD-NE-CZ	6.16	132.22	123.60
1	O	140	SER	CA-C-N	6.15	130.73	117.20
1	J	80	TYR	CA-CB-CG	6.15	125.08	113.40
1	A	33	ASP	N-CA-CB	6.13	121.63	110.60
1	H	136	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	U	58	ASP	CB-CG-OD1	6.11	123.80	118.30
1	P	82	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	V	139	LEU	CB-CG-CD1	6.11	121.38	111.00
1	R	13	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	97	GLU	OE1-CD-OE2	-6.10	115.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	139	LEU	N-CA-CB	6.10	122.60	110.40
1	O	14	LEU	CA-CB-CG	6.10	129.32	115.30
1	Q	58	ASP	CB-CG-OD2	6.09	123.78	118.30
1	R	109	PHE	CB-CG-CD1	6.09	125.06	120.80
1	O	110	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	T	140	SER	CA-C-N	6.08	130.58	117.20
1	K	80	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	I	136	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	L	17	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
1	A	83	ALA	N-CA-CB	6.04	118.55	110.10
1	C	106	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	P	107	GLU	OE1-CD-OE2	-6.03	116.06	123.30
1	H	131	TYR	CB-CG-CD1	6.02	124.61	121.00
1	M	24	ARG	CG-CD-NE	6.00	124.41	111.80
1	H	13	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	R	17	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	S	58	ASP	CB-CG-OD1	5.97	123.67	118.30
1	T	98	VAL	O-C-N	-5.96	113.16	122.70
1	N	82	TYR	CG-CD1-CE1	5.96	126.07	121.30
1	I	58	ASP	CB-CG-OD2	5.96	123.66	118.30
1	V	53	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	S	53	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	D	97	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	Y	29	ASP	CB-CG-OD2	5.92	123.63	118.30
1	E	80	TYR	CG-CD1-CE1	5.91	126.03	121.30
1	G	118	VAL	O-C-N	-5.88	113.30	122.70
1	M	139	LEU	CA-C-N	5.86	130.09	117.20
1	D	112[A]	GLN	CB-CG-CD	5.85	126.80	111.60
1	D	112[B]	GLN	CB-CG-CD	5.85	126.80	111.60
1	G	23	GLY	N-CA-C	5.85	127.72	113.10
1	Q	14	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	86	ASP	CB-CG-OD2	5.84	123.56	118.30
1	L	25	GLN	CA-CB-CG	5.81	126.17	113.40
1	O	31	GLU	CA-CB-CG	5.81	126.17	113.40
1	H	17	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	T	80	TYR	CB-CG-CD1	5.79	124.47	121.00
1	G	131	TYR	CB-CG-CD1	5.79	124.47	121.00
1	U	42	HIS	N-CA-CB	5.78	121.01	110.60
1	L	17	ARG	CG-CD-NE	5.77	123.92	111.80
1	R	58	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	T	35	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	B	4	LEU	CB-CA-C	-5.76	99.26	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	136	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	C	137	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	104	TYR	CB-CG-CD1	5.75	124.45	121.00
1	M	13	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	M	136	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	R	41	LEU	CA-C-O	5.73	132.14	120.10
1	P	33	ASP	CA-CB-CG	5.73	126.00	113.40
1	L	22	PHE	CA-C-O	5.71	132.10	120.10
1	F	135	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	H	72	LEU	O-C-N	5.71	131.83	122.70
1	A	89	SER	CB-CA-C	-5.70	99.28	110.10
1	Y	14	LEU	CA-CB-CG	5.70	128.40	115.30
1	F	53	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	A	110	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	L	23	GLY	N-CA-C	5.69	127.32	113.10
1	O	85	ARG	CD-NE-CZ	5.69	131.56	123.60
1	S	134	ALA	N-CA-CB	5.68	118.05	110.10
1	X	106	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	F	17	ARG	CA-CB-CG	5.67	125.88	113.40
1	S	24	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	J	13	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	E	110	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	J	6	LEU	CA-CB-CG	5.64	128.28	115.30
1	N	1	PRO	CA-N-CD	-5.64	103.61	111.50
1	E	80	TYR	CB-CG-CD1	5.64	124.38	121.00
1	J	80	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	K	106	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	K	110	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	M	31	GLU	CA-CB-CG	5.61	125.73	113.40
1	X	136	ARG	CD-NE-CZ	5.61	131.45	123.60
1	I	17	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	T	136	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	I	3	PHE	CB-CG-CD1	-5.59	116.89	120.80
1	C	85	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	J	74	PRO	C-N-CA	-5.58	110.58	122.30
1	E	33	ASP	CB-CA-C	-5.58	99.25	110.40
1	R	4	LEU	CB-CG-CD2	5.57	120.47	111.00
1	K	98	VAL	O-C-N	-5.57	113.79	122.70
1	Y	33	ASP	CB-CG-OD1	5.56	123.31	118.30
1	S	141	GLN	CG-CD-OE1	-5.56	110.48	121.60
1	B	4	LEU	CB-CG-CD2	5.55	120.44	111.00
1	B	131	TYR	CZ-CE2-CD2	5.55	124.80	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	TYR	CG-CD1-CE1	5.54	125.73	121.30
1	S	42	HIS	CA-CB-CG	-5.54	104.18	113.60
1	O	140	SER	O-C-N	-5.53	113.84	122.70
1	L	6	LEU	CA-CB-CG	5.53	128.01	115.30
1	H	106	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	N	58	ASP	CB-CG-OD1	5.52	123.27	118.30
1	Y	96	VAL	CA-CB-CG1	5.51	119.17	110.90
1	X	53	GLU	CG-CD-OE2	5.51	129.32	118.30
1	P	3	PHE	CB-CG-CD1	-5.51	116.95	120.80
1	H	37	PHE	CB-CG-CD2	5.50	124.65	120.80
1	X	80	TYR	CA-CB-CG	5.50	123.85	113.40
1	D	129	GLU	O-C-N	-5.50	113.86	123.20
1	R	131	TYR	CB-CG-CD2	5.49	124.30	121.00
1	K	68	SER	O-C-N	-5.49	113.86	123.20
1	E	53	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	V	120	LYS	CB-CG-CD	-5.48	97.35	111.60
1	K	58	ASP	OD1-CG-OD2	-5.47	112.90	123.30
1	X	82	TYR	CB-CG-CD2	5.47	124.28	121.00
1	N	39	GLU	CA-C-N	5.47	129.23	117.20
1	T	82	TYR	CB-CG-CD2	5.47	124.28	121.00
1	O	106	ARG	CD-NE-CZ	5.46	131.25	123.60
1	P	97	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	X	86	ASP	O-C-N	-5.46	113.96	122.70
1	K	4	LEU	CA-CB-CG	5.46	127.85	115.30
1	P	1	PRO	CA-N-CD	-5.46	103.86	111.50
1	R	140	SER	CA-C-N	5.45	129.19	117.20
1	Y	39	GLU	C-N-CA	5.45	135.33	121.70
1	E	16[A]	SER	C-N-CA	5.44	135.30	121.70
1	E	16[B]	SER	C-N-CA	5.44	135.30	121.70
1	Q	131	TYR	CB-CG-CD1	5.44	124.27	121.00
1	V	141	GLN	N-CA-C	5.44	125.70	111.00
1	K	104	TYR	CB-CG-CD1	5.43	124.26	121.00
1	E	55	ASP	OD1-CG-OD2	-5.43	112.98	123.30
1	X	82	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	K	110	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	I	34	LEU	O-C-N	-5.42	114.03	122.70
1	S	80	TYR	CA-CB-CG	5.42	123.69	113.40
1	T	53	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	K	59	ALA	O-C-N	-5.41	114.05	122.70
1	T	31	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	R	75	GLY	CA-C-O	5.40	130.32	120.60
1	S	55	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	86	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	X	82	TYR	CD1-CE1-CZ	-5.38	114.95	119.80
1	M	29	ASP	CA-CB-CG	5.38	125.24	113.40
1	I	114	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	X	55	ASP	OD1-CG-OD2	-5.37	113.09	123.30
1	G	136	ARG	O-C-N	-5.37	114.11	122.70
