Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:36 AM GMT

PDB ID	:	3P9Q
Title	:	Structure of I274C variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on	:	2010-10-18
Resolution	:	1.48 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 ⓘ symbol.

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

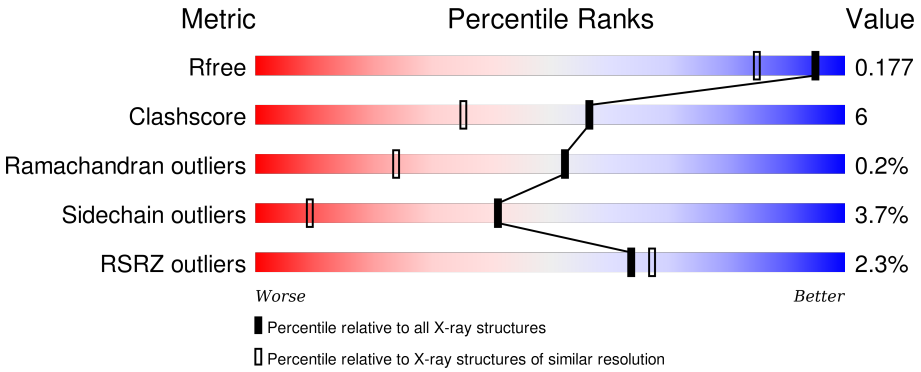
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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

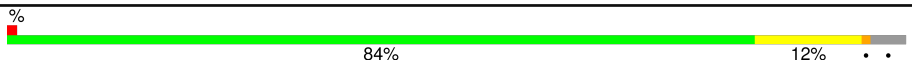
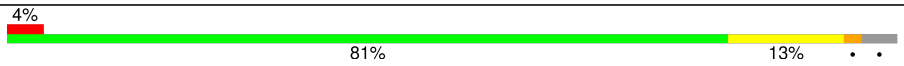
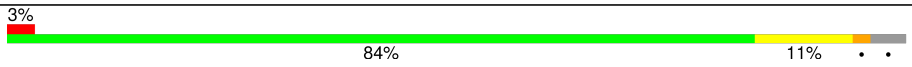
The reported resolution of this entry is 1.48 Å.

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))
R_{free}	91344	3129 (1.50-1.46)
Clashscore	102246	3380 (1.50-1.46)
Ramachandran outliers	100387	3310 (1.50-1.46)
Sidechain outliers	100360	3308 (1.50-1.46)
RSRZ outliers	91569	3133 (1.50-1.46)

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.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

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
3	HDE	A	761[B]	X	-	-	-
4	H2S	A	754[A]	-	-	X	X
4	H2S	B	754[A]	-	-	X	X
4	H2S	C	754[A]	-	-	X	X
4	H2S	D	754[A]	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 26893 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.

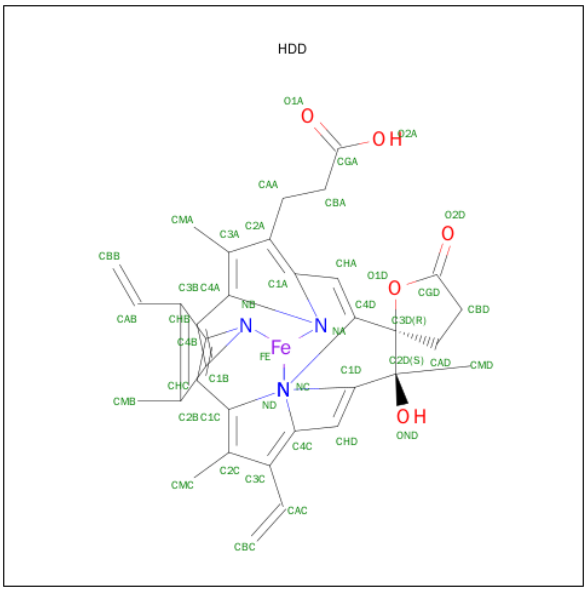
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	5	0
			5755	3652	1009	1083	11			
1	B	726	Total	C	N	O	S	0	5	0
			5757	3654	1009	1083	11			
1	C	726	Total	C	N	O	S	0	4	0
			5760	3658	1010	1081	11			
1	D	726	Total	C	N	O	S	0	8	0
			5769	3661	1012	1085	11			

There are 12 discrepancies between the modelled and reference sequences:

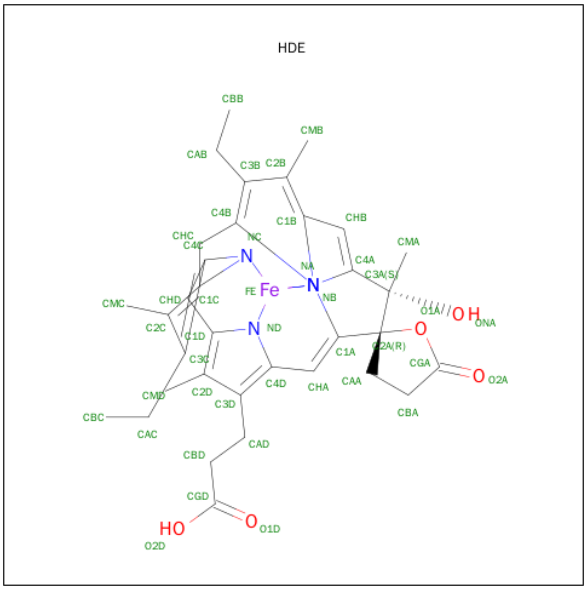
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
A	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
A	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
B	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
B	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
C	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
C	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
C	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179
D	274	CYS	ILE	ENGINEERED MUTATION	UNP P21179
D	438	ALA	CYS	ENGINEERED MUTATION	UNP P21179
D	669	ALA	CYS	ENGINEERED MUTATION	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



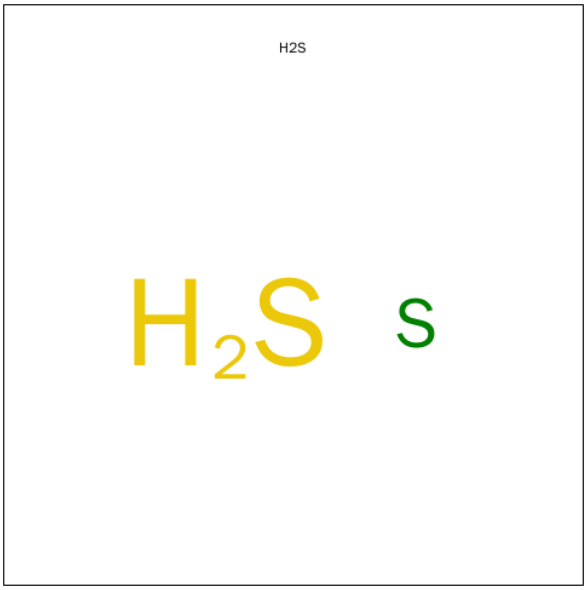
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (three-letter code: HDE) (formula: $C_{34}H_{38}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	S	0	1
			1	1		
4	B	1	Total	S	0	1
			1	1		
4	C	1	Total	S	0	1
			1	1		
4	D	1	Total	S	0	1
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	895	Total	O	0	0
			895	895		
5	B	803	Total	O	0	0
			803	803		

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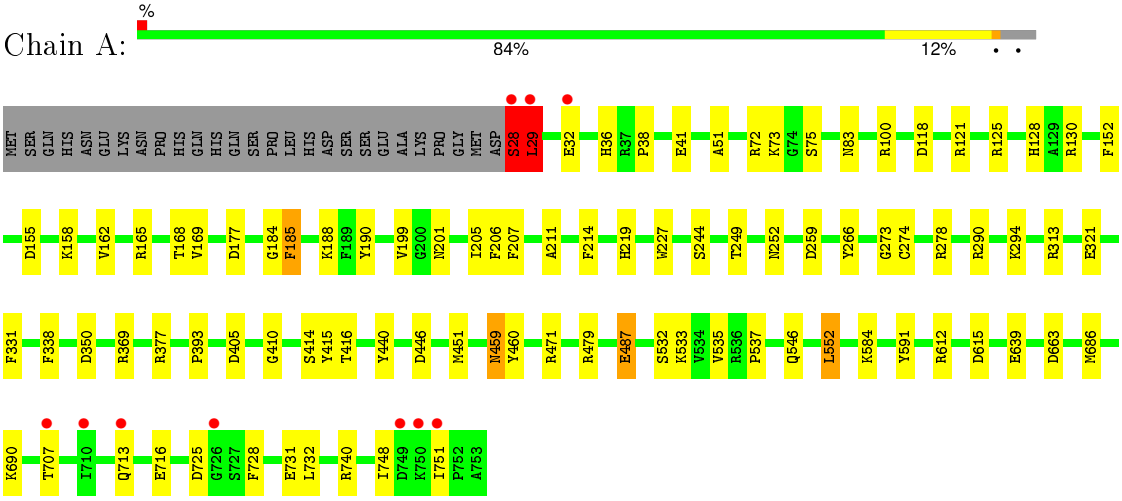
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	865	Total O 865 865	0	0
5	D	933	Total O 933 933	0	0

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.