1	J	14	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	17	ARG	C-N-CA	5.36	135.11	121.70
1	E	56	LEU	CB-CG-CD2	5.36	120.12	111.00
1	D	136	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	P	34	LEU	CA-C-N	5.35	128.98	117.20
1	Q	38	ALA	CB-CA-C	-5.35	102.07	110.10
1	S	110	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	I	104	TYR	CB-CG-CD2	5.35	124.21	121.00
1	V	110	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	K	137	TYR	CG-CD2-CE2	-5.34	117.03	121.30
1	T	80	TYR	CA-CB-CG	5.33	123.54	113.40
1	O	53	GLU	CG-CD-OE2	5.33	128.97	118.30
1	O	106	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
1	H	34	LEU	O-C-N	-5.33	114.17	122.70
1	R	41	LEU	O-C-N	-5.33	114.17	122.70
1	O	13	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	103	LEU	O-C-N	-5.32	114.18	122.70
1	P	13	ARG	O-C-N	-5.32	114.19	122.70
1	Q	14	LEU	C-N-CA	5.31	133.46	122.30
1	T	53	GLU	CG-CD-OE2	5.31	128.92	118.30
1	B	58	ASP	CB-CG-OD1	5.30	123.08	118.30
1	L	103	LEU	O-C-N	-5.30	114.21	122.70
1	L	138	LEU	CA-CB-CG	5.30	127.50	115.30
1	Y	42	HIS	CA-CB-CG	-5.30	104.59	113.60
1	R	26	THR	CA-CB-CG2	-5.30	104.98	112.40
1	D	108	GLU	O-C-N	-5.30	114.23	122.70
1	L	14	LEU	CA-CB-CG	5.29	127.47	115.30
1	C	14	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	4	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	86	ASP	CB-CG-OD1	5.28	123.05	118.30
1	Q	58	ASP	OD1-CG-OD2	-5.27	113.29	123.30
1	G	29	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	41	LEU	O-C-N	-5.26	114.28	122.70
1	G	80	TYR	CA-CB-CG	5.26	123.39	113.40
1	K	29	ASP	CB-CG-OD1	5.26	123.03	118.30
1	I	130	GLY	O-C-N	-5.26	114.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	42	HIS	CA-CB-CG	-5.25	104.67	113.60
1	G	98	VAL	O-C-N	-5.25	114.30	122.70
1	B	140	SER	CB-CA-C	-5.25	100.13	110.10
1	I	121	GLY	O-C-N	5.25	131.09	122.70
1	K	112	GLN	CB-CG-CD	5.24	125.23	111.60
1	V	84	ILE	O-C-N	-5.24	114.31	122.70
1	D	113	SER	N-CA-CB	5.24	118.36	110.50
1	V	137	TYR	O-C-N	-5.24	114.32	122.70
1	K	110	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
1	C	110	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	E	99	HIS	N-CA-CB	5.23	120.01	110.60
1	V	128	ALA	N-CA-CB	5.23	117.42	110.10
1	Y	97	GLU	O-C-N	-5.22	114.35	122.70
1	G	80	TYR	CB-CG-CD1	5.21	124.13	121.00
1	C	17	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	V	16	SER	CA-C-N	5.21	128.66	117.20
1	V	16	SER	N-CA-C	5.21	125.06	111.00
1	B	82	TYR	CB-CG-CD2	5.20	124.12	121.00
1	H	34	LEU	CA-C-N	5.20	128.64	117.20
1	X	112	GLN	CB-CG-CD	5.20	125.11	111.60
1	E	18	GLU	N-CA-C	5.19	125.01	111.00
1	V	62	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	L	80	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	25	GLN	CA-CB-CG	5.18	124.80	113.40
1	L	104	TYR	CG-CD2-CE2	5.18	125.44	121.30
1	M	96	VAL	CG1-CB-CG2	-5.18	102.62	110.90
1	S	82	TYR	CB-CG-CD2	5.18	124.11	121.00
1	T	97	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	J	86	ASP	CB-CG-OD1	5.17	122.96	118.30
1	L	55	ASP	CB-CG-OD1	5.17	122.95	118.30
1	J	109	PHE	CB-CG-CD1	5.17	124.42	120.80
1	L	82	TYR	CG-CD2-CE2	5.16	125.43	121.30
1	V	55	ASP	CB-CG-OD1	5.16	122.94	118.30
1	R	28	THR	N-CA-CB	5.16	120.10	110.30
1	P	80	TYR	CA-CB-CG	5.15	123.19	113.40
1	X	25	GLN	N-CA-CB	-5.15	101.34	110.60
1	G	14	LEU	CA-CB-CG	5.15	127.14	115.30
1	L	31	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	L	114	VAL	CA-CB-CG2	5.14	118.62	110.90
1	M	33	ASP	CA-CB-CG	5.14	124.71	113.40
1	F	1	PRO	O-C-N	5.14	130.92	122.70
1	X	13	ARG	NE-CZ-NH2	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	81	SER	O-C-N	-5.13	114.50	122.70
1	E	98	VAL	CA-CB-CG1	-5.13	103.21	110.90
1	O	6	LEU	CA-CB-CG	5.12	127.08	115.30
1	Q	58	ASP	CB-CG-OD1	5.12	122.91	118.30
1	H	140	SER	N-CA-CB	5.12	118.18	110.50
1	H	37	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	K	89	SER	CB-CA-C	-5.12	100.38	110.10
1	I	53	GLU	CG-CD-OE2	5.12	128.53	118.30
1	N	112	GLN	CB-CG-CD	5.12	124.91	111.60
1	D	139	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	K	24	ARG	CA-C-O	5.11	130.84	120.10
1	H	26	THR	CA-CB-CG2	-5.11	105.25	112.40
1	H	80	TYR	CB-CG-CD1	5.10	124.06	121.00
1	E	31	GLU	CA-CB-CG	5.10	124.62	113.40
1	F	13	ARG	CD-NE-CZ	5.10	130.73	123.60
1	O	97	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	R	77	LEU	O-C-N	-5.07	114.59	122.70
1	X	38	ALA	N-CA-CB	-5.07	103.00	110.10
1	H	34	LEU	N-CA-CB	5.07	120.54	110.40
1	K	7	ASN	CB-CG-OD1	5.06	131.72	121.60
1	T	88	VAL	O-C-N	-5.06	114.60	122.70
1	I	24	ARG	N-CA-C	5.06	124.65	111.00
1	Y	53	GLU	CG-CD-OE2	5.05	128.40	118.30
1	I	17	ARG	O-C-N	-5.04	114.63	122.70
1	O	80	TYR	CA-CB-CG	5.04	122.98	113.40
1	L	112[A]	GLN	CB-CG-CD	5.04	124.71	111.60
1	L	112[B]	GLN	CB-CG-CD	5.04	124.71	111.60
1	M	14	LEU	C-N-CA	5.04	132.88	122.30
1	U	38	ALA	CB-CA-C	-5.04	102.54	110.10
1	L	104	TYR	CZ-CE2-CD2	-5.03	115.27	119.80
1	H	42	HIS	CA-C-O	5.03	130.66	120.10
1	T	28	THR	N-CA-CB	5.03	119.85	110.30
1	L	36	GLN	CG-CD-NE2	5.03	128.76	116.70
1	J	49	GLN	CA-CB-CG	5.02	124.45	113.40
1	D	85	ARG	CD-NE-CZ	5.02	130.63	123.60
1	M	107	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	Q	110	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	S	58	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	N	109	PHE	CB-CG-CD2	5.01	124.31	120.80
1	G	35	PHE	CA-CB-CG	-5.01	101.87	113.90
1	L	63	ALA	N-CA-CB	5.01	117.12	110.10
1	R	82	TYR	N-CA-CB	5.00	119.61	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	85	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	141	GLN	Mainchain
1	H	40	ALA	Mainchain
1	I	115	ILE	Mainchain
1	K	12	ASN	Mainchain
1	R	111	HIS	Mainchain
1	X	109	PHE	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1094	0	1059	31	0
1	B	1105	0	1065	27	0
1	C	1093	0	1064	23	0
1	D	1094	0	1059	22	0
1	E	1108	0	1078	24	0
1	F	1107	0	1076	18	0
1	G	1101	0	1067	21	0
1	H	1096	0	1061	31	0
1	I	1090	0	1055	32	0
1	J	1093	0	1064	23	0
1	K	1051	0	1021	17	0
1	L	1085	0	1050	26	0
1	M	1098	0	1069	24	0
1	N	1028	0	1006	15	0
1	O	1096	0	1066	24	0
1	P	1099	0	1071	25	0
1	Q	1109	0	1086	18	0
1	R	1094	0	1055	23	0
1	S	1108	0	1084	25	0
1	T	1104	0	1076	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	1093	0	1064	35	0
1	V	1056	0	1034	21	0
1	X	1034	0	1012	17	0
1	Y	1096	0	1062	28	0
2	A	18	0	24	5	0
2	B	18	0	24	5	0
2	C	18	0	24	7	0
2	D	18	0	23	5	0
2	E	17	0	21	3	0
2	F	17	0	20	3	0
2	G	18	0	24	6	0
2	H	18	0	24	5	0
2	I	18	0	24	4	0
2	J	18	0	24	2	0
2	K	18	0	24	6	0
2	L	18	0	23	7	0
2	M	18	0	24	3	0
2	N	18	0	23	3	0
2	O	18	0	24	8	0
2	P	18	0	24	6	0
2	Q	18	0	24	11	0
2	R	18	0	24	6	0
2	S	18	0	24	9	0
2	T	18	0	24	4	0
2	U	18	0	24	10	0
2	V	18	0	24	5	0
2	X	18	0	23	3	0
2	Y	18	0	24	7	0
3	A	90	0	0	14	0
3	B	98	0	0	10	0
3	C	100	0	0	12	0
3	D	96	0	0	6	0
3	E	93	0	0	9	0
3	F	91	0	0	8	0
3	G	91	0	0	9	0
3	H	75	0	0	12	0
3	I	91	0	0	8	0
3	J	91	0	0	10	0
3	K	83	0	0	2	0
3	L	86	0	0	8	0
3	M	97	0	0	8	0
3	N	96	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	89	0	0	9	0
3	P	97	0	0	10	0
3	Q	97	0	0	9	0
3	R	103	0	0	13	0
3	S	84	0	0	10	0
3	T	87	0	0	8	0
3	U	101	0	0	13	0
3	V	107	0	0	9	0
3	X	79	0	0	10	0
3	Y	80	0	0	12	0
All	All	28764	0	25969	589	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:141:GLN:HA	1:N:142:GLN:N	1.42	1.23
1:F:142:GLN:N	3:F:2084:HOH:O	1.69	1.20
1:U:140:SER:O	1:U:142:GLN:N	1.81	1.13
1:U:117:PRO:HG3	2:U:151:GOL:H11	1.36	1.06
1:M:14:LEU:HD13	2:M:152:GOL:H11	1.38	1.04
1:N:141:GLN:CA	1:N:142:GLN:N	2.15	0.99
1:C:141:GLN:HE21	1:C:142:GLN:N	1.60	0.98
1:D:112[B]:GLN:HG3	2:D:151:GOL:H31	1.49	0.93
1:G:112[B]:GLN:HG3	2:G:151:GOL:H2	1.49	0.93
1:K:1:PRO:H2	1:K:43:ILE:HG22	1.35	0.92
3:F:2067:HOH:O	2:H:151:GOL:H2	1.67	0.92
1:M:98:VAL:HG13	3:M:2086:HOH:O	1.71	0.90
1:F:98:VAL:HG13	3:F:2075:HOH:O	1.73	0.89
1:U:112:GLN:HG3	3:U:2099:HOH:O	1.73	0.87
1:Q:14:LEU:HD13	2:Q:152:GOL:H2	1.57	0.87
1:X:98:VAL:HG13	3:X:2065:HOH:O	1.75	0.86
1:H:1:PRO:HG2	1:H:43:ILE:HG22	1.57	0.86
1:C:98:VAL:HG13	3:C:2088:HOH:O	1.74	0.86
1:E:123:ILE:HG22	3:E:2083:HOH:O	1.74	0.85
1:R:113:SER:HB2	3:R:2084:HOH:O	1.75	0.85
1:A:98:VAL:HG13	3:A:2077:HOH:O	1.77	0.84
1:U:43:ILE:HG21	1:U:139:LEU:HD11	1.59	0.84
1:D:62:GLU:OE1	1:Q:22:PHE:HA	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:113:SER:HB2	3:I:2073:HOH:O	1.77	0.83
1:P:132:LYS:HG3	3:P:2085:HOH:O	1.78	0.82
1:L:123:ILE:HG22	3:L:2080:HOH:O	1.80	0.82
1:J:98:VAL:HG13	3:J:2080:HOH:O	1.78	0.82
1:H:132:LYS:HG3	3:H:2068:HOH:O	1.77	0.81
1:U:80:TYR:HB2	3:U:2053:HOH:O	1.80	0.81
1:L:20:GLU:HA	1:L:23:GLY:HA2	1.60	0.81
1:Q:123:ILE:HG22	3:Q:2083:HOH:O	1.77	0.81
1:K:14:LEU:HD13	2:K:152:GOL:H2	1.61	0.81
1:F:113:SER:HA	3:F:2044:HOH:O	1.80	0.80
1:E:141:GLN:CB	1:E:142:GLN:N	2.18	0.80
1:G:141:GLN:CA	1:G:142:GLN:N	2.31	0.80
1:Y:79:HIS:HE1	3:Y:2059:HOH:O	1.64	0.80
1:J:141:GLN:HB3	1:J:142:GLN:N	1.97	0.80
1:D:98:VAL:HG13	3:D:2085:HOH:O	1.82	0.79
1:T:1:PRO:HD2	1:T:43:ILE:HG22	1.63	0.79
1:P:98:VAL:HG13	3:P:2081:HOH:O	1.83	0.79
1:K:141:GLN:NE2	1:K:142:GLN:N	2.31	0.78
1:B:14:LEU:HA	2:B:152:GOL:H11	1.64	0.78
1:I:80:TYR:HB2	3:I:2041:HOH:O	1.82	0.78
1:B:80:TYR:HB2	3:B:2044:HOH:O	1.82	0.78
1:I:141:GLN:NE2	1:I:142:GLN:N	2.31	0.78
1:U:117:PRO:CG	2:U:151:GOL:H11	2.15	0.77
1:A:53:GLU:HB3	3:A:2035:HOH:O	1.85	0.77
1:A:80:TYR:HB2	3:A:2049:HOH:O	1.84	0.76
1:L:117:PRO:HG3	2:L:151:GOL:H12	1.65	0.76
1:G:141:GLN:HA	1:G:142:GLN:N	2.01	0.76
1:H:141:GLN:O	1:H:142:GLN:N	2.04	0.76
1:R:117:PRO:HG3	2:R:151:GOL:H11	1.67	0.75
1:C:103:LEU:HB2	3:C:2068:HOH:O	1.85	0.75
1:M:41:LEU:O	1:M:42:HIS:HB2	1.85	0.75
1:P:112:GLN:HG3	3:P:2072:HOH:O	1.86	0.74
1:P:100:LEU:HD23	3:P:2087:HOH:O	1.86	0.74
1:S:80:TYR:HB2	3:S:2043:HOH:O	1.87	0.74
1:O:133:LEU:HD23	3:O:2083:HOH:O	1.87	0.74
1:V:112:GLN:HG3	3:V:2086:HOH:O	1.88	0.74
1:F:112[B]:GLN:HB2	3:F:2089:HOH:O	1.87	0.74
1:B:116:ALA:HB3	3:B:2098:HOH:O	1.88	0.74
1:M:1:PRO:HG2	1:M:43:ILE:HG22	1.69	0.73
1:U:24:ARG:HA	3:U:2014:HOH:O	1.87	0.73
1:A:133:LEU:HD23	3:A:2085:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:53:GLU:HB3	3:J:2037:HOH:O	1.88	0.73
1:L:80:TYR:HB2	3:L:2043:HOH:O	1.89	0.72
1:A:25:GLN:HG3	3:A:2008:HOH:O	1.89	0.72
1:Y:103:LEU:HD13	3:Y:2059:HOH:O	1.87	0.72
1:F:112[A]:GLN:HB2	3:F:2089:HOH:O	1.88	0.72
1:D:105:ALA:HB2	3:D:2063:HOH:O	1.90	0.72
1:A:4:LEU:HD13	3:A:2001:HOH:O	1.90	0.71
1:T:113:SER:O	2:T:151:GOL:H12	1.90	0.71
1:T:98:VAL:HG13	3:T:2074:HOH:O	1.91	0.71
1:S:113:SER:HB2	3:S:2073:HOH:O	1.90	0.71
1:A:6:LEU:HB2	3:A:2001:HOH:O	1.89	0.70
1:A:70:ILE:HG23	3:A:2001:HOH:O	1.89	0.70
1:F:113:SER:O	2:F:151:GOL:H11	1.92	0.70
1:P:34:LEU:HG	3:P:2015:HOH:O	1.91	0.70
1:N:117:PRO:HG2	3:N:2093:HOH:O	1.90	0.70
1:P:132:LYS:HD3	3:P:2025:HOH:O	1.91	0.69
1:E:141:GLN:HB3	1:E:142:GLN:N	2.05	0.69
1:D:17:ARG:HH11	1:D:17:ARG:HG2	1.58	0.69
1:E:113:SER:HB2	3:E:2080:HOH:O	1.91	0.69
1:M:88:VAL:HG12	3:M:2077:HOH:O	1.92	0.69
1:N:112:GLN:HG3	3:N:2090:HOH:O	1.93	0.69
1:N:14:LEU:HD13	2:N:152:GOL:H31	1.74	0.68
2:U:151:GOL:H12	3:U:2081:HOH:O	1.93	0.68
1:S:1:PRO:HA	3:S:2001:HOH:O	1.93	0.68
1:U:113:SER:O	2:U:151:GOL:H12	1.93	0.68
1:Y:117:PRO:HG3	2:Y:151:GOL:H12	1.74	0.68
1:D:112[B]:GLN:HG3	2:D:151:GOL:C3	2.24	0.68
1:N:113:SER:O	2:N:151:GOL:H31	1.94	0.67
2:Q:151:GOL:C1	1:Y:111:HIS:HB3	2.24	0.67
1:U:79:HIS:HE1	3:U:2079:HOH:O	1.75	0.67
1:T:1:PRO:HD2	1:T:43:ILE:CG2	2.24	0.67
1:F:79:HIS:ND1	3:F:2044:HOH:O	2.27	0.67
1:G:35:PHE:HA	3:G:2023:HOH:O	1.94	0.66
1:H:22:PHE:HA	3:H:2004:HOH:O	1.95	0.66
1:I:140:SER:O	1:I:142:GLN:N	2.30	0.66
1:T:14:LEU:HA	2:T:152:GOL:H11	1.78	0.66
1:J:80:TYR:HB2	3:J:2050:HOH:O	1.94	0.65
1:Y:14:LEU:HA	2:Y:152:GOL:H11	1.77	0.65
1:P:112:GLN:HB2	2:P:151:GOL:H31	1.78	0.65
1:X:103:LEU:HD12	3:X:2064:HOH:O	1.97	0.65
1:D:21:VAL:HG12	1:D:101:SER:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:112:GLN:HG3	3:Q:2093:HOH:O	1.97	0.65
1:V:25:GLN:HE21	1:V:30:ILE:CG1	2.10	0.65
1:B:112:GLN:HB2	2:B:151:GOL:O2	1.97	0.64
1:V:53:GLU:HB2	3:X:2025:HOH:O	1.96	0.64
1:O:10:ASN:O	2:O:152:GOL:H2	1.97	0.64
1:I:111:HIS:ND1	2:K:151:GOL:H2	2.13	0.64
1:H:132:LYS:HB3	3:H:2071:HOH:O	1.97	0.63
1:B:15:GLY:HA2	3:B:2011:HOH:O	1.98	0.63
1:G:103:LEU:HD12	3:G:2079:HOH:O	1.96	0.63
2:Q:151:GOL:H11	1:Y:111:HIS:CG	2.33	0.63
1:H:88:VAL:HG12	3:H:2058:HOH:O	1.98	0.63
1:H:43:ILE:HG21	1:H:139:LEU:HD21	1.81	0.63
3:N:2072:HOH:O	2:S:151:GOL:H2	1.99	0.63
2:Y:151:GOL:H31	3:Y:2038:HOH:O	1.98	0.62
1:U:105:ALA:HB2	3:U:2066:HOH:O	1.98	0.62
1:E:31:GLU:HB2	3:E:2016:HOH:O	1.99	0.62
2:S:150:GOL:H11	2:S:152:GOL:H31	1.80	0.62
1:I:1:PRO:HG2	1:I:43:ILE:HG22	1.81	0.62
1:A:141:GLN:NE2	1:A:142:GLN:N	2.47	0.62
1:G:112[B]:GLN:HG2	1:G:113:SER:N	2.14	0.62
1:B:132:LYS:HG3	3:B:2088:HOH:O	2.00	0.62
1:I:14:LEU:HD13	2:I:152:GOL:H32	1.79	0.62
2:B:151:GOL:H2	3:G:2071:HOH:O	1.98	0.62
1:R:1:PRO:HD2	1:R:43:ILE:HG22	1.81	0.61
2:Q:151:GOL:H11	1:Y:111:HIS:HB3	1.82	0.61
1:M:111:HIS:ND1	2:P:151:GOL:O2	2.34	0.61
1:B:142:GLN:N	1:B:143:GLY:O	2.33	0.61
1:X:89:SER:HA	3:X:2042:HOH:O	2.00	0.61
1:B:43:ILE:HG21	1:B:139:LEU:HD21	1.83	0.61
3:C:2090:HOH:O	1:J:136:ARG:HB3	2.00	0.61
1:H:22:PHE:CE2	2:H:152:GOL:H12	2.36	0.60
1:M:72:LEU:HG	1:M:74:PRO:HD3	1.83	0.60
1:K:38:ALA:HB1	1:K:43:ILE:O	2.02	0.60
1:C:88:VAL:HG12	3:C:2081:HOH:O	2.01	0.60
1:S:22:PHE:CE2	2:S:152:GOL:H32	2.35	0.60
1:B:30:ILE:HG22	1:B:34:LEU:HD12	1.83	0.60
1:I:113:SER:HB2	3:I:2074:HOH:O	2.01	0.60
2:P:151:GOL:H2	3:P:2095:HOH:O	2.01	0.60
3:C:2077:HOH:O	2:J:151:GOL:H2	2.01	0.60
1:F:112[B]:GLN:HG3	2:F:151:GOL:O2	2.02	0.60
1:I:38:ALA:HB1	1:I:43:ILE:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1:PRO:CG	1:P:43:ILE:HG22	2.31	0.60
1:G:20:GLU:OE1	1:G:21:VAL:HG23	2.03	0.59
1:D:46:THR:HG21	1:Q:20:GLU:OE2	2.03	0.59
1:C:141:GLN:NE2	1:C:142:GLN:N	2.41	0.59
1:I:14:LEU:HA	2:I:152:GOL:H11	1.85	0.59