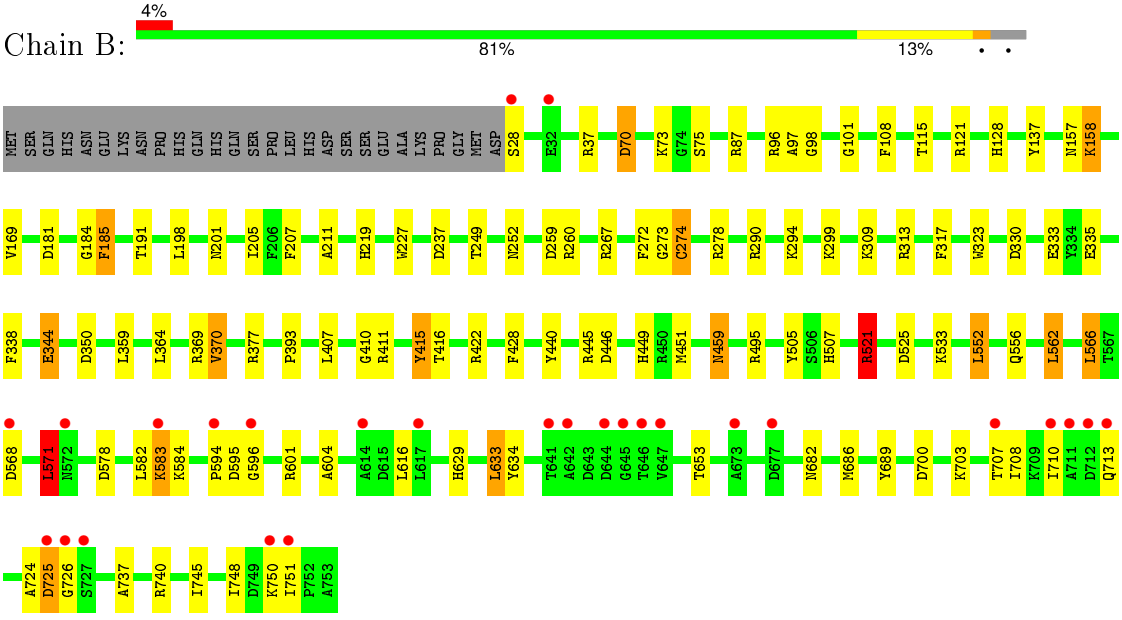
- Molecule 1: Catalase HPII

Chain A:



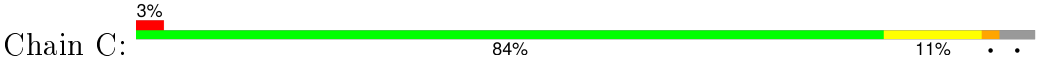
- Molecule 1: Catalase HPII

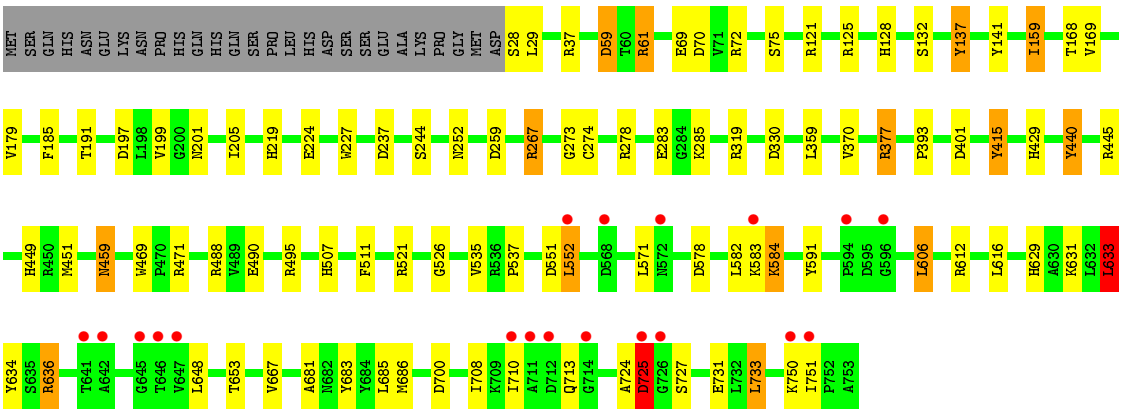
Chain B:



- Molecule 1: Catalase HPII

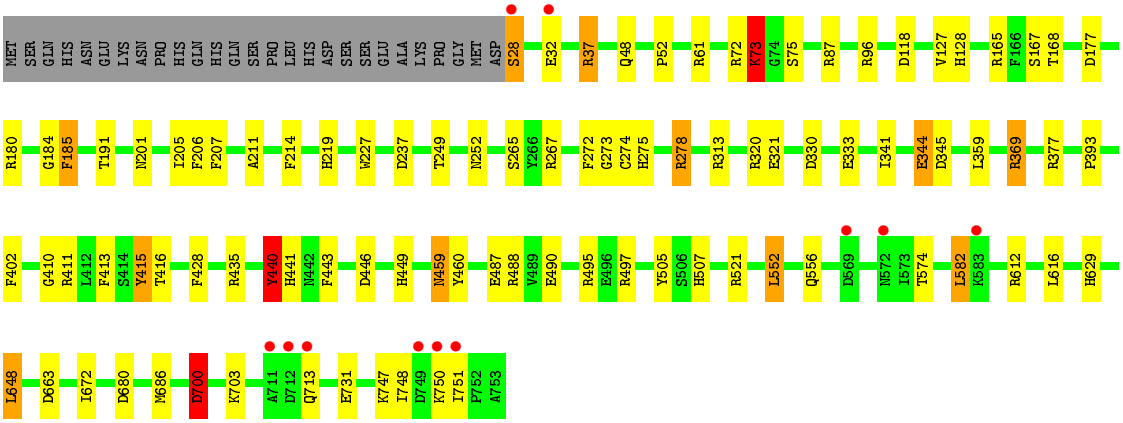
Chain C:





- Molecule 1: Catalase HPII

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.66Å 133.02Å 122.59Å 90.00° 109.59° 90.00°	Depositor
Resolution (Å)	28.55 – 1.48 28.55 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.7 (28.55-1.48) 91.7 (28.55-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.143 , 0.177 0.143 , 0.177	Depositor DCC
R_{free} test set	21507 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	10.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 429789 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26893	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HDE, HDD, H2S

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	1.37	11/5932 (0.2%)	1.22	34/8064 (0.4%)
1	B	1.32	15/5931 (0.3%)	1.20	43/8062 (0.5%)
1	C	1.30	18/5932 (0.3%)	1.20	33/8065 (0.4%)
1	D	1.40	24/5957 (0.4%)	1.23	33/8098 (0.4%)
All	All	1.35	68/23752 (0.3%)	1.21	143/32289 (0.4%)

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	A	0	1
1	B	0	1
1	C	1	3
All	All	1	5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	CD-OE1	9.75	1.36	1.25
1	D	28	SER	CB-OG	9.68	1.54	1.42
1	D	321	GLU	CD-OE1	8.88	1.35	1.25
1	C	59	ASP	CB-CG	8.65	1.70	1.51
1	D	440	TYR	CE1-CZ	7.54	1.48	1.38
1	B	37	ARG	CZ-NH2	7.37	1.42	1.33
1	D	333	GLU	CD-OE2	-7.02	1.18	1.25
1	A	460	TYR	CE1-CZ	6.97	1.47	1.38
1	B	521	ARG	CG-CD	6.90	1.69	1.51
1	D	206	PHE	CD1-CE1	6.88	1.53	1.39
1	A	29	LEU	N-CA	-6.61	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	ASP	CG-OD1	6.41	1.40	1.25
1	C	377	ARG	CZ-NH1	6.32	1.41	1.33
1	D	214	PHE	CE2-CZ	6.30	1.49	1.37
1	B	333	GLU	CD-OE1	-6.30	1.18	1.25
1	D	369	ARG	CG-CD	6.18	1.67	1.51
1	B	272	PHE	CE2-CZ	6.18	1.49	1.37
1	C	495	ARG	CZ-NH1	6.10	1.41	1.33
1	D	415	TYR	CE1-CZ	6.08	1.46	1.38
1	B	415	TYR	CE2-CZ	5.90	1.46	1.38
1	D	377	ARG	CZ-NH2	5.90	1.40	1.33
1	C	244	SER	CA-CB	5.75	1.61	1.52
1	C	377	ARG	CZ-NH2	5.74	1.40	1.33
1	C	415	TYR	CE2-CZ	5.74	1.46	1.38
1	B	37	ARG	CG-CD	5.70	1.66	1.51
1	D	505	TYR	CD1-CE1	5.68	1.47	1.39
1	C	591	TYR	CD2-CE2	5.65	1.47	1.39
1	C	132	SER	CB-OG	5.57	1.49	1.42
1	B	98	GLY	N-CA	5.57	1.54	1.46
1	D	272	PHE	CE2-CZ	5.56	1.48	1.37
1	A	350	ASP	CB-CG	-5.56	1.40	1.51
1	C	667	VAL	CB-CG2	5.46	1.64	1.52
1	C	179	VAL	CB-CG2	5.40	1.64	1.52
1	D	443	PHE	CE2-CZ	5.38	1.47	1.37
1	C	683	TYR	CE2-CZ	5.37	1.45	1.38
1	D	413	PHE	CG-CD1	5.37	1.46	1.38
1	A	190	TYR	CG-CD2	5.33	1.46	1.39
1	D	402	PHE	CE1-CZ	5.32	1.47	1.37
1	B	377	ARG	CG-CD	-5.32	1.38	1.51
1	A	331	PHE	CD1-CE1	5.29	1.49	1.39
1	C	370	VAL	CA-CB	5.29	1.65	1.54
1	C	526	GLY	N-CA	5.28	1.53	1.46
1	B	505	TYR	CD2-CE2	5.21	1.47	1.39
1	B	87	ARG	CZ-NH1	-5.19	1.26	1.33
1	B	338	PHE	CE1-CZ	5.19	1.47	1.37
1	D	28	SER	CA-C	5.18	1.66	1.52
1	D	344	GLU	CD-OE2	5.18	1.31	1.25
1	A	41	GLU	CG-CD	5.16	1.59	1.51
1	D	428	PHE	CG-CD2	5.15	1.46	1.38
1	C	511	PHE	CE1-CZ	5.14	1.47	1.37
1	D	167	SER	CB-OG	5.13	1.49	1.42
1	D	265	SER	CA-CB	5.13	1.60	1.52
1	A	377	ARG	CZ-NH1	5.12	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	460	TYR	CD1-CE1	5.12	1.47	1.39
1	A	740	ARG	CZ-NH2	5.09	1.39	1.33
1	B	335	GLU	CB-CG	-5.08	1.42	1.52
1	B	317	PHE	CD1-CE1	5.07	1.49	1.39
1	B	689	TYR	CG-CD1	5.07	1.45	1.39
1	D	320	ARG	CZ-NH1	5.06	1.39	1.33
1	A	487	GLU	CD-OE1	-5.04	1.20	1.25
1	B	323	TRP	CE3-CZ3	5.04	1.47	1.38
1	C	141	TYR	CG-CD2	5.04	1.45	1.39
1	C	469	TRP	CE3-CZ3	5.04	1.47	1.38
1	A	731	GLU	CD-OE2	-5.03	1.20	1.25
1	D	87	ARG	CZ-NH1	-5.02	1.26	1.33
1	C	69	GLU	CB-CG	5.01	1.61	1.52
1	D	73	LYS	CD-CE	5.01	1.63	1.51
1	D	377	ARG	CZ-NH1	5.01	1.39	1.33

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	636	ARG	NE-CZ-NH1	15.89	128.25	120.30
1	C	37	ARG	NE-CZ-NH2	-15.18	112.71	120.30
1	C	636	ARG	NE-CZ-NH2	-14.19	113.21	120.30
1	B	521	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	C	59	ASP	CB-CG-OD1	10.46	127.72	118.30
1	D	521	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	D	435	ARG	NE-CZ-NH2	-9.61	115.49	120.30
1	D	377	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	700	ASP	CB-CG-OD1	9.04	126.43	118.30
1	B	740	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	D	686	MET	CG-SD-CE	8.77	114.22	100.20
1	A	479	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	A	471	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	130	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	B	495	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	D	177	ASP	CB-CG-OD1	-8.04	111.06	118.30
1	B	313	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	70	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	A	663	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	C	37	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	377	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	96	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	D	61	ARG	NE-CZ-NH1	-7.61	116.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	582	LEU	CB-CG-CD1	7.49	123.74	111.00
1	A	28	SER	C-N-CA	-7.34	103.34	121.70
1	D	313	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	D	612	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	C	471	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	59	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	D	72	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	118	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	C	267	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	C	125	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	445	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	70	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	165	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	369	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	D	663	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	D	185	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	B	369	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	D	278	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	D	648	LEU	CB-CG-CD2	6.63	122.28	111.00
1	C	612	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	319	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	130	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	70	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	278	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	552	LEU	CB-CG-CD1	6.43	121.94	111.00
1	A	612	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	D	411	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	158	LYS	CA-CB-CG	-6.38	99.37	113.40
1	A	177	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	A	377	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	344	GLU	CA-CB-CG	6.20	127.03	113.40
1	B	686	MET	CG-SD-CE	-6.15	90.35	100.20
1	A	313	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	C	606	LEU	CB-CG-CD1	6.14	121.43	111.00
1	B	108	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	D	180	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	497	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	37	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	B	181	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	552	LEU	CB-CG-CD2	5.97	121.15	111.00
1	A	377	ARG	CG-CD-NE	-5.95	99.31	111.80
1	C	259	ASP	CB-CG-OD1	-5.94	112.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	290	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	260	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	740	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	525	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	495	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	266	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	A	338	PHE	CB-CG-CD1	-5.84	116.71	120.80
1	B	198	LEU	CB-CG-CD1	5.82	120.89	111.00
1	A	294	LYS	CD-CE-NZ	-5.80	98.37	111.70
1	B	370	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	C	278	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	D	612	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	D	37	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	185	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	C	733	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	680	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	725	ASP	N-CA-C	5.69	126.37	111.00
1	B	446	ASP	CB-CG-OD1	5.67	123.41	118.30
1	C	278	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	290	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	C	197	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	595	ASP	CB-CA-C	5.62	121.64	110.40
1	D	345	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	D	495	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	405	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	72	ARG	CG-CD-NE	-5.53	100.18	111.80
1	A	29	LEU	CB-CA-C	5.53	120.71	110.20
1	B	338	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	B	377	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	B	571	LEU	CB-CG-CD1	5.51	120.36	111.00
1	C	61	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	D	377	ARG	NH1-CZ-NH2	5.45	125.40	119.40
1	B	445	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	259	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	344	GLU	CA-CB-CG	5.42	125.32	113.40
1	B	137	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
1	B	259	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	B	601	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	552	LEU	CB-CG-CD1	5.40	120.17	111.00
1	A	185	PHE	CB-CG-CD2	-5.39	117.02	120.80
1	A	206	PHE	CB-CG-CD2	-5.39	117.02	120.80
1	A	446	ASP	CB-CG-OD1	5.39	123.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	D	446	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	96	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	428	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	615	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	96	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	299	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	C	633	LEU	CB-CG-CD1	5.33	120.06	111.00
1	B	313	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	445	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	72	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	562	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	551	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	100	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	612	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	B	267	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	497	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	377	ARG	CG-CD-NE	-5.20	100.89	111.80
1	C	377	ARG	NH1-CZ-NH2	5.20	125.11	119.40
1	D	118	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	C	137	TYR	CZ-CE2-CD2	-5.17	115.14	119.80
1	D	490	GLU	OE1-CD-OE2	5.15	129.49	123.30
1	D	435	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	479	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	165	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	309	LYS	CD-CE-NZ	-5.11	99.94	111.70
1	A	686	MET	CG-SD-CE	5.11	108.37	100.20
1	B	267	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	401	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	591	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	B	422	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	37	ARG	CB-CG-CD	-5.05	98.47	111.60
1	A	152	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	B	350	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	C	29	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	B	137	TYR	CG-CD1-CE1	-5.01	117.29	121.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	159	ILE	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5755	0	5582	61	0
1	B	5757	0	5587	63	0
1	C	5760	0	5591	59	0
1	D	5769	0	5597	53	0
2	A	44	0	31	12	0
2	B	44	0	31	19	0
2	C	44	0	31	19	0
2	D	44	0	31	11	0
3	A	44	0	36	10	0
3	B	44	0	36	10	0
3	C	44	0	36	8	0
3	D	44	0	36	9	0
4	A	1	0	0	5	0
4	B	1	0	0	4	0
4	C	1	0	0	5	0
4	D	1	0	0	4	0
5	A	895	0	0	9	1
5	B	803	0	0	19	0
5	C	865	0	0	20	0
5	D	933	0	0	25	1
All	All	26893	0	22625	282	1

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 6.