1:B:20:GLU:OE1	1:B:21:VAL:HG23	2.02	0.59
1:V:112:GLN:HA	3:V:2087:HOH:O	2.03	0.58
1:F:1:PRO:HD2	1:F:43:ILE:HG22	1.85	0.58
1:D:112[B]:GLN:CG	2:D:151:GOL:H31	2.28	0.58
1:B:1:PRO:HD2	1:B:43:ILE:HG22	1.84	0.58
1:U:17:ARG:HH11	1:U:17:ARG:HG2	1.68	0.58
1:O:112:GLN:HG3	3:O:2070:HOH:O	2.02	0.58
1:R:40:ALA:C	1:R:42:HIS:H	2.05	0.58
1:U:103:LEU:HD13	3:U:2079:HOH:O	2.04	0.58
1:K:141:GLN:HE21	1:K:142:GLN:N	2.02	0.58
1:B:111:HIS:ND1	2:G:151:GOL:H12	2.18	0.58
2:C:151:GOL:O1	1:J:104:TYR:HB3	2.03	0.57
1:C:124:VAL:HG11	3:C:2068:HOH:O	2.03	0.57
1:K:43:ILE:HD13	1:K:139:LEU:HD11	1.87	0.57
1:H:38:ALA:HB1	1:H:43:ILE:O	2.05	0.57
1:P:1:PRO:HG2	1:P:43:ILE:HG22	1.86	0.57
1:H:23:GLY:HA3	3:H:2005:HOH:O	2.04	0.57
1:A:141:GLN:HA	1:A:142:GLN:N	2.20	0.57
1:Y:126:LEU:N	3:Y:2045:HOH:O	2.38	0.57
1:V:27:LEU:O	1:V:31:GLU:HG3	2.05	0.56
1:E:17:ARG:HA	3:E:2009:HOH:O	2.04	0.56
1:L:19:PRO:O	1:L:20:GLU:CB	2.53	0.56
1:Q:10:ASN:O	2:Q:152:GOL:O2	2.23	0.56
1:I:141:GLN:HE22	1:I:142:GLN:N	2.03	0.56
1:O:14:LEU:HD13	2:O:152:GOL:H11	1.86	0.56
1:O:6:LEU:HD22	1:O:56:LEU:HD22	1.86	0.56
1:F:111:HIS:ND1	2:H:151:GOL:H11	2.21	0.56
1:U:130:GLY:HA3	3:U:2091:HOH:O	2.05	0.56
1:K:1:PRO:N	1:K:43:ILE:HG22	2.14	0.56
1:X:2:HIS:HA	1:X:44:GLN:O	2.05	0.56
1:X:132:LYS:HB3	3:X:2074:HOH:O	2.05	0.56
1:A:82:TYR:CD1	3:A:2048:HOH:O	2.53	0.56
1:H:1:PRO:HG2	1:H:43:ILE:CG2	2.32	0.56
1:A:141:GLN:CD	1:A:142:GLN:N	2.58	0.56
1:F:38:ALA:HB1	1:F:43:ILE:HG13	1.87	0.56
1:B:27:LEU:HG	1:B:31:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:151:GOL:H31	3:R:2101:HOH:O	2.06	0.56
1:N:10:ASN:O	2:N:152:GOL:H2	2.04	0.56
1:U:102:ASN:ND2	3:U:2066:HOH:O	2.39	0.56
1:S:2:HIS:HA	1:S:44:GLN:O	2.06	0.56
2:L:150:GOL:H11	2:L:152:GOL:H31	1.87	0.56
1:R:112:GLN:HG3	3:R:2077:HOH:O	2.06	0.55
1:I:81:SER:HB2	3:I:2042:HOH:O	2.06	0.55
1:H:44:GLN:HA	3:H:2015:HOH:O	2.07	0.55
1:V:17:ARG:HB3	3:V:2007:HOH:O	2.06	0.55
1:A:111:HIS:ND1	2:D:151:GOL:H11	2.22	0.55
1:O:14:LEU:HA	2:O:152:GOL:H12	1.88	0.55
1:G:17:ARG:HA	3:G:2009:HOH:O	2.07	0.55
1:U:14:LEU:HG	3:U:2015:HOH:O	2.06	0.55
2:R:151:GOL:H12	3:R:2100:HOH:O	2.06	0.55
2:U:151:GOL:HO2	1:X:111:HIS:CG	2.24	0.54
1:D:112[B]:GLN:HG2	1:D:113:SER:N	2.23	0.54
1:H:1:PRO:CG	1:H:43:ILE:HG22	2.35	0.54
1:B:31:GLU:HG2	1:B:47:PHE:CD2	2.43	0.54
1:T:31:GLU:HG2	1:T:47:PHE:CD2	2.42	0.54
1:R:132:LYS:HD3	3:R:2094:HOH:O	2.07	0.54
1:E:111:HIS:ND1	2:L:151:GOL:H2	2.22	0.54
1:Y:38:ALA:HB1	1:Y:43:ILE:O	2.08	0.54
1:C:17:ARG:HA	3:C:2006:HOH:O	2.08	0.54
1:D:102:ASN:ND2	3:D:2063:HOH:O	2.41	0.54
2:G:152:GOL:H32	3:G:2002:HOH:O	2.08	0.54
1:E:110:ARG:NH1	2:E:150:GOL:H12	2.22	0.54
1:J:141:GLN:OE1	1:J:142:GLN:N	2.41	0.54
1:U:17:ARG:HG2	1:U:17:ARG:NH1	2.23	0.54
1:Q:2:HIS:HA	1:Q:44:GLN:O	2.09	0.53
1:J:37:PHE:O	1:J:41:LEU:HB2	2.07	0.53
1:O:111:HIS:ND1	2:V:151:GOL:H12	2.23	0.53
3:B:2075:HOH:O	2:G:151:GOL:H11	2.07	0.53
1:X:64:GLU:HB3	3:X:2032:HOH:O	2.07	0.53
1:J:1:PRO:HD2	1:J:43:ILE:HG22	1.90	0.53
1:X:77:LEU:HD22	3:X:2026:HOH:O	2.09	0.53
1:M:1:PRO:CG	1:M:43:ILE:HG22	2.37	0.53
1:Q:117:PRO:HG3	2:Q:151:GOL:O2	2.09	0.53
1:S:19:PRO:HA	1:S:23:GLY:H	1.74	0.53
1:E:117:PRO:HG3	2:E:151:GOL:H11	1.91	0.53
1:Y:113:SER:O	2:Y:151:GOL:H32	2.08	0.53
1:X:120:LYS:HE3	3:X:2060:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:PHE:HB2	1:Q:21:VAL:HG21	1.89	0.53
1:P:38:ALA:HB1	1:P:43:ILE:O	2.09	0.53
1:E:1:PRO:HG2	1:E:43:ILE:HG21	1.90	0.53
2:Q:151:GOL:H11	1:Y:111:HIS:ND1	2.23	0.53
1:I:77:LEU:HA	3:I:2042:HOH:O	2.09	0.52
1:P:14:LEU:HD13	2:P:152:GOL:H32	1.90	0.52
1:F:1:PRO:CD	1:F:43:ILE:HG22	2.39	0.52
1:E:141:GLN:HG2	3:E:2089:HOH:O	2.09	0.52
1:C:14:LEU:HD13	2:C:152:GOL:H2	1.92	0.52
1:E:14:LEU:HD13	2:E:152:GOL:H11	1.92	0.52
1:C:2:HIS:HA	1:C:44:GLN:O	2.08	0.52
1:B:79:HIS:CE1	3:B:2073:HOH:O	2.62	0.52
1:A:19:PRO:HA	1:A:23:GLY:O	2.10	0.52
1:U:31:GLU:HG2	1:U:47:PHE:CD2	2.45	0.52
1:X:13:ARG:O	1:X:16:SER:HB3	2.10	0.52
1:H:124:VAL:HG21	3:H:2042:HOH:O	2.09	0.52
1:F:22:PHE:CE2	2:F:152:GOL:H2	2.45	0.52
1:S:32:THR:HA	3:S:2018:HOH:O	2.10	0.51
1:J:79:HIS:CE1	3:J:2060:HOH:O	2.63	0.51
1:P:15:GLY:O	1:P:17:ARG:N	2.43	0.51
1:I:34:LEU:HD11	1:I:131:TYR:HB3	1.91	0.51
1:T:19:PRO:HD3	3:T:2007:HOH:O	2.09	0.51
1:A:14:LEU:HD13	2:A:152:GOL:H2	1.91	0.51
1:K:2:HIS:HA	1:K:44:GLN:O	2.11	0.51
2:O:151:GOL:H11	1:V:111:HIS:ND1	2.25	0.51
1:C:2:HIS:HE2	1:C:46:THR:HG1	1.59	0.51
1:J:88:VAL:HG12	3:J:2073:HOH:O	2.11	0.51
1:U:25:GLN:HB2	1:U:29:ASP:HB2	1.91	0.51
1:C:53:GLU:HB3	3:C:2041:HOH:O	2.11	0.51
1:J:2:HIS:HA	1:J:44:GLN:O	2.10	0.51
1:S:81:SER:HB2	3:S:2044:HOH:O	2.10	0.51
1:S:25:GLN:HB3	1:S:29:ASP:HB2	1.91	0.51
1:T:17:ARG:HA	3:T:2008:HOH:O	2.11	0.51
1:I:38:ALA:CA	1:I:43:ILE:HG13	2.41	0.51
3:S:2033:HOH:O	1:U:80:TYR:HE1	1.93	0.51
1:O:137:TYR:CZ	1:O:141:GLN:HG3	2.46	0.51
1:N:33:ASP:HA	1:N:36:GLN:NE2	2.25	0.50
1:O:43:ILE:HD13	1:O:139:LEU:HD11	1.93	0.50
1:I:64:GLU:HB3	3:I:2034:HOH:O	2.12	0.50
1:A:130:GLY:HA3	3:A:2077:HOH:O	2.12	0.50
1:J:99:HIS:CE1	3:J:2060:HOH:O	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:TYR:CD2	3:N:2047:HOH:O	2.63	0.50
1:E:19:PRO:HB3	1:E:24:ARG:HA	1.92	0.50
1:P:112:GLN:CB	2:P:151:GOL:H31	2.41	0.50
1:U:47:PHE:HD2	3:U:2001:HOH:O	1.95	0.50
1:Q:47:PHE:O	3:Q:2025:HOH:O	2.19	0.50
1:L:113:SER:HB2	3:L:2078:HOH:O	2.12	0.50
1:D:19:PRO:HA	1:D:23:GLY:O	2.11	0.50
3:Q:2074:HOH:O	2:Y:151:GOL:H2	2.11	0.50
2:X:150:GOL:H12	3:X:2048:HOH:O	2.10	0.50
1:L:117:PRO:HG3	2:L:151:GOL:C1	2.38	0.50
2:L:150:GOL:C1	2:L:152:GOL:H31	2.42	0.50
1:J:75:GLY:HA2	3:J:2003:HOH:O	2.11	0.50
1:R:43:ILE:HG21	1:R:139:LEU:HD21	1.93	0.50
1:U:25:GLN:HB2	1:U:29:ASP:CB	2.42	0.50
1:O:43:ILE:HG21	1:O:139:LEU:HD11	1.92	0.50
1:G:19:PRO:HB3	3:G:2012:HOH:O	2.11	0.50
3:E:2026:HOH:O	1:L:102:ASN:HB3	2.11	0.50
1:I:53:GLU:HB3	3:I:2027:HOH:O	2.11	0.50
1:K:141:GLN:CD	1:K:142:GLN:N	2.42	0.50
1:U:79:HIS:CE1	3:U:2079:HOH:O	2.59	0.50
1:I:112:GLN:HG3	2:I:151:GOL:O3	2.12	0.50
1:B:30:ILE:HG22	1:B:34:LEU:CD1	2.42	0.49
1:V:17:ARG:HA	3:V:2008:HOH:O	2.12	0.49
2:A:151:GOL:H11	1:D:104:TYR:CD2	2.47	0.49
1:N:64:GLU:HB3	3:N:2041:HOH:O	2.11	0.49
1:L:103:LEU:HB2	3:L:2068:HOH:O	2.11	0.49
1:H:6:LEU:HD22	1:H:56:LEU:HD22	1.94	0.49
1:D:21:VAL:HG11	1:D:106:ARG:HD2	1.93	0.49
1:U:10:ASN:O	2:U:152:GOL:H2	2.12	0.49
1:I:29:ASP:N	1:I:29:ASP:OD1	2.45	0.49
1:B:78:SER:HA	1:B:115:ILE:HD12	1.94	0.49
1:I:38:ALA:HA	1:I:43:ILE:HG13	1.94	0.49
1:L:12:ASN:HA	1:L:27:LEU:HD22	1.93	0.49
2:Y:150:GOL:H32	3:Y:2034:HOH:O	2.12	0.49
1:O:41:LEU:O	1:O:43:ILE:HG23	2.12	0.49
1:E:18:GLU:O	1:E:22:PHE:HB2	2.12	0.49
2:U:151:GOL:HO2	1:X:111:HIS:CE1	2.31	0.49
1:C:111:HIS:ND1	2:J:151:GOL:H2	2.28	0.49
1:J:7:ASN:O	1:J:49:GLN:HA	2.13	0.49
1:Y:88:VAL:HG12	3:Y:2061:HOH:O	2.13	0.49
1:V:14:LEU:HD13	2:V:152:GOL:H2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:GLU:H	1:F:20:GLU:CD	2.15	0.48
1:C:117:PRO:HG3	2:C:151:GOL:O1	2.13	0.48