All (282) 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)
2:C:760[A]:HDD:HBB2	4:C:754[A]:H2S:S	1.30	1.70
2:B:760[A]:HDD:HBB2	4:B:754[A]:H2S:S	1.22	1.68
1:A:274:CYS:HB3	4:A:754[A]:H2S:S	1.34	1.63
1:B:274:CYS:HB3	4:B:754[A]:H2S:S	1.35	1.63
1:C:274:CYS:HB3	4:C:754[A]:H2S:S	1.32	1.62
1:D:274:CYS:HB3	4:D:754[A]:H2S:S	1.36	1.60
2:B:760[A]:HDD:CBB	4:B:754[A]:H2S:S	2.08	1.38
2:C:760[A]:HDD:CBB	4:C:754[A]:H2S:S	2.17	1.33
5:B:2705:HOH:O	1:D:73:LYS:HD3	1.26	1.30
3:B:761[B]:HDE:CBC	3:B:761[B]:HDE:HMC	1.59	1.29
1:C:578:ASP:HB3	5:C:2919:HOH:O	1.12	1.27
1:C:274:CYS:CB	4:C:754[A]:H2S:S	2.26	1.24
1:A:201:ASN:CG	2:A:760[A]:HDD:HMB2	1.58	1.23
1:B:274:CYS:CB	4:B:754[A]:H2S:S	2.27	1.21
1:A:274:CYS:CB	4:A:754[A]:H2S:S	2.28	1.20
1:D:274:CYS:CB	4:D:754[A]:H2S:S	2.31	1.18
1:A:29:LEU:HD22	5:C:2405:HOH:O	1.43	1.17
1:B:201:ASN:CG	2:B:760[A]:HDD:HMB2	1.63	1.16
1:B:451:MET:SD	5:B:3614:HOH:O	2.05	1.13
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:HMC	1.28	1.13
1:A:73:LYS:CD	5:C:3442:HOH:O	1.94	1.13
1:C:451:MET:SD	5:C:3612:HOH:O	2.10	1.09
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.26	1.08
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.51	1.08
2:A:760[A]:HDD:HBB2	4:A:754[A]:H2S:S	1.94	1.08
3:B:761[B]:HDE:HBCB	3:B:761[B]:HDE:HMC	1.16	1.07
1:A:201:ASN:ND2	2:A:760[A]:HDD:HMB2	1.68	1.06
1:D:201:ASN:CG	2:D:760[A]:HDD:HMB2	1.75	1.06
1:D:416[A]:THR:CG2	5:D:3576:HOH:O	2.03	1.05
1:B:416:THR:HG21	5:D:2464:HOH:O	1.55	1.04
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.20	1.03
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:HBCB	1.07	1.02
1:C:201:ASN:CG	2:C:760[A]:HDD:HMB2	1.80	1.02
1:D:416[A]:THR:HG23	5:D:3576:HOH:O	1.59	1.02
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCB	1.85	1.00
3:B:761[B]:HDE:HBCA	3:B:761[B]:HDE:HMC	1.45	0.98
1:A:451:MET:SD	5:A:3609:HOH:O	2.20	0.96
1:A:416[A]:THR:HG21	5:A:3313:HOH:O	1.65	0.96
3:D:761[B]:HDE:HMC	3:D:761[B]:HDE:CBC	1.96	0.96
2:A:760[A]:HDD:CBB	4:A:754[A]:H2S:S	2.54	0.95
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:HBCB	1.89	0.92
1:B:73:LYS:HE3	5:D:3517:HOH:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	1:B:745:ILE:HG21	1.85	0.90
1:A:73:LYS:HD3	5:C:3442:HOH:O	1.64	0.89
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:HMB	1.55	0.89
1:C:440[B]:TYR:CZ	5:C:1792:HOH:O	2.24	0.88
1:A:716:GLU:HG2	5:A:3090:HOH:O	1.73	0.88
1:A:28:SER:OG	1:A:28:SER:O	1.86	0.87
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:HBCA	2.02	0.87
1:A:639:GLU:HG3	5:A:2414:HOH:O	1.74	0.87
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.59	0.84
1:C:713:GLN:HB3	5:C:3004:HOH:O	1.78	0.84
3:C:761[B]:HDE:HBBB	3:C:761[B]:HDE:HMB	1.60	0.82
2:B:760[A]:HDD:HBB1	2:B:760[A]:HDD:HMB1	1.61	0.81
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:HMC	2.10	0.80
1:B:748:ILE:O	1:B:751:ILE:HG22	1.78	0.80
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB3	2.21	0.80
1:D:28:SER:HA	5:D:2467:HOH:O	1.81	0.79
1:D:274:CYS:SG	2:D:760[A]:HDD:CMB	2.71	0.79
3:B:761[B]:HDE:CMC	3:B:761[B]:HDE:CBC	2.31	0.78
3:B:761[B]:HDE:HBBB	3:B:761[B]:HDE:HMB	1.65	0.78
1:C:201:ASN:ND2	2:C:760[A]:HDD:HMB2	1.99	0.77
1:B:201:ASN:ND2	2:B:760[A]:HDD:HMB2	1.99	0.77
1:D:416[A]:THR:HG21	5:D:3334:HOH:O	1.84	0.77
1:A:751:ILE:O	1:A:751:ILE:HD12	1.83	0.77
2:C:760[A]:HDD:HBB1	2:C:760[A]:HDD:HMB1	1.66	0.75
1:C:685:LEU:N	1:C:685:LEU:HD22	2.02	0.73
1:D:700:ASP:OD1	5:D:3236:HOH:O	2.07	0.73
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB3	2.29	0.72
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.07	0.72
2:C:760[A]:HDD:CBB	2:C:760[A]:HDD:HMB1	2.20	0.71
1:D:274:CYS:SG	2:D:760[A]:HDD:HMB1	2.29	0.71
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB3	2.30	0.71
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	1.91	0.71
1:D:440:TYR:CZ	5:D:3517:HOH:O	2.42	0.71
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB3	2.31	0.71
2:C:760[A]:HDD:CBC	2:C:760[A]:HDD:HMC1	2.21	0.70
1:A:274:CYS:SG	2:A:760[A]:HDD:CMB	2.79	0.70
2:B:760[A]:HDD:CBB	2:B:760[A]:HDD:HMB1	2.22	0.70
3:B:761[B]:HDE:CBB	3:B:761[B]:HDE:HMB	2.21	0.70
1:D:416[A]:THR:HG21	5:D:3576:HOH:O	1.76	0.69
3:D:761[B]:HDE:CMC	3:D:761[B]:HDE:CBC	2.62	0.69
1:C:578:ASP:OD1	5:C:3157:HOH:O	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760[A]:HDD:CMB	2:B:760[A]:HDD:HBB1	2.23	0.69
2:C:760[A]:HDD:CMB	2:C:760[A]:HDD:HBB1	2.21	0.68
1:C:274:CYS:SG	2:C:760[A]:HDD:CMB	2.83	0.67
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.78	0.67
2:C:760[A]:HDD:HMC1	2:C:760[A]:HDD:HBC1	1.77	0.67
1:D:703:LYS:NZ	5:D:2744:HOH:O	2.26	0.67
1:D:201:ASN:ND2	2:D:760[A]:HDD:HMB2	2.10	0.66
1:B:274:CYS:SG	2:B:760[A]:HDD:CMB	2.83	0.65
1:C:274:CYS:HB3	2:C:760[A]:HDD:CBB	2.26	0.65
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.26	0.65
2:C:760[A]:HDD:CMC	2:C:760[A]:HDD:HBC1	2.27	0.64
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.80	0.64
1:C:725:ASP:O	5:C:2403:HOH:O	2.14	0.64
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:HBCB	2.06	0.64
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.27	0.64
1:B:700:ASP:HB2	5:B:3595:HOH:O	1.97	0.63
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.80	0.63
1:B:533[A]:LYS:HE2	5:B:3100:HOH:O	1.98	0.63
1:C:578:ASP:HB2	1:C:582:LEU:O	1.98	0.63
1:B:70:ASP:OD1	5:B:2761:HOH:O	2.15	0.63
1:A:201:ASN:ND2	2:A:760[A]:HDD:CMB	2.53	0.62
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.62
1:C:583:LYS:O	1:C:584:LYS:HB3	2.00	0.61
1:A:532:SER:OG	5:A:2410:HOH:O	2.15	0.61
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.84	0.60
1:B:449[B]:HIS:HE1	5:D:1789:HOH:O	1.84	0.60
1:D:267:ARG:HG3	5:D:1920:HOH:O	2.01	0.60
1:D:341:ILE:HD12	5:D:3022:HOH:O	2.02	0.59
1:B:274:CYS:HB3	2:B:760[A]:HDD:CBB	2.33	0.59
1:D:440:TYR:CE2	5:D:3517:HOH:O	2.55	0.59
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.84	0.58
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:CMC	2.12	0.58
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.86	0.58
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.86	0.58
1:A:416[B]:THR:HG22	5:A:901:HOH:O	2.03	0.58
1:C:274:CYS:SG	2:C:760[A]:HDD:HBB1	2.45	0.57
1:B:521:ARG:NH2	1:B:745:ILE:CG2	2.64	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.57
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.32	0.57
1:B:115:THR:CG2	5:B:3420:HOH:O	2.54	0.56
1:B:726:GLY:HA2	5:B:3590:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:761[B]:HDE:CMC	3:C:761[B]:HDE:CBC	2.82	0.56
2:B:760[A]:HDD:CBC	2:B:760[A]:HDD:HMC1	2.35	0.56
1:B:359:LEU:H	1:B:507:HIS:HD2	1.54	0.56
1:C:59:ASP:OD2	5:C:2529:HOH:O	2.17	0.56
1:B:274:CYS:SG	2:B:760[A]:HDD:HBB1	2.47	0.55
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:HMC1	1.89	0.55
1:C:681:ALA:O	1:C:685:LEU:HD23	2.05	0.55
1:D:672:ILE:HG12	1:D:700:ASP:OD2	2.06	0.55
1:D:449[A]:HIS:HE1	5:D:1789:HOH:O	1.90	0.55
1:B:629:HIS:HD2	5:B:1054:HOH:O	1.89	0.55
1:D:127:VAL:HG22	3:D:761[B]:HDE:HMAB	1.88	0.54
1:A:73:LYS:HD2	5:C:3442:HOH:O	1.79	0.54
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.89	0.54
1:C:273:GLY:C	1:C:274:CYS:SG	2.86	0.54
1:A:273:GLY:C	1:A:274:CYS:SG	2.85	0.54
1:B:583:LYS:NZ	1:B:583:LYS:H	2.05	0.54
1:A:201:ASN:CG	2:A:760[A]:HDD:CMB	2.53	0.54
1:D:37:ARG:HD2	5:D:2157:HOH:O	2.08	0.54
2:D:760[A]:HDD:CBB	4:D:754[A]:H2S:S	2.96	0.53
1:D:748:ILE:O	1:D:751:ILE:HG22	2.08	0.53
1:A:725:ASP:H	1:A:728:PHE:HB3	1.72	0.53
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.39	0.53
1:A:29:LEU:HD23	5:C:3144:HOH:O	2.08	0.53
1:D:275:HIS:CE1	2:D:760[A]:HDD:HBB2	2.44	0.53
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.90	0.53
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.38	0.53
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.24	0.53
1:A:214:PHE:CD2	3:A:761[B]:HDE:HAB	2.45	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.52
1:B:201:ASN:ND2	2:B:760[A]:HDD:CMB	2.72	0.52
1:A:184:GLY:HA3	2:A:760[A]:HDD:HMA2	1.90	0.52
2:C:760[A]:HDD:CMB	2:C:760[A]:HDD:CBB	2.85	0.52
1:C:700:ASP:HB2	5:C:3596:HOH:O	2.08	0.52
2:D:760[A]:HDD:HBB2	4:D:754[A]:H2S:S	2.49	0.52
2:D:760[A]:HDD:HMC1	2:D:760[A]:HDD:CBC	2.40	0.52
1:A:274:CYS:CA	4:A:754[A]:H2S:S	2.99	0.51
1:C:634:TYR:O	1:C:653:THR:HA	2.10	0.51
2:B:760[A]:HDD:HBC1	2:B:760[A]:HDD:CMC	2.41	0.51
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.45	0.51
3:A:761[B]:HDE:CBC	3:A:761[B]:HDE:CMC	2.81	0.50
2:C:760[A]:HDD:CMC	2:C:760[A]:HDD:CBC	2.86	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:HG12	3:C:761[B]:HDE:HHDA	1.93	0.50
1:C:274:CYS:CB	2:C:760[A]:HDD:CBB	2.90	0.49
1:B:274:CYS:SG	2:B:760[A]:HDD:HMB1	2.52	0.49
1:A:748:ILE:O	1:A:751:ILE:HG13	2.13	0.49
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.16	0.49
1:A:73:LYS:CE	5:C:3442:HOH:O	2.40	0.49
1:B:201:ASN:OD1	2:B:760[A]:HDD:HMB2	2.08	0.49
1:B:115:THR:HG21	5:B:3420:HOH:O	2.11	0.48
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.29	0.48
1:B:578:ASP:HB2	5:B:2590:HOH:O	2.12	0.48
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.44	0.48
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.48
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.48	0.48
3:D:761[B]:HDE:HMAA	3:D:761[B]:HDE:HAAA	1.67	0.48
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.48
1:C:727:SER:O	1:C:731:GLU:HG3	2.13	0.47
1:C:274:CYS:SG	2:C:760[A]:HDD:HMB1	2.50	0.47
1:D:341:ILE:CG1	5:D:3022:HOH:O	2.63	0.47
1:B:556:GLN:HG2	1:B:566:LEU:HD22	1.96	0.47
1:C:681:ALA:O	1:C:685:LEU:CD2	2.63	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.30	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.14	0.47
1:C:685:LEU:H	1:C:685:LEU:HD22	1.76	0.47
3:D:761[B]:HDE:CMB	3:D:761[B]:HDE:CBB	2.91	0.47
1:C:685:LEU:CD2	1:C:685:LEU:N	2.73	0.47
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.50	0.47
1:A:201:ASN:CB	2:A:760[A]:HDD:HMB2	2.44	0.46
1:D:341:ILE:HG13	5:D:3022:HOH:O	2.15	0.46
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.50	0.46
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMC	2.19	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.97	0.46
1:C:274:CYS:CA	4:C:754[A]:H2S:S	3.02	0.46
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.98	0.46
1:B:158:LYS:HG2	5:B:975:HOH:O	2.15	0.46
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.97	0.46
1:C:584:LYS:HB2	1:C:584:LYS:HE3	1.78	0.45
1:B:552:LEU:HD22	1:B:552:LEU:O	2.16	0.45
1:A:533:LYS:HE3	5:A:2410:HOH:O	2.17	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
3:A:761[B]:HDE:HBBB	3:A:761[B]:HDE:HMB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.52	0.45
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.99	0.45
1:B:596:GLY:HA3	1:B:737:ALA:O	2.17	0.45
1:D:672:ILE:CG1	1:D:700:ASP:OD2	2.65	0.45
1:B:459:ASN:H	1:B:459:ASN:HD22	1.64	0.45
5:B:983:HOH:O	1:D:52:PRO:HG3	2.17	0.45
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:A:414:SER:OG	3:A:761[B]:HDE:HHB	2.18	0.44
1:D:341:ILE:CD1	5:D:3022:HOH:O	2.62	0.44
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.52	0.44
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.47	0.44
1:C:137:TYR:CB	1:C:159:ILE:HD11	2.41	0.44
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.99	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.17	0.44
1:A:274:CYS:SG	2:A:760[A]:HDD:HMB1	2.54	0.44
1:B:407:LEU:HG	3:B:761[B]:HDE:HABA	1.99	0.44
1:A:29:LEU:HD12	1:A:29:LEU:N	2.33	0.43
1:B:583:LYS:O	1:B:584:LYS:HB3	2.18	0.43
1:A:155:ASP:CG	5:A:3378:HOH:O	2.56	0.43
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.19	0.43
1:B:273:GLY:C	1:B:274:CYS:SG	2.96	0.43
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.43
1:C:583:LYS:O	1:C:584:LYS:CB	2.67	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.43
1:B:28:SER:HA	5:B:2571:HOH:O	2.18	0.43
1:A:29:LEU:HD12	1:A:29:LEU:H	1.83	0.43
1:C:128:HIS:HA	1:C:168:THR:O	2.18	0.43
1:C:224:GLU:HB3	5:C:3120:HOH:O	2.19	0.43
5:B:3557:HOH:O	1:C:686:MET:HE1	2.18	0.43
5:B:3376:HOH:O	1:D:28:SER:HB3	2.19	0.43
2:A:760[A]:HDD:HMC1	2:A:760[A]:HDD:CBC	2.49	0.43
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.52	0.43
1:B:115:THR:HG23	5:B:3420:HOH:O	2.17	0.42
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.01	0.42
1:D:393:PRO:HD2	1:D:415:TYR:CD2	2.54	0.42
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.42
1:C:490:GLU:OE1	1:D:488[B]:ARG:NH2	2.28	0.42
1:D:552:LEU:HA	1:D:552:LEU:HD22	1.88	0.42
1:C:267:ARG:HD2	1:C:267:ARG:HH11	1.63	0.42
1:C:201:ASN:ND2	2:C:760[A]:HDD:CMB	2.77	0.42
1:A:125:ARG:HG2	3:A:761[B]:HDE:HBA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.23	0.42
1:D:273:GLY:C	1:D:274:CYS:SG	2.98	0.42
1:D:184:GLY:HA3	2:D:760[A]:HDD:HMA2	2.01	0.42
1:A:535:VAL:O	1:A:537:PRO:HD3	2.20	0.42
3:A:761[B]:HDE:HABA	3:A:761[B]:HDE:HHCA	1.85	0.41
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.41
1:D:275:HIS:NE2	2:D:760[A]:HDD:CBB	2.83	0.41
1:C:685:LEU:CD2	1:C:685:LEU:H	2.33	0.41
1:B:724:ALA:O	1:B:725:ASP:O	2.38	0.41
3:C:761[B]:HDE:HMAA	3:C:761[B]:HDE:HAAA	1.60	0.41
1:A:83:ASN:HB3	1:C:429:HIS:CG	2.55	0.41
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.56	0.41
1:B:751:ILE:HG23	1:B:751:ILE:O	2.21	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.20	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.21	0.41
1:B:521:ARG:HG3	5:B:3553:HOH:O	2.21	0.41
1:A:244:SER:HA	1:A:546[B]:GLN:NE2	2.36	0.41
1:A:36:HIS:HD2	1:A:36:HIS:H	1.66	0.40
1:B:294:LYS:NZ	5:B:2778:HOH:O	2.53	0.40
1:C:507:HIS:HE1	5:C:926:HOH:O	2.04	0.40
1:D:369:ARG:CG	5:D:3574:HOH:O	2.68	0.40
1:B:184:GLY:HA3	2:B:760[A]:HDD:HMA2	2.02	0.40
1:A:83:ASN:HB3	1:C:429:HIS:CD2	2.56	0.40
1:B:364:LEU:HG	1:B:582:LEU:HD11	2.04	0.40
1:A:199:VAL:HG12	3:A:761[B]:HDE:HHDA	2.02	0.40
1:A:751:ILE:O	1:A:751:ILE:CD1	2.64	0.40
1:C:631:LYS:HG3	1:C:633:LEU:CD1	2.51	0.40
1:D:207:PHE:O	1:D:249:THR:HA	2.21	0.40
2:B:760[A]:HDD:CBC	2:B:760[A]:HDD:CMC	2.99	0.40
1:A:162:VAL:HA	1:A:188:LYS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3241:HOH:O	5:D:2457:HOH:O[2_646]	1.92	0.28