1:O:126:LEU:HB3	1:V:137:TYR:CD1	2.48	0.48
1:M:38:ALA:HB1	1:M:43:ILE:HG13	1.94	0.48
2:Q:151:GOL:H11	1:Y:111:HIS:CB	2.42	0.48
1:X:15:GLY:O	1:X:16:SER:C	2.51	0.48
1:B:113:SER:HB3	3:B:2098:HOH:O	2.12	0.48
1:A:82:TYR:HD1	3:A:2048:HOH:O	1.95	0.48
1:S:113:SER:CB	3:S:2073:HOH:O	2.55	0.48
1:N:114:VAL:HA	3:N:2093:HOH:O	2.14	0.48
1:E:2:HIS:HA	1:E:44:GLN:O	2.13	0.48
1:E:112:GLN:HA	3:E:2091:HOH:O	2.14	0.48
1:V:25:GLN:HE21	1:V:30:ILE:HG13	1.79	0.48
1:P:1:PRO:HB2	1:P:43:ILE:HG22	1.96	0.48
1:H:31:GLU:HG3	1:H:47:PHE:CE1	2.48	0.48
2:P:151:GOL:H32	3:P:2096:HOH:O	2.12	0.48
1:H:19:PRO:HA	1:H:23:GLY:O	2.14	0.48
1:O:1:PRO:HD2	1:O:43:ILE:HG22	1.95	0.48
1:B:77:LEU:HA	3:B:2046:HOH:O	2.12	0.48
1:K:140:SER:O	1:K:142:GLN:N	2.32	0.48
2:O:151:GOL:H11	1:V:111:HIS:CE1	2.48	0.48
1:Y:88:VAL:HG13	1:Y:95:VAL:HG21	1.96	0.48
1:G:116:ALA:N	1:G:117:PRO:CD	2.77	0.48
1:Y:113:SER:HB2	3:Y:2033:HOH:O	2.13	0.48
1:V:25:GLN:HG3	1:V:30:ILE:HD11	1.95	0.48
1:L:10:ASN:O	2:L:152:GOL:H12	2.14	0.48
1:O:111:HIS:ND1	2:V:151:GOL:H2	2.29	0.48
1:H:25:GLN:HB3	1:H:29:ASP:HB2	1.95	0.47
1:U:104:TYR:CD2	2:X:151:GOL:H11	2.48	0.47
1:A:2:HIS:HA	1:A:44:GLN:O	2.14	0.47
1:D:38:ALA:O	1:D:39:GLU:C	2.51	0.47
1:H:22:PHE:CZ	2:H:152:GOL:H12	2.49	0.47
1:H:10:ASN:HB2	3:H:2001:HOH:O	2.14	0.47
1:L:6:LEU:HD22	1:L:56:LEU:HD22	1.96	0.47
1:M:113:SER:HB2	3:M:2084:HOH:O	2.14	0.47
1:L:15:GLY:O	1:L:16:SER:C	2.52	0.47
1:O:9:PRO:HA	1:O:51:ASN:OD1	2.14	0.47
1:C:123:ILE:HB	3:C:2088:HOH:O	2.14	0.47
1:H:28:THR:O	1:H:29:ASP:C	2.50	0.47
1:P:80:TYR:HE1	3:Q:2031:HOH:O	1.96	0.47
1:E:99:HIS:CG	1:E:103:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:LEU:CD1	2:K:152:GOL:H2	2.37	0.47
1:O:99:HIS:CE1	3:O:2055:HOH:O	2.67	0.47
1:R:34:LEU:HG	3:R:2024:HOH:O	2.13	0.47
1:Y:43:ILE:HD12	1:Y:139:LEU:HD21	1.97	0.47
1:L:21:VAL:O	1:L:22:PHE:CB	2.62	0.47
1:D:103:LEU:HD12	3:D:2065:HOH:O	2.15	0.47
1:U:17:ARG:HH11	1:U:17:ARG:CG	2.27	0.47
1:S:90:SER:HA	1:U:17:ARG:NH1	2.29	0.47
1:P:113:SER:HB2	3:P:2079:HOH:O	2.15	0.47
1:R:78:SER:HA	1:R:115:ILE:HD12	1.97	0.47
1:N:78:SER:HA	1:N:115:ILE:HD12	1.97	0.47
1:B:35:PHE:HE2	3:B:2029:HOH:O	1.98	0.47
1:L:120:LYS:HA	3:L:2076:HOH:O	2.15	0.47
1:V:53:GLU:OE2	1:V:81:SER:OG	2.27	0.47
1:Y:13:ARG:O	1:Y:16:SER:OG	2.31	0.47
1:Y:17:ARG:HA	3:Y:2004:HOH:O	2.14	0.47
1:N:6:LEU:HD13	1:N:72:LEU:HD13	1.97	0.47
1:D:113:SER:HA	3:D:2047:HOH:O	2.15	0.47
2:C:151:GOL:H12	3:C:2098:HOH:O	2.14	0.47
1:G:78:SER:HA	1:G:115:ILE:HD12	1.97	0.47
1:G:3:PHE:HE1	1:G:139:LEU:CD2	2.27	0.47
1:I:72:LEU:O	1:I:97:GLU:HA	2.15	0.46
2:Q:151:GOL:C1	3:Q:2094:HOH:O	2.63	0.46
1:C:17:ARG:NH1	3:C:2009:HOH:O	2.48	0.46
1:L:16:SER:O	1:L:17:ARG:HB2	2.14	0.46
1:R:132:LYS:HB3	3:R:2094:HOH:O	2.15	0.46
1:O:103:LEU:HB2	3:O:2068:HOH:O	2.15	0.46
1:A:90:SER:HB2	3:C:2009:HOH:O	2.16	0.46
2:U:151:GOL:O2	1:X:111:HIS:ND1	2.49	0.46
1:Y:99:HIS:CE1	3:Y:2034:HOH:O	2.67	0.46
1:S:112:GLN:HG3	2:S:151:GOL:H31	1.97	0.46
1:D:38:ALA:HB1	1:D:43:ILE:O	2.15	0.46
1:G:77:LEU:HA	3:G:2046:HOH:O	2.14	0.46
1:M:80:TYR:HD1	3:M:2021:HOH:O	1.98	0.46
1:V:15:GLY:O	1:V:17:ARG:N	2.48	0.46
1:F:18:GLU:HA	1:F:19:PRO:HD2	1.77	0.46
1:Q:14:LEU:CD1	2:Q:152:GOL:H2	2.39	0.46
1:A:124:VAL:HG21	3:A:2062:HOH:O	2.15	0.46
1:M:81:SER:HB2	3:M:2051:HOH:O	2.15	0.46
3:A:2048:HOH:O	1:C:80:TYR:CD2	2.56	0.45
2:O:151:GOL:H32	3:O:2087:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:113:SER:H	2:X:151:GOL:H12	1.80	0.45
1:B:26:THR:O	1:B:29:ASP:HB2	2.15	0.45
1:R:81:SER:HA	3:R:2040:HOH:O	2.16	0.45
1:J:123:ILE:HB	3:J:2080:HOH:O	2.15	0.45
1:Y:112:GLN:HG3	2:Y:151:GOL:O3	2.16	0.45
1:A:36:GLN:HE21	1:A:36:GLN:HB2	1.35	0.45
1:T:14:LEU:CD1	2:T:152:GOL:H11	2.46	0.45
1:S:77:LEU:HA	3:S:2044:HOH:O	2.16	0.45
1:G:2:HIS:HA	1:G:44:GLN:O	2.17	0.45
1:J:20:GLU:H	1:J:20:GLU:CD	2.19	0.45
1:P:2:HIS:HA	1:P:44:GLN:O	2.17	0.45
1:C:17:ARG:HH11	1:C:17:ARG:HG2	1.81	0.45
1:I:41:LEU:O	1:I:42:HIS:HB2	2.17	0.45
1:N:99:HIS:CG	1:N:103:LEU:HD11	2.52	0.45
1:A:64:GLU:HB3	3:A:2040:HOH:O	2.16	0.45
1:S:99:HIS:CG	1:S:103:LEU:HD11	2.51	0.45
2:C:151:GOL:H31	3:J:2071:HOH:O	2.16	0.45
1:Y:2:HIS:HA	1:Y:44:GLN:O	2.16	0.45
1:I:15:GLY:O	1:I:17:ARG:N	2.50	0.45
1:Q:41:LEU:O	1:Q:42:HIS:HB2	2.16	0.45
1:Q:37:PHE:CZ	1:Q:41:LEU:HD11	2.52	0.45
1:C:43:ILE:HG21	1:C:139:LEU:HD21	1.99	0.45
1:U:38:ALA:O	1:U:39:GLU:C	2.56	0.45
2:U:151:GOL:O2	1:X:111:HIS:CG	2.70	0.45
1:I:38:ALA:HB1	1:I:43:ILE:HG13	1.98	0.45
1:A:38:ALA:O	1:A:39:GLU:C	2.53	0.45
1:B:32:THR:O	1:B:36:GLN:HG3	2.16	0.45
1:A:6:LEU:HD22	1:A:56:LEU:HD22	2.00	0.44
1:R:19:PRO:HA	1:R:23:GLY:O	2.17	0.44
2:V:152:GOL:H31	3:V:2012:HOH:O	2.17	0.44
1:D:79:HIS:CE1	1:D:110:ARG:HA	2.52	0.44
1:T:103:LEU:HD12	3:T:2054:HOH:O	2.17	0.44
1:M:41:LEU:O	1:M:42:HIS:CB	2.57	0.44
1:R:139:LEU:HD23	1:R:139:LEU:HA	1.84	0.44
1:O:111:HIS:HA	3:O:2068:HOH:O	2.17	0.44
1:A:36:GLN:O	1:A:37:PHE:C	2.55	0.44
1:H:79:HIS:CE1	3:H:2038:HOH:O	2.70	0.44
1:Q:103:LEU:HD12	3:Q:2082:HOH:O	2.17	0.44
1:G:95:VAL:HB	3:G:2056:HOH:O	2.17	0.44
1:X:130:GLY:HA3	3:X:2065:HOH:O	2.16	0.44
1:B:22:PHE:CE2	2:B:152:GOL:H32	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1:PRO:HG2	1:M:43:ILE:CG2	2.45	0.44
2:Q:151:GOL:H12	3:Q:2094:HOH:O	2.17	0.44
2:V:151:GOL:H32	3:V:2062:HOH:O	2.18	0.44
1:P:13:ARG:O	1:P:14:LEU:C	2.56	0.44
1:I:13:ARG:O	1:I:15:GLY:N	2.51	0.44
1:S:31:GLU:HB2	3:S:2017:HOH:O	2.18	0.44
1:L:2:HIS:HA	1:L:44:GLN:O	2.17	0.44
1:T:25:GLN:HB2	3:T:2011:HOH:O	2.18	0.44
1:A:113:SER:O	2:A:151:GOL:H12	2.18	0.44
1:P:74:PRO:HG2	1:P:78:SER:HB2	2.00	0.43
1:Y:78:SER:HA	1:Y:115:ILE:HD12	2.00	0.43
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.62	0.43
1:Q:139:LEU:HD23	1:Q:139:LEU:HA	1.79	0.43
1:E:126:LEU:HG	3:E:2083:HOH:O	2.18	0.43
1:S:22:PHE:HE2	2:S:150:GOL:HO1	1.65	0.43
1:I:38:ALA:CB	1:I:43:ILE:HG13	2.48	0.43
1:K:53:GLU:HB2	3:L:2032:HOH:O	2.18	0.43
1:M:14:LEU:CD1	2:M:152:GOL:H11	2.28	0.43
1:R:18:GLU:HA	1:R:20:GLU:OE2	2.18	0.43
1:V:25:GLN:HE21	1:V:30:ILE:HG12	1.82	0.43
1:I:79:HIS:CE1	1:I:110:ARG:HA	2.53	0.43
2:K:152:GOL:H32	3:K:2082:HOH:O	2.19	0.43
1:B:81:SER:HB2	3:B:2046:HOH:O	2.17	0.43
1:X:53:GLU:HB2	3:Y:2025:HOH:O	2.17	0.43
1:M:2:HIS:HA	1:M:44:GLN:O	2.18	0.43
1:O:53:GLU:HB3	3:O:2035:HOH:O	2.19	0.43
1:M:123:ILE:HG22	3:M:2086:HOH:O	2.18	0.43
1:L:117:PRO:CG	2:L:151:GOL:H12	2.43	0.43
1:O:53:GLU:HB3	3:O:2034:HOH:O	2.18	0.43
1:H:100:LEU:HG	3:H:2066:HOH:O	2.18	0.43
1:S:24:ARG:HB2	1:S:24:ARG:HE	1.62	0.43
2:R:151:GOL:H32	3:R:2099:HOH:O	2.18	0.43
1:T:2:HIS:HA	1:T:44:GLN:O	2.19	0.43
1:S:79:HIS:CE1	3:S:2039:HOH:O	2.71	0.43
1:H:75:GLY:HA2	2:H:150:GOL:O2	2.19	0.43
1:S:112:GLN:HB2	2:S:151:GOL:H31	2.00	0.43
1:C:22:PHE:CD2	2:C:152:GOL:H12	2.54	0.43
1:Y:30:ILE:HG22	1:Y:34:LEU:HD12	2.00	0.43
1:R:40:ALA:O	1:R:42:HIS:N	2.48	0.43
1:Y:43:ILE:CD1	1:Y:139:LEU:HD21	2.48	0.43
1:Y:16:SER:O	1:Y:17:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:17:ARG:O	1:Y:18:GLU:C	2.57	0.43