5.3 Torsion angles

5.3.1 Protein backbone

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	729/753 (97%)	711 (98%)	17 (2%)	1 (0%)	56	25
1	B	729/753 (97%)	713 (98%)	14 (2%)	2 (0%)	46	18
1	C	728/753 (97%)	707 (97%)	20 (3%)	1 (0%)	56	25
1	D	732/753 (97%)	714 (98%)	17 (2%)	1 (0%)	56	25
All	All	2918/3012 (97%)	2845 (98%)	68 (2%)	5 (0%)	52	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	D	75	SER
1	B	75	SER

5.3.2 Protein sidechains

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	614/634 (97%)	599 (98%)	15 (2%)	57	21
1	B	614/634 (97%)	589 (96%)	25 (4%)	37	7
1	C	613/634 (97%)	583 (95%)	30 (5%)	31	4
1	D	617/634 (97%)	596 (97%)	21 (3%)	44	11
All	All	2458/2536 (97%)	2367 (96%)	91 (4%)	41	9

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	32	GLU
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	584	LYS
1	A	707	THR
1	A	713	GLN
1	A	732	LEU
1	B	157	ASN
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	274	CYS
1	B	344	GLU
1	B	370	VAL
1	B	440	TYR
1	B	459	ASN
1	B	521	ARG
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	594	PRO
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	750	LYS
1	C	28	SER
1	C	61	ARG

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Mol	Chain	Res	Type
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440[A]	TYR
1	C	440[B]	TYR
1	C	459	ASN
1	C	488[A]	ARG
1	C	488[B]	ARG
1	C	521	ARG
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	32	GLU
1	D	48	GLN
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	344	GLU
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	574	THR

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Mol	Chain	Res	Type
1	D	582	LEU
1	D	616	LEU
1	D	648	LEU
1	D	700	ASP
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	B	157	ASN
1	B	252	ASN
1	B	368	GLN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

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)

Of 12 ligands modelled in this entry, 4 are modelled with single atom - leaving 8 for Mogul analysis.

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	HDD	A	760[A]	1,5	30,52,52	2.43	12 (40%)	20,89,89	3.97	10 (50%)
3	HDE	A	761[B]	1,5	34,52,52	3.67	13 (38%)	27,89,89	3.48	17 (62%)
2	HDD	B	760[A]	1,5	30,52,52	2.12	9 (30%)	20,89,89	4.32	11 (55%)
3	HDE	B	761[B]	1,5	34,52,52	3.21	13 (38%)	27,89,89	3.31	15 (55%)
2	HDD	C	760[A]	1,5	30,52,52	2.40	9 (30%)	20,89,89	3.79	10 (50%)
3	HDE	C	761[B]	1,5	34,52,52	3.08	14 (41%)	27,89,89	2.81	15 (55%)
2	HDD	D	760[A]	1,5	30,52,52	2.54	9 (30%)	20,89,89	4.30	10 (50%)
3	HDE	D	761[B]	1,5	34,52,52	2.76	13 (38%)	27,89,89	2.65	15 (55%)

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	HDD	A	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	A	761[B]	1,5	1/1/8/10	0/7/89/89	0/1/9/9
2	HDD	B	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	B	761[B]	1,5	-	2/7/89/89	0/1/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HDD	C	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	C	761[B]	1,5	-	0/7/89/89	0/1/9/9
2	HDD	D	760[A]	1,5	-	0/3/89/89	0/1/9/9
3	HDE	D	761[B]	1,5	-	0/7/89/89	0/1/9/9

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760[A]	HDD	C3C-C2C	-4.71	1.34	1.40
2	C	760[A]	HDD	C3B-C2B	-4.68	1.34	1.40
2	B	760[A]	HDD	C3C-C2C	-4.59	1.34	1.40
2	C	760[A]	HDD	C3C-C2C	-4.42	1.34	1.40
2	A	760[A]	HDD	O1D-C3D	-3.82	1.40	1.46
2	A	760[A]	HDD	C3C-C2C	-3.73	1.35	1.40
2	D	760[A]	HDD	C3B-C2B	-3.63	1.35	1.40
2	B	760[A]	HDD	C3B-C2B	-3.63	1.35	1.40
2	A	760[A]	HDD	C3B-C2B	-3.04	1.36	1.40
2	C	760[A]	HDD	O1D-C3D	-2.94	1.41	1.46
3	C	761[B]	HDE	C1D-C2D	2.07	1.40	1.37
2	A	760[A]	HDD	CAA-C2A	2.11	1.55	1.52
3	C	761[B]	HDE	C4A-NA	2.20	1.41	1.38
3	B	761[B]	HDE	C1D-C2D	2.20	1.40	1.37
3	B	761[B]	HDE	C3D-C2D	2.36	1.44	1.37
3	D	761[B]	HDE	C1C-C2C	2.40	1.41	1.37
2	B	760[A]	HDD	C3B-CAB	2.41	1.52	1.47
3	D	761[B]	HDE	C3D-C2D	2.47	1.45	1.37
2	A	760[A]	HDD	CMD-C2D	2.49	1.56	1.53
2	C	760[A]	HDD	C3B-CAB	2.50	1.52	1.47
2	C	760[A]	HDD	CMC-C2C	2.55	1.56	1.51
2	B	760[A]	HDD	C4D-ND	2.58	1.42	1.38
2	A	760[A]	HDD	C3B-CAB	2.67	1.53	1.47
2	A	760[A]	HDD	CMC-C2C	2.68	1.57	1.51
2	B	760[A]	HDD	CAA-C2A	2.70	1.56	1.52
2	A	760[A]	HDD	C3C-CAC	2.75	1.53	1.47
2	D	760[A]	HDD	CMA-C3A	2.76	1.57	1.51
3	C	761[B]	HDE	CMA-C3A	2.78	1.57	1.53
2	B	760[A]	HDD	CMC-C2C	2.80	1.57	1.51
3	A	761[B]	HDE	C1D-ND	2.81	1.38	1.34
3	D	761[B]	HDE	C1A-NA	2.85	1.42	1.38
3	C	761[B]	HDE	C4D-CHA	2.88	1.47	1.39
3	C	761[B]	HDE	C3C-C2C	2.93	1.46	1.37
2	B	760[A]	HDD	C3C-CAC	3.00	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	CMA-C3A	3.01	1.57	1.53
2	B	760[A]	HDD	CMD-C2D	3.03	1.57	1.53
3	A	761[B]	HDE	C1B-CHB	3.11	1.48	1.39
3	B	761[B]	HDE	C3C-C2C	3.23	1.47	1.37
3	C	761[B]	HDE	C1A-NA	3.29	1.43	1.38
2	A	760[A]	HDD	CMB-C2B	3.39	1.59	1.51
3	D	761[B]	HDE	C4D-CHA	3.39	1.49	1.39
3	C	761[B]	HDE	C3D-C2D	3.41	1.47	1.37
3	A	761[B]	HDE	C4D-CHA	3.45	1.49	1.39
3	D	761[B]	HDE	C3C-C2C	3.49	1.48	1.37
2	D	760[A]	HDD	OND-C2D	3.51	1.49	1.42
2	D	760[A]	HDD	CMC-C2C	3.52	1.58	1.51
2	D	760[A]	HDD	C3B-CAB	3.53	1.55	1.47
3	B	761[B]	HDE	O1A-CGA	3.58	1.41	1.35
3	B	761[B]	HDE	C4D-CHA	3.63	1.49	1.39
2	C	760[A]	HDD	C3C-CAC	3.67	1.55	1.47
2	D	760[A]	HDD	C3C-CAC	3.67	1.55	1.47
2	C	760[A]	HDD	C4B-NB	3.82	1.41	1.36
3	B	761[B]	HDE	C3B-C2B	3.88	1.49	1.37
3	A	761[B]	HDE	C3D-C2D	3.89	1.49	1.37
3	B	761[B]	HDE	C1A-NA	3.95	1.44	1.38
3	A	761[B]	HDE	C3C-C2C	3.97	1.49	1.37
3	C	761[B]	HDE	C1C-C2C	3.99	1.43	1.37
3	C	761[B]	HDE	O1A-CGA	4.00	1.42	1.35
3	D	761[B]	HDE	C4A-NA	4.04	1.44	1.38
2	C	760[A]	HDD	CMD-C2D	4.06	1.59	1.53
3	B	761[B]	HDE	C4A-NA	4.09	1.44	1.38
3	D	761[B]	HDE	C3B-C2B	4.14	1.49	1.37
3	C	761[B]	HDE	C3B-C2B	4.16	1.50	1.37
3	D	761[B]	HDE	C4B-NB	4.17	1.39	1.34
2	A	760[A]	HDD	C4B-NB	4.23	1.42	1.36
3	D	761[B]	HDE	O1A-CGA	4.25	1.42	1.35
3	A	761[B]	HDE	C3B-C2B	4.57	1.51	1.37
2	A	760[A]	HDD	OND-C2D	4.60	1.52	1.42
3	B	761[B]	HDE	C1C-C2C	4.73	1.44	1.37
2	D	760[A]	HDD	CMD-C2D	4.75	1.60	1.53
3	C	761[B]	HDE	C4C-NC	4.99	1.40	1.34
3	A	761[B]	HDE	C1A-NA	5.07	1.45	1.38
3	B	761[B]	HDE	C4B-NB	5.15	1.41	1.34
2	B	760[A]	HDD	FE-ND	5.19	2.16	1.95
3	B	761[B]	HDE	C4C-NC	5.42	1.41	1.34
3	A	761[B]	HDE	C4B-NB	5.47	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	761[B]	HDE	C4C-NC	5.54	1.41	1.34
3	C	761[B]	HDE	C4B-NB	5.62	1.41	1.34
3	A	761[B]	HDE	C1C-C2C	5.80	1.45	1.37
2	A	760[A]	HDD	FE-ND	5.97	2.19	1.95
2	C	760[A]	HDD	FE-ND	6.26	2.20	1.95
3	D	761[B]	HDE	C1C-NC	6.58	1.42	1.34
3	A	761[B]	HDE	O1A-CGA	6.59	1.46	1.35
2	D	760[A]	HDD	FE-ND	7.05	2.23	1.95
3	D	761[B]	HDE	C4C-C3C	7.07	1.47	1.37
3	A	761[B]	HDE	C4C-NC	8.33	1.44	1.34
3	C	761[B]	HDE	C4C-C3C	8.39	1.48	1.37
3	C	761[B]	HDE	C1C-NC	8.55	1.45	1.34
3	A	761[B]	HDE	C4C-C3C	8.65	1.49	1.37
3	B	761[B]	HDE	C1C-NC	8.82	1.45	1.34
3	B	761[B]	HDE	C4C-C3C	8.82	1.49	1.37
3	A	761[B]	HDE	C1C-NC	9.25	1.45	1.34

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	760[A]	HDD	C3B-CAB-CBB	-9.13	107.65	126.32
2	A	760[A]	HDD	C3B-CAB-CBB	-8.69	108.53	126.32
2	C	760[A]	HDD	C3C-CAC-CBC	-8.66	108.60	126.32
2	C	760[A]	HDD	C3B-CAB-CBB	-8.20	109.53	126.32
2	B	760[A]	HDD	O1D-CGD-CBD	-7.76	101.11	110.20
2	B	760[A]	HDD	C3C-CAC-CBC	-7.02	111.95	126.32
2	B	760[A]	HDD	C3B-CAB-CBB	-6.39	113.24	126.32
3	B	761[B]	HDE	CAD-CBD-CGD	-6.22	101.35	112.75
3	B	761[B]	HDE	C1C-C2C-C3C	-6.20	99.98	105.67
3	A	761[B]	HDE	CAD-CBD-CGD	-6.19	101.41	112.75
2	A	760[A]	HDD	CAD-CBD-CGD	-6.09	94.10	104.64
2	D	760[A]	HDD	O1D-CGD-CBD	-5.97	103.20	110.20
2	D	760[A]	HDD	CAA-C2A-C1A	-5.85	120.66	127.01
2	B	760[A]	HDD	CAA-CBA-CGA	-5.82	102.07	112.75
3	B	761[B]	HDE	CBC-CAC-C3C	-5.45	98.14	112.40
2	D	760[A]	HDD	C3C-CAC-CBC	-5.41	115.25	126.32
3	A	761[B]	HDE	CAB-C3B-C4B	-5.30	120.42	127.12
3	B	761[B]	HDE	C4A-NA-C1A	-5.26	103.97	107.36
3	D	761[B]	HDE	CBC-CAC-C3C	-4.90	99.58	112.40
3	C	761[B]	HDE	C1C-C2C-C3C	-4.89	101.18	105.67
2	D	760[A]	HDD	CAA-CBA-CGA	-4.78	103.99	112.75
2	A	760[A]	HDD	CAA-CBA-CGA	-4.66	104.21	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760[A]	HDD	OND-C2D-CMD	-4.47	101.34	109.41
3	C	761[B]	HDE	CMB-C2B-C1B	-4.35	121.17	128.36
3	D	761[B]	HDE	CBB-CAB-C3B	-4.33	101.07	112.40
3	C	761[B]	HDE	CBC-CAC-C3C	-4.29	101.16	112.40
2	C	760[A]	HDD	CAA-CBA-CGA	-4.21	105.04	112.75
3	A	761[B]	HDE	CMB-C2B-C1B	-4.14	121.51	128.36
3	C	761[B]	HDE	CAD-CBD-CGD	-4.11	105.21	112.75
2	B	760[A]	HDD	C3B-C4B-NB	-4.10	103.21	110.94
3	A	761[B]	HDE	O1A-CGA-CBA	-4.06	105.45	110.20
2	B	760[A]	HDD	CMC-C2C-C1C	-3.94	121.84	128.36
3	A	761[B]	HDE	C4A-NA-C1A	-3.82	104.90	107.36
2	A	760[A]	HDD	C3C-CAC-CBC	-3.78	118.59	126.32
3	D	761[B]	HDE	C3A-C4A-CHB	-3.75	117.63	123.48
3	D	761[B]	HDE	CAD-CBD-CGD	-3.72	105.93	112.75
2	B	760[A]	HDD	OND-C2D-CMD	-3.69	102.74	109.41
2	C	760[A]	HDD	O1D-CGD-CBD	-3.55	106.04	110.20
3	A	761[B]	HDE	ONA-C3A-CMA	-3.53	103.04	109.41
2	A	760[A]	HDD	C3B-C4B-NB	-3.37	104.59	110.94
3	D	761[B]	HDE	CMB-C2B-C1B	-3.24	123.00	128.36
2	C	760[A]	HDD	C3B-C4B-NB	-3.22	104.87	110.94
3	A	761[B]	HDE	CAD-C3D-C4D	-3.12	123.62	127.01
3	C	761[B]	HDE	CBB-CAB-C3B	-3.01	104.52	112.40
2	B	760[A]	HDD	CAA-C2A-C1A	-2.97	123.78	127.01
2	D	760[A]	HDD	C3B-C4B-NB	-2.96	105.36	110.94
3	A	761[B]	HDE	C1C-C2C-C3C	-2.91	103.00	105.67
3	A	761[B]	HDE	CBC-CAC-C3C	-2.83	105.00	112.40
3	B	761[B]	HDE	ONA-C3A-CMA	-2.80	104.35	109.41
3	C	761[B]	HDE	CMD-C2D-C1D	-2.80	124.32	127.14
2	D	760[A]	HDD	CMA-C3A-C4A	-2.78	123.77	128.36
3	D	761[B]	HDE	CAB-C3B-C4B	-2.73	123.67	127.12
3	C	761[B]	HDE	C3A-C4A-CHB	-2.65	119.35	123.48
2	D	760[A]	HDD	OND-C2D-CMD	-2.54	104.83	109.41
3	B	761[B]	HDE	CAA-CBA-CGA	-2.43	100.44	104.64
2	C	760[A]	HDD	CMC-C2C-C1C	-2.39	124.41	128.36
3	C	761[B]	HDE	CAC-C3C-C4C	-2.38	124.12	127.12
2	B	760[A]	HDD	C3C-C4C-NC	-2.36	106.17	109.21
3	D	761[B]	HDE	C1C-C2C-C3C	-2.31	103.55	105.67
3	B	761[B]	HDE	C3A-C4A-CHB	-2.28	119.93	123.48
2	A	760[A]	HDD	CMA-C3A-C4A	-2.17	124.77	128.36
2	A	760[A]	HDD	CMB-C2B-C3B	-2.13	120.91	125.09
2	A	760[A]	HDD	CAA-C2A-C1A	-2.07	124.76	127.01
3	A	761[B]	HDE	C1D-C2D-C3D	-2.03	103.81	105.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	761[B]	HDE	C4A-NA-C1A	-2.02	106.06	107.36
3	B	761[B]	HDE	CMC-C2C-C3C	2.01	129.43	125.24
3	D	761[B]	HDE	CAD-C3D-C4D	2.16	129.36	127.01
3	D	761[B]	HDE	CAB-C3B-C2B	2.25	129.64	124.01
3	C	761[B]	HDE	CAB-C3B-C2B	2.28	129.72	124.01
2	C	760[A]	HDD	C2D-C1D-CHD	2.31	127.08	123.48
3	A	761[B]	HDE	CMD-C2D-C3D	2.37	130.19	125.24
3	C	761[B]	HDE	O1A-CGA-O2A	2.38	123.06	120.80
3	B	761[B]	HDE	CMD-C2D-C1D	2.41	129.58	127.14
3	D	761[B]	HDE	ONA-C3A-CMA	2.68	114.25	109.41
3	C	761[B]	HDE	CMC-C2C-C3C	2.76	131.01	125.24
3	B	761[B]	HDE	CMB-C2B-C3B	2.81	131.11	125.24
3	D	761[B]	HDE	O1A-CGA-O2A	2.87	123.53	120.80
3	C	761[B]	HDE	CMD-C2D-C3D	2.99	131.49	125.24
3	B	761[B]	HDE	O1A-CGA-CBA	3.16	113.91	110.20
2	C	760[A]	HDD	C4D-ND-C1D	3.27	109.47	107.36
2	A	760[A]	HDD	C2D-C1D-CHD	3.28	128.59	123.48
3	B	761[B]	HDE	CMC-C2C-C1C	3.32	130.49	127.14
3	C	761[B]	HDE	CMB-C2B-C3B	3.81	133.20	125.24
3	A	761[B]	HDE	CMB-C2B-C3B	3.87	133.33	125.24
3	A	761[B]	HDE	C4C-CHD-C1D	4.13	120.98	112.50
3	A	761[B]	HDE	CMC-C2C-C1C	4.13	131.31	127.14
3	D	761[B]	HDE	CMB-C2B-C3B	4.16	133.93	125.24
3	D	761[B]	HDE	C4C-CHD-C1D	4.24	121.21	112.50
3	A	761[B]	HDE	CAB-C3B-C2B	4.39	134.99	124.01
3	D	761[B]	HDE	C4B-CHC-C1C	4.72	122.19	112.50
3	B	761[B]	HDE	C4B-CHC-C1C	4.72	122.20	112.50
3	C	761[B]	HDE	C4B-CHC-C1C	4.84	122.44	112.50
3	B	761[B]	HDE	CAD-C3D-C4D	4.94	132.38	127.01
3	C	761[B]	HDE	C4C-CHD-C1D	5.39	123.57	112.50
3	A	761[B]	HDE	C4B-CHC-C1C	5.41	123.60	112.50
3	B	761[B]	HDE	C4C-CHD-C1D	5.82	124.44	112.50
2	B	760[A]	HDD	C4D-ND-C1D	6.18	111.35	107.36
2	C	760[A]	HDD	O1D-CGD-O2D	7.13	127.58	120.80
3	A	761[B]	HDE	O1A-CGA-O2A	7.19	127.64	120.80
2	D	760[A]	HDD	O1D-CGD-O2D	8.00	128.41	120.80
2	D	760[A]	HDD	C4D-ND-C1D	8.02	112.54	107.36
2	B	760[A]	HDD	O1D-CGD-O2D	8.89	129.26	120.80
2	A	760[A]	HDD	C4D-ND-C1D	10.93	114.41	107.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	761[B]	HDE	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	761[B]	HDE	C2B-C3B-CAB-CBB
3	B	761[B]	HDE	C2C-C3C-CAC-CBC