1:S:79:HIS:CE1	1:S:110:ARG:HA	2.54	0.43
1:J:122:GLN:HG2	1:J:124:VAL:HG23	2.01	0.43
1:P:136:ARG:O	1:P:139:LEU:HB2	2.19	0.43
1:D:22:PHE:CE2	2:D:152:GOL:H32	2.54	0.43
1:R:113:SER:O	2:R:151:GOL:H12	2.18	0.42
1:O:14:LEU:HD13	2:O:152:GOL:C1	2.49	0.42
1:N:82:TYR:HD1	3:N:2047:HOH:O	1.96	0.42
1:L:120:LYS:HA	1:L:120:LYS:HD3	1.90	0.42
2:S:150:GOL:C1	2:S:152:GOL:H31	2.47	0.42
1:T:103:LEU:HB2	3:T:2054:HOH:O	2.19	0.42
1:H:99:HIS:CG	1:H:103:LEU:HD11	2.54	0.42
2:M:151:GOL:H2	1:P:111:HIS:ND1	2.33	0.42
1:U:17:ARG:HG3	1:U:18:GLU:N	2.34	0.42
1:L:53:GLU:OE2	1:L:81:SER:OG	2.22	0.42
1:A:106:ARG:HH12	2:A:150:GOL:H12	1.84	0.42
1:B:6:LEU:HD22	1:B:56:LEU:HD22	2.02	0.42
1:R:141:GLN:HA	1:R:142:GLN:N	2.33	0.42
1:I:112:GLN:HB2	2:I:151:GOL:H32	2.01	0.42
1:A:34:LEU:HA	1:A:37:PHE:HB3	2.01	0.42
1:U:6:LEU:HD22	1:U:56:LEU:HD22	2.00	0.42
1:D:30:ILE:HA	3:D:2021:HOH:O	2.19	0.42
1:F:43:ILE:HG21	1:F:139:LEU:HD21	2.02	0.42
1:L:99:HIS:CG	1:L:103:LEU:HD11	2.54	0.42
1:K:34:LEU:HD11	1:K:131:TYR:HB3	2.01	0.42
1:M:7:ASN:O	1:M:49:GLN:HA	2.19	0.42
1:T:79:HIS:CE1	3:T:2039:HOH:O	2.71	0.42
1:N:116:ALA:N	1:N:117:PRO:CD	2.83	0.42
1:O:79:HIS:CE1	3:O:2055:HOH:O	2.71	0.42
1:G:81:SER:HB2	3:G:2046:HOH:O	2.19	0.42
1:U:78:SER:HA	1:U:115:ILE:HD12	2.01	0.42
2:R:152:GOL:H32	3:R:2006:HOH:O	2.19	0.42
1:J:80:TYR:HD1	3:J:2050:HOH:O	2.03	0.42
2:O:151:GOL:H2	1:V:111:HIS:ND1	2.35	0.42
1:K:25:GLN:H	1:K:25:GLN:HG2	1.67	0.42
1:R:112:GLN:HB2	3:R:2099:HOH:O	2.18	0.42
1:A:22:PHE:CE2	2:A:152:GOL:H32	2.55	0.42
1:P:97:GLU:O	1:P:122:GLN:HA	2.20	0.42
1:R:103:LEU:HD12	3:R:2065:HOH:O	2.19	0.42
1:P:42:HIS:N	1:P:42:HIS:ND1	2.65	0.42
1:B:111:HIS:CG	2:G:151:GOL:H12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1:PRO:CB	1:P:43:ILE:HG22	2.50	0.42
1:C:1:PRO:HG2	1:C:43:ILE:HG22	2.00	0.42
3:P:2033:HOH:O	1:R:77:LEU:CD2	2.67	0.42
1:K:36:GLN:HB3	3:K:2018:HOH:O	2.20	0.42
1:V:103:LEU:HB2	3:V:2075:HOH:O	2.19	0.42
1:U:7:ASN:ND2	3:U:2001:HOH:O	2.52	0.41
1:L:15:GLY:O	1:L:16:SER:O	2.38	0.41
1:V:66:GLN:HG3	3:V:2052:HOH:O	2.19	0.41
1:V:84:ILE:O	1:V:85:ARG:C	2.56	0.41
1:F:7:ASN:O	1:F:49:GLN:HA	2.19	0.41
1:S:22:PHE:CE2	2:S:152:GOL:H11	2.55	0.41
1:J:78:SER:HA	1:J:115:ILE:HD12	2.01	0.41
1:G:112[B]:GLN:CG	2:G:151:GOL:H2	2.35	0.41
1:U:43:ILE:HD13	1:U:139:LEU:HD11	2.02	0.41
1:K:113:SER:O	2:K:151:GOL:O1	2.37	0.41
1:M:6:LEU:HD13	1:M:72:LEU:HD13	2.01	0.41
1:C:22:PHE:CE2	2:C:152:GOL:H12	2.55	0.41
1:R:79:HIS:CE1	1:R:110:ARG:HA	2.55	0.41
1:R:128:ALA:HA	3:R:2087:HOH:O	2.19	0.41
1:S:43:ILE:HD13	1:S:139:LEU:HD21	2.01	0.41
1:R:99:HIS:CG	1:R:103:LEU:HD11	2.55	0.41
1:G:6:LEU:HD22	1:G:56:LEU:HD22	2.03	0.41
1:Q:103:LEU:HB2	3:Q:2073:HOH:O	2.20	0.41
1:M:99:HIS:CG	1:M:103:LEU:HD11	2.56	0.41
1:Y:103:LEU:CD1	3:Y:2059:HOH:O	2.58	0.41
1:S:25:GLN:HB3	1:S:29:ASP:CB	2.50	0.41
1:G:23:GLY:O	1:G:24:ARG:CB	2.68	0.41
3:M:2021:HOH:O	1:O:80:TYR:HD1	2.04	0.41
1:T:124:VAL:HG21	3:T:2054:HOH:O	2.21	0.41
1:I:31:GLU:HG3	1:I:47:PHE:CE1	2.55	0.41
1:E:80:TYR:HE1	3:F:2034:HOH:O	2.02	0.41
1:G:35:PHE:O	1:G:38:ALA:HB3	2.21	0.41
1:U:18:GLU:O	1:U:22:PHE:HB2	2.21	0.41
1:H:40:ALA:C	1:H:42:HIS:N	2.73	0.41
1:P:6:LEU:HD22	1:P:56:LEU:HD22	2.03	0.41
1:T:14:LEU:HD13	2:T:152:GOL:H11	2.03	0.41
1:C:116:ALA:N	1:C:117:PRO:CD	2.84	0.41
1:S:19:PRO:HA	1:S:23:GLY:N	2.36	0.41
1:C:2:HIS:NE2	1:C:46:THR:OG1	2.49	0.41
1:G:13:ARG:HD3	1:H:61:HIS:CG	2.56	0.41
1:L:43:ILE:CG2	1:L:139:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:LEU:HD11	3:H:2070:HOH:O	2.21	0.41
1:J:43:ILE:HG21	1:J:139:LEU:HD11	2.03	0.41
1:E:1:PRO:H2	1:E:43:ILE:HG22	1.86	0.41
1:J:79:HIS:CE1	1:J:110:ARG:HA	2.56	0.41
1:L:7:ASN:O	1:L:49:GLN:HA	2.21	0.41
1:I:108:GLU:HG2	3:I:2062:HOH:O	2.21	0.41
1:U:1:PRO:HD2	1:U:43:ILE:HG22	2.03	0.40
1:B:112:GLN:HG3	2:B:151:GOL:H31	2.02	0.40
1:U:14:LEU:HA	2:U:152:GOL:H11	2.04	0.40
1:J:99:HIS:CG	1:J:103:LEU:HD11	2.55	0.40
1:H:40:ALA:O	1:H:41:LEU:CB	2.69	0.40
1:M:18:GLU:HA	1:M:19:PRO:HD3	1.93	0.40
1:E:81:SER:HB2	3:E:2034:HOH:O	2.21	0.40
1:F:25:GLN:HE21	1:F:25:GLN:HB3	1.71	0.40
1:O:2:HIS:HA	1:O:44:GLN:O	2.21	0.40
1:L:17:ARG:NH1	3:L:2009:HOH:O	2.53	0.40
1:E:30:ILE:O	1:E:34:LEU:HG	2.21	0.40
1:M:120:LYS:NZ	3:M:2082:HOH:O	2.53	0.40
1:Q:12:ASN:HA	1:Q:27:LEU:CD2	2.52	0.40
1:Q:12:ASN:HA	1:Q:27:LEU:HD23	2.03	0.40
1:Y:79:HIS:CE1	3:Y:2034:HOH:O	2.74	0.40
1:I:138:LEU:O	1:I:141:GLN:HB2	2.20	0.40
1:S:112:GLN:CG	2:S:151:GOL:H31	2.52	0.40
1:L:10:ASN:HB2	3:L:2003:HOH:O	2.20	0.40
1:V:79:HIS:CE1	3:V:2058:HOH:O	2.74	0.40
1:A:18:GLU:OE1	1:A:21:VAL:HG21	2.22	0.40
1:H:43:ILE:CD1	1:H:139:LEU:HD11	2.51	0.40
1:K:10:ASN:O	2:K:152:GOL:O2	2.39	0.40
1:I:141:GLN:HE21	1:I:142:GLN:N	2.14	0.40
1:H:99:HIS:CE1	3:H:2038:HOH:O	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/143 (97%)	131 (94%)	8 (6%)	0	100 100
1	B	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	26 21
1	C	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	D	140/143 (98%)	132 (94%)	7 (5%)	1 (1%)	26 21
1	E	142/143 (99%)	130 (92%)	10 (7%)	2 (1%)	14 7
1	F	142/143 (99%)	133 (94%)	7 (5%)	2 (1%)	14 7
1	G	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	14 7
1	H	140/143 (98%)	132 (94%)	8 (6%)	0	100 100
1	I	139/143 (97%)	130 (94%)	5 (4%)	4 (3%)	6 2
1	J	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	K	132/143 (92%)	127 (96%)	5 (4%)	0	100 100
1	L	140/143 (98%)	128 (91%)	6 (4%)	6 (4%)	3 1
1	M	140/143 (98%)	133 (95%)	5 (4%)	2 (1%)	14 7
1	N	128/143 (90%)	124 (97%)	4 (3%)	0	100 100
1	O	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	P	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	14 7
1	Q	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	R	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	26 21
1	S	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	T	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	26 21
1	U	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	14 7
1	V	131/143 (92%)	125 (95%)	5 (4%)	1 (1%)	24 17
1	X	129/143 (90%)	122 (95%)	7 (5%)	0	100 100
1	Y	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	26 21
All	All	3314/3432 (97%)	3130 (94%)	156 (5%)	28 (1%)	24 17

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	16	SER
1	L	22	PHE
1	L	23	GLY

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Mol	Chain	Res	Type
1	P	16	SER
1	V	16	SER
1	E	16[A]	SER
1	E	16[B]	SER
1	G	24	ARG
1	I	14	LEU
1	I	25	GLN
1	L	16	SER
1	L	20	GLU
1	L	24	ARG
1	M	22	PHE
1	P	25	GLN
1	F	25	GLN
1	U	16	SER
1	F	18	GLU
1	I	18	GLU
1	R	26	THR
1	B	18	GLU
1	T	18	GLU
1	U	18	GLU
1	Y	18	GLU
1	D	18	GLU
1	G	18	GLU
1	M	21	VAL
1	L	19	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	115/120 (96%)	105 (91%)	10 (9%)	13 8
1	B	115/120 (96%)	106 (92%)	9 (8%)	16 11
1	C	115/120 (96%)	108 (94%)	7 (6%)	23 19
1	D	115/120 (96%)	102 (89%)	13 (11%)	7 4
1	E	119/120 (99%)	110 (92%)	9 (8%)	16 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	119/120 (99%)	112 (94%)	7 (6%)	24 20
1	G	117/120 (98%)	108 (92%)	9 (8%)	16 12
1	H	115/120 (96%)	102 (89%)	13 (11%)	7 4
1	I	114/120 (95%)	105 (92%)	9 (8%)	15 11
1	J	115/120 (96%)	107 (93%)	8 (7%)	19 15
1	K	110/120 (92%)	101 (92%)	9 (8%)	14 10
1	L	113/120 (94%)	104 (92%)	9 (8%)	15 11
1	M	116/120 (97%)	107 (92%)	9 (8%)	16 11
1	N	109/120 (91%)	102 (94%)	7 (6%)	22 18
1	O	115/120 (96%)	108 (94%)	7 (6%)	23 19
1	P	116/120 (97%)	105 (90%)	11 (10%)	11 7
1	Q	118/120 (98%)	110 (93%)	8 (7%)	20 16
1	R	115/120 (96%)	105 (91%)	10 (9%)	13 8
1	S	118/120 (98%)	105 (89%)	13 (11%)	8 4
1	T	118/120 (98%)	108 (92%)	10 (8%)	13 9
1	U	115/120 (96%)	108 (94%)	7 (6%)	23 19
1	V	112/120 (93%)	105 (94%)	7 (6%)	22 18
1	X	110/120 (92%)	103 (94%)	7 (6%)	22 18
1	Y	115/120 (96%)	100 (87%)	15 (13%)	5 2
All	All	2759/2880 (96%)	2536 (92%)	223 (8%)	15 10

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LEU
1	A	14	LEU
1	A	16	SER
1	A	17	ARG
1	A	22	PHE
1	A	33	ASP
1	A	42	HIS
1	A	112	GLN
1	A	138	LEU
1	B	1	PRO

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Mol	Chain	Res	Type
1	B	4	LEU
1	B	6	LEU
1	B	14	LEU
1	B	16	SER
1	B	20	GLU
1	B	25	GLN
1	B	112	GLN
1	B	138	LEU
1	C	4	LEU
1	C	6	LEU
1	C	14	LEU
1	C	17	ARG
1	C	20	GLU
1	C	112	GLN
1	C	138	LEU
1	D	4	LEU
1	D	6	LEU
1	D	14	LEU
1	D	17	ARG
1	D	20	GLU
1	D	21	VAL
1	D	22	PHE
1	D	25	GLN
1	D	42	HIS
1	D	74	PRO
1	D	112[A]	GLN
1	D	112[B]	GLN
1	D	138	LEU
1	E	4	LEU
1	E	6	LEU
1	E	14	LEU
1	E	25	GLN
1	E	33	ASP
1	E	41	LEU
1	E	43	ILE
1	E	112	GLN
1	E	138	LEU
1	F	4	LEU
1	F	6	LEU
1	F	14	LEU
1	F	68	SER
1	F	112[A]	GLN

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Mol	Chain	Res	Type
1	F	112[B]	GLN
1	F	138	LEU
1	G	4	LEU
1	G	6	LEU
1	G	14	LEU
1	G	16[A]	SER
1	G	16[B]	SER
1	G	20	GLU
1	G	112[A]	GLN
1	G	112[B]	GLN
1	G	138	LEU
1	H	4	LEU
1	H	6	LEU
1	H	14	LEU
1	H	17	ARG
1	H	33	ASP
1	H	35	PHE
1	H	37	PHE
1	H	42	HIS
1	H	43	ILE
1	H	64	GLU
1	H	112	GLN
1	H	138	LEU
1	H	140	SER
1	I	4	LEU
1	I	6	LEU
1	I	14	LEU
1	I	25	GLN
1	I	33	ASP
1	I	37	PHE
1	I	112	GLN
1	I	138	LEU
1	I	140	SER
1	J	4	LEU
1	J	6	LEU
1	J	14	LEU
1	J	25	GLN
1	J	36	GLN
1	J	41	LEU
1	J	112	GLN
1	J	138	LEU
1	K	1	PRO

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Mol	Chain	Res	Type
1	K	4	LEU
1	K	6	LEU
1	K	14	LEU
1	K	17	ARG
1	K	25	GLN
1	K	42	HIS
1	K	112	GLN
1	K	138	LEU
1	L	4	LEU
1	L	6	LEU
1	L	14	LEU
1	L	16	SER
1	L	36	GLN
1	L	112[A]	GLN
1	L	112[B]	GLN
1	L	138	LEU
1	L	140	SER
1	M	4	LEU
1	M	6	LEU
1	M	14	LEU
1	M	17	ARG
1	M	31	GLU
1	M	80	TYR
1	M	112	GLN
1	M	138	LEU
1	M	140	SER
1	N	4	LEU
1	N	6	LEU
1	N	14	LEU
1	N	25	GLN
1	N	112	GLN
1	N	138	LEU
1	N	140	SER
1	O	4	LEU
1	O	6	LEU
1	O	14	LEU
1	O	24	ARG
1	O	64	GLU
1	O	112	GLN
1	O	138	LEU
1	P	4	LEU
1	P	6	LEU

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Mol	Chain	Res	Type
1	P	14	LEU
1	P	16	SER
1	P	17	ARG
1	P	20	GLU
1	P	43	ILE
1	P	64	GLU
1	P	112	GLN
1	P	138	LEU
1	P	140	SER
1	Q	4	LEU
1	Q	6	LEU
1	Q	14	LEU
1	Q	24	ARG
1	Q	35	PHE
1	Q	74	PRO
1	Q	112	GLN
1	Q	138	LEU
1	R	1	PRO
1	R	4	LEU
1	R	6	LEU
1	R	14	LEU
1	R	20	GLU
1	R	25	GLN
1	R	64	GLU
1	R	112	GLN
1	R	138	LEU
1	R	140	SER
1	S	1	PRO
1	S	4	LEU
1	S	6	LEU
1	S	14	LEU
1	S	17	ARG
1	S	19	PRO
1	S	20	GLU
1	S	24	ARG
1	S	25	GLN
1	S	35	PHE
1	S	64	GLU
1	S	112	GLN
1	S	138	LEU
1	T	4	LEU
1	T	6	LEU

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Mol	Chain	Res	Type
1	T	14	LEU
1	T	18	GLU
1	T	20	GLU
1	T	35	PHE
1	T	43	ILE
1	T	112	GLN
1	T	138	LEU
1	T	139	LEU
1	U	4	LEU
1	U	6	LEU
1	U	14	LEU
1	U	17	ARG
1	U	20	GLU
1	U	112	GLN
1	U	138	LEU
1	V	4	LEU
1	V	6	LEU
1	V	14	LEU
1	V	25	GLN
1	V	35	PHE
1	V	112	GLN
1	V	138	LEU
1	X	4	LEU
1	X	6	LEU
1	X	14	LEU
1	X	16	SER
1	X	68	SER
1	X	112	GLN
1	X	138	LEU
1	Y	1	PRO
1	Y	4	LEU
1	Y	6	LEU
1	Y	14	LEU
1	Y	20	GLU
1	Y	25	GLN
1	Y	34	LEU
1	Y	35	PHE
1	Y	37	PHE
1	Y	42	HIS
1	Y	43	ILE
1	Y	74	PRO
1	Y	112	GLN

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Mol	Chain	Res	Type
1	Y	138	LEU
1	Y	140	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	141	GLN
1	B	66	GLN
1	C	66	GLN
1	D	25	GLN
1	D	66	GLN
1	G	66	GLN
1	H	66	GLN
1	H	141	GLN
1	I	25	GLN
1	I	36	GLN
1	I	66	GLN
1	I	141	GLN
1	J	66	GLN
1	J	141	GLN
1	L	66	GLN
1	M	36	GLN
1	M	66	GLN
1	O	66	GLN
1	P	36	GLN
1	P	66	GLN
1	Q	36	GLN
1	Q	66	GLN
1	R	36	GLN
1	S	25	GLN
1	S	66	GLN
1	T	66	GLN
1	U	66	GLN
1	V	25	GLN
1	V	66	GLN
1	X	36	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

72 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	150	-	5,5,5	0.91	0	5,5,5	0.51	0
2	GOL	A	151	-	5,5,5	0.64	0	5,5,5	1.95	2 (40%)
2	GOL	A	152	-	5,5,5	0.73	0	5,5,5	1.00	0
2	GOL	B	150	-	5,5,5	0.79	0	5,5,5	1.11	0
2	GOL	B	151	-	5,5,5	0.84	0	5,5,5	1.20	0
2	GOL	B	152	-	5,5,5	0.60	0	5,5,5	0.47	0
2	GOL	C	150	-	5,5,5	1.04	0	5,5,5	1.10	1 (20%)
2	GOL	C	151	-	5,5,5	0.76	0	5,5,5	0.98	0
2	GOL	C	152	-	5,5,5	0.78	0	5,5,5	0.73	0
2	GOL	D	150	-	5,5,5	1.02	0	5,5,5	2.20	2 (40%)
2	GOL	D	151	-	5,5,5	0.84	0	5,5,5	0.74	0
2	GOL	D	152	-	5,5,5	0.52	0	5,5,5	1.95	4 (80%)
2	GOL	E	150	-	5,5,5	1.04	1 (20%)	5,5,5	0.80	0
2	GOL	E	151	-	5,5,5	0.57	0	5,5,5	0.86	0
2	GOL	E	152	-	4,4,5	0.99	0	2,4,5	0.67	0
2	GOL	F	150	-	5,5,5	1.17	0	5,5,5	1.82	2 (40%)
2	GOL	F	151	-	5,5,5	0.53	0	5,5,5	0.79	0
2	GOL	F	152	-	4,4,5	1.07	0	2,4,5	0.26	0
2	GOL	G	150	-	5,5,5	0.56	0	5,5,5	1.15	1 (20%)
2	GOL	G	151	-	5,5,5	0.59	0	5,5,5	1.39	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	G	152	-	5,5,5	0.68	0	5,5,5	1.84	2 (40%)
2	GOL	H	150	-	5,5,5	0.90	0	5,5,5	1.44	1 (20%)
2	GOL	H	151	-	5,5,5	0.69	0	5,5,5	0.74	0
2	GOL	H	152	-	5,5,5	0.78	0	5,5,5	1.18	0
2	GOL	I	150	-	5,5,5	0.76	0	5,5,5	1.69	2 (40%)
2	GOL	I	151	-	5,5,5	0.59	0	5,5,5	0.91	0
2	GOL	I	152	-	5,5,5	0.52	0	5,5,5	1.04	0
2	GOL	J	150	-	5,5,5	0.92	0	5,5,5	2.29	2 (40%)
2	GOL	J	151	-	5,5,5	0.65	0	5,5,5	1.24	1 (20%)
2	GOL	J	152	-	5,5,5	0.76	0	5,5,5	1.06	1 (20%)
2	GOL	K	150	-	5,5,5	1.06	1 (20%)	5,5,5	1.21	0
2	GOL	K	151	-	5,5,5	0.65	0	5,5,5	0.61	0
2	GOL	K	152	-	5,5,5	0.79	0	5,5,5	1.04	0
2	GOL	L	150	-	5,5,5	0.96	0	5,5,5	2.26	2 (40%)
2	GOL	L	151	-	5,5,5	0.54	0	5,5,5	0.88	0
2	GOL	L	152	-	5,5,5	0.50	0	5,5,5	1.15	0
2	GOL	M	150	-	5,5,5	1.04	0	5,5,5	1.14	0
2	GOL	M	151	-	5,5,5	0.57	0	5,5,5	0.94	0
2	GOL	M	152	-	5,5,5	0.51	0	5,5,5	0.98	0
2	GOL	N	150	-	5,5,5	1.13	0	5,5,5	1.46	1 (20%)
2	GOL	N	151	-	5,5,5	0.71	0	5,5,5	1.50	1 (20%)
2	GOL	N	152	-	5,5,5	0.63	0	5,5,5	0.91	0
2	GOL	O	150	-	5,5,5	1.22	1 (20%)	5,5,5	1.60	1 (20%)
2	GOL	O	151	-	5,5,5	0.78	0	5,5,5	1.01	0
2	GOL	O	152	-	5,5,5	0.72	0	5,5,5	0.56	0
2	GOL	P	150	-	5,5,5	1.11	1 (20%)	5,5,5	1.10	0
2	GOL	P	151	-	5,5,5	0.73	0	5,5,5	0.78	0
2	GOL	P	152	-	5,5,5	0.64	0	5,5,5	0.72	0
2	GOL	Q	150	-	5,5,5	1.12	0	5,5,5	1.42	1 (20%)
2	GOL	Q	151	-	5,5,5	0.71	0	5,5,5	0.47	0
2	GOL	Q	152	-	5,5,5	0.90	0	5,5,5	0.78	0
2	GOL	R	150	-	5,5,5	1.80	2 (40%)	5,5,5	2.17	3 (60%)
2	GOL	R	151	-	5,5,5	0.41	0	5,5,5	1.48	1 (20%)
2	GOL	R	152	-	5,5,5	0.61	0	5,5,5	0.80	0
2	GOL	S	150	-	5,5,5	1.80	1 (20%)	5,5,5	1.38	1 (20%)
2	GOL	S	151	-	5,5,5	0.75	0	5,5,5	1.71	2 (40%)
2	GOL	S	152	-	5,5,5	0.54	0	5,5,5	0.97	0
2	GOL	T	150	-	5,5,5	1.00	0	5,5,5	1.60	1 (20%)
2	GOL	T	151	-	5,5,5	0.59	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	T	152	-	5,5,5	0.65	0	5,5,5	0.63	0
2	GOL	U	150	-	5,5,5	0.93	0	5,5,5	1.44	1 (20%)
2	GOL	U	151	-	5,5,5	0.36	0	5,5,5	0.73	0
2	GOL	U	152	-	5,5,5	0.72	0	5,5,5	0.60	0
2	GOL	V	150	-	5,5,5	0.54	0	5,5,5	1.11	0
2	GOL	V	151	-	5,5,5	0.71	0	5,5,5	1.89	1 (20%)
2	GOL	V	152	-	5,5,5	0.70	0	5,5,5	1.26	0
2	GOL	X	150	-	5,5,5	1.33	1 (20%)	5,5,5	0.94	0
2	GOL	X	151	-	5,5,5	0.76	0	5,5,5	1.69	1 (20%)
2	GOL	X	152	-	5,5,5	0.78	0	5,5,5	0.44	0
2	GOL	Y	150	-	5,5,5	0.70	0	5,5,5	1.60	2 (40%)
2	GOL	Y	151	-	5,5,5	0.52	0	5,5,5	0.94	0
2	GOL	Y	152	-	5,5,5	0.93	0	5,5,5	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	150	-	-	0/4/4/4	0/0/0/0
2	GOL	A	151	-	-	0/4/4/4	0/0/0/0
2	GOL	A	152	-	-	0/4/4/4	0/0/0/0
2	GOL	B	150	-	-	0/4/4/4	0/0/0/0
2	GOL	B	151	-	-	0/4/4/4	0/0/0/0
2	GOL	B	152	-	-	0/4/4/4	0/0/0/0
2	GOL	C	150	-	-	0/4/4/4	0/0/0/0
2	GOL	C	151	-	-	0/4/4/4	0/0/0/0
2	GOL	C	152	-	-	0/4/4/4	0/0/0/0
2	GOL	D	150	-	-	0/4/4/4	0/0/0/0
2	GOL	D	151	-	-	0/4/4/4	0/0/0/0
2	GOL	D	152	-	-	0/4/4/4	0/0/0/0
2	GOL	E	150	-	-	0/4/4/4	0/0/0/0
2	GOL	E	151	-	-	0/4/4/4	0/0/0/0
2	GOL	E	152	-	-	0/2/2/4	0/0/0/0
2	GOL	F	150	-	-	0/4/4/4	0/0/0/0
2	GOL	F	151	-	-	0/4/4/4	0/0/0/0
2	GOL	F	152	-	-	0/2/2/4	0/0/0/0
2	GOL	G	150	-	-	0/4/4/4	0/0/0/0
2	GOL	G	151	-	-	0/4/4/4	0/0/0/0
2	GOL	G	152	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	H	150	-	-	0/4/4/4	0/0/0/0
2	GOL	H	151	-	-	0/4/4/4	0/0/0/0
2	GOL	H	152	-	-	0/4/4/4	0/0/0/0
2	GOL	I	150	-	-	0/4/4/4	0/0/0/0
2	GOL	I	151	-	-	0/4/4/4	0/0/0/0
2	GOL	I	152	-	-	0/4/4/4	0/0/0/0
2	GOL	J	150	-	-	0/4/4/4	0/0/0/0
2	GOL	J	151	-	-	0/4/4/4	0/0/0/0
2	GOL	J	152	-	-	0/4/4/4	0/0/0/0
2	GOL	K	150	-	-	0/4/4/4	0/0/0/0
2	GOL	K	151	-	-	0/4/4/4	0/0/0/0
2	GOL	K	152	-	-	0/4/4/4	0/0/0/0
2	GOL	L	150	-	-	0/4/4/4	0/0/0/0
2	GOL	L	151	-	-	0/4/4/4	0/0/0/0
2	GOL	L	152	-	-	0/4/4/4	0/0/0/0
2	GOL	M	150	-	-	0/4/4/4	0/0/0/0
2	GOL	M	151	-	-	0/4/4/4	0/0/0/0
2	GOL	M	152	-	-	0/4/4/4	0/0/0/0
2	GOL	N	150	-	-	0/4/4/4	0/0/0/0
2	GOL	N	151	-	-	0/4/4/4	0/0/0/0
2	GOL	N	152	-	-	0/4/4/4	0/0/0/0
2	GOL	O	150	-	-	0/4/4/4	0/0/0/0
2	GOL	O	151	-	-	0/4/4/4	0/0/0/0
2	GOL	O	152	-	-	0/4/4/4	0/0/0/0
2	GOL	P	150	-	-	0/4/4/4	0/0/0/0
2	GOL	P	151	-	-	0/4/4/4	0/0/0/0
2	GOL	P	152	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	150	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	151	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	152	-	-	0/4/4/4	0/0/0/0
2	GOL	R	150	-	-	0/4/4/4	0/0/0/0
2	GOL	R	151	-	-	0/4/4/4	0/0/0/0
2	GOL	R	152	-	-	0/4/4/4	0/0/0/0
2	GOL	S	150	-	-	0/4/4/4	0/0/0/0
2	GOL	S	151	-	-	0/4/4/4	0/0/0/0
2	GOL	S	152	-	-	0/4/4/4	0/0/0/0
2	GOL	T	150	-	-	0/4/4/4	0/0/0/0
2	GOL	T	151	-	-	0/4/4/4	0/0/0/0
2	GOL	T	152	-	-	0/4/4/4	0/0/0/0
2	GOL	U	150	-	-	0/4/4/4	0/0/0/0
2	GOL	U	151	-	-	0/4/4/4	0/0/0/0
2	GOL	U	152	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	V	150	-	-	0/4/4/4	0/0/0/0
2	GOL	V	151	-	-	0/4/4/4	0/0/0/0
2	GOL	V	152	-	-	0/4/4/4	0/0/0/0
2	GOL	X	150	-	-	0/4/4/4	0/0/0/0
2	GOL	X	151	-	-	0/4/4/4	0/0/0/0
2	GOL	X	152	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	150	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	151	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	152	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	150	GOL	C1-C2	2.01	1.60	1.52
2	E	150	GOL	C1-C2	2.02	1.60	1.52
2	P	150	GOL	O1-C1	2.05	1.51	1.42
2	R	150	GOL	O1-C1	2.07	1.51	1.42
2	K	150	GOL	O1-C1	2.08	1.51	1.42
2	R	150	GOL	C1-C2	2.63	1.62	1.52
2	X	150	GOL	O1-C1	2.66	1.53	1.42
2	S	150	GOL	O1-C1	3.58	1.57	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	150	GOL	O1-C1-C2	-3.32	94.07	110.18
2	R	150	GOL	O1-C1-C2	-2.93	96.00	110.18
2	Q	150	GOL	O1-C1-C2	-2.56	97.78	110.18
2	U	150	GOL	O1-C1-C2	-2.52	97.94	110.18
2	R	150	GOL	C3-C2-C1	-2.44	101.55	111.12
2	N	150	GOL	O1-C1-C2	-2.37	98.69	110.18
2	C	150	GOL	O2-C2-C3	-2.36	97.81	108.65
2	S	150	GOL	O1-C1-C2	-2.26	99.24	110.18
2	I	150	GOL	O1-C1-C2	-2.16	99.72	110.18
2	D	152	GOL	C3-C2-C1	2.08	119.27	111.12
2	R	151	GOL	O1-C1-C2	2.08	120.28	110.18
2	D	152	GOL	O2-C2-C3	2.08	118.20	108.65
2	I	150	GOL	C3-C2-C1	2.10	119.33	111.12
2	G	150	GOL	O2-C2-C1	2.10	118.27	108.65
2	Y	150	GOL	O2-C2-C1	2.10	118.30	108.65
2	D	152	GOL	O3-C3-C2	2.16	120.67	110.18
2	J	152	GOL	O3-C3-C2	2.23	121.00	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	150	GOL	O2-C2-C1	2.24	118.91	108.65
2	A	151	GOL	O1-C1-C2	2.36	121.62	110.18
2	D	152	GOL	O2-C2-C1	2.37	119.53	108.65
2	R	150	GOL	O3-C3-C2	2.42	121.94	110.18
2	O	150	GOL	O3-C3-C2	2.44	122.03	110.18
2	S	151	GOL	O2-C2-C3	2.48	120.04	108.65
2	G	152	GOL	O2-C2-C3	2.51	120.17	108.65
2	J	150	GOL	O3-C3-C2	2.60	122.77	110.18
2	J	151	GOL	O2-C2-C1	2.60	120.57	108.65
2	N	151	GOL	O2-C2-C1	2.69	121.01	108.65
2	F	150	GOL	C3-C2-C1	2.71	121.76	111.12
2	S	151	GOL	O2-C2-C1	2.72	121.14	108.65
2	Y	150	GOL	O3-C3-C2	2.75	123.50	110.18
2	D	150	GOL	O2-C2-C3	2.79	121.45	108.65
2	H	150	GOL	O3-C3-C2	2.83	123.92	110.18
2	L	150	GOL	O3-C3-C2	2.88	124.17	110.18
2	G	152	GOL	O2-C2-C1	2.92	122.06	108.65
2	G	151	GOL	O2-C2-C1	2.93	122.08	108.65
2	X	151	GOL	C3-C2-C1	3.20	123.67	111.12
2	T	150	GOL	O3-C3-C2	3.23	125.83	110.18
2	A	151	GOL	O2-C2-C1	3.28	123.68	108.65
2	V	151	GOL	O2-C2-C1	3.72	125.71	108.65
2	L	150	GOL	C3-C2-C1	3.78	125.92	111.12
2	J	150	GOL	C3-C2-C1	4.22	127.66	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

53 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	150	GOL	1	0
2	A	151	GOL	2	0
2	A	152	GOL	2	0
2	B	151	GOL	3	0
2	B	152	GOL	2	0
2	C	151	GOL	4	0
2	C	152	GOL	3	0
2	D	151	GOL	4	0
2	D	152	GOL	1	0
2	E	150	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	151	GOL	1	0
2	E	152	GOL	1	0
2	F	151	GOL	2	0
2	F	152	GOL	1	0
2	G	151	GOL	5	0
2	G	152	GOL	1	0
2	H	150	GOL	1	0
2	H	151	GOL	2	0
2	H	152	GOL	2	0
2	I	151	GOL	2	0
2	I	152	GOL	2	0
2	J	151	GOL	2	0
2	K	151	GOL	2	0
2	K	152	GOL	4	0
2	L	150	GOL	2	0
2	L	151	GOL	4	0
2	L	152	GOL	3	0
2	M	151	GOL	1	0
2	M	152	GOL	2	0
2	N	151	GOL	1	0
2	N	152	GOL	2	0
2	O	151	GOL	4	0
2	O	152	GOL	4	0
2	P	151	GOL	5	0
2	P	152	GOL	1	0
2	Q	151	GOL	8	0
2	Q	152	GOL	3	0
2	R	151	GOL	5	0
2	R	152	GOL	1	0
2	S	150	GOL	3	0
2	S	151	GOL	4	0
2	S	152	GOL	4	0
2	T	151	GOL	1	0
2	T	152	GOL	3	0
2	U	151	GOL	8	0
2	U	152	GOL	2	0
2	V	151	GOL	3	0
2	V	152	GOL	2	0
2	X	150	GOL	1	0
2	X	151	GOL	2	0
2	Y	150	GOL	1	0
2	Y	151	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	152	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.