There are no ring outliers.

8 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760[A]	HDD	12	0
3	A	761[B]	HDE	10	0
2	B	760[A]	HDD	19	0
3	B	761[B]	HDE	10	0
2	C	760[A]	HDD	19	0
3	C	761[B]	HDE	8	0
2	D	760[A]	HDD	11	0
3	D	761[B]	HDE	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	726/753 (96%)	-0.39	10 (1%)	78	80	4, 10, 25, 45	2 (0%)
1	B	726/753 (96%)	-0.22	27 (3%)	45	47	5, 12, 32, 47	2 (0%)
1	C	726/753 (96%)	-0.29	19 (2%)	59	62	5, 12, 31, 46	2 (0%)
1	D	726/753 (96%)	-0.39	11 (1%)	76	79	4, 10, 26, 45	1 (0%)
All	All	2904/3012 (96%)	-0.32	67 (2%)	64	67	4, 11, 29, 47	7 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	6.9
1	B	713	GLN	4.3
1	B	28	SER	4.3
1	D	28	SER	4.3
1	C	594	PRO	4.2
1	A	32	GLU	3.9
1	A	28	SER	3.9
1	B	712	ASP	3.8
1	B	32	GLU	3.8
1	B	711	ALA	3.7
1	B	647	VAL	3.7
1	C	711	ALA	3.6
1	C	726	GLY	3.6
1	D	750	LYS	3.5
1	D	713	GLN	3.4
1	C	725	ASP	3.4
1	B	645	GLY	3.3
1	B	646	THR	3.3
1	B	725	ASP	3.2
1	A	726	GLY	3.1
1	B	572	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	710	ILE	3.1
1	C	750	LYS	3.1
1	B	750	LYS	3.0
1	A	713	GLN	3.0
1	C	751	ILE	3.0
1	D	711	ALA	3.0
1	B	614	ALA	3.0
1	B	673	ALA	3.0
1	D	712	ASP	2.9
1	D	749	ASP	2.9
1	D	751	ILE	2.9
1	B	641	THR	2.9
1	B	642	ALA	2.8
1	C	596	GLY	2.8
1	B	568	ASP	2.8
1	C	714	GLY	2.6
1	D	572	ASN	2.6
1	B	583	LYS	2.6
1	A	749	ASP	2.6
1	C	712	ASP	2.6
1	B	596	GLY	2.6
1	C	572	ASN	2.6
1	B	617	LEU	2.6
1	C	641	THR	2.4
1	D	32	GLU	2.4
1	A	750	LYS	2.4
1	C	583	LYS	2.4
1	B	677	ASP	2.4
1	C	646	THR	2.4
1	C	645	GLY	2.4
1	D	583	LYS	2.3
1	C	568	ASP	2.3
1	A	710	ILE	2.3
1	A	751	ILE	2.3
1	C	642	ALA	2.3
1	A	29	LEU	2.3
1	B	594	PRO	2.3
1	B	644	ASP	2.3
1	B	707	THR	2.3
1	C	647	VAL	2.2
1	B	751	ILE	2.2
1	C	710	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	727	SER	2.1
1	C	552	LEU	2.1
1	A	707	THR	2.0
1	D	569	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	H2S	D	754[A]	1/1	0.94	0.23	13.59	23,23,23,23	1
4	H2S	A	754[A]	1/1	0.97	0.17	7.60	21,21,21,21	1
4	H2S	C	754[A]	1/1	0.92	0.17	6.46	21,21,21,21	1
4	H2S	B	754[A]	1/1	0.93	0.13	3.58	22,22,22,22	1
3	HDE	B	761[B]	44/44	0.99	0.07	0.68	2,11,15,18	44
2	HDD	A	760[A]	44/44	0.99	0.07	0.56	2,3,10,14	44
3	HDE	A	761[B]	44/44	0.99	0.07	0.44	4,10,13,14	44
3	HDE	C	761[B]	44/44	0.99	0.06	0.40	4,11,14,15	44
3	HDE	D	761[B]	44/44	0.99	0.06	0.34	4,11,15,19	44
2	HDD	B	760[A]	44/44	0.99	0.07	0.33	2,4,8,12	44
2	HDD	C	760[A]	44/44	0.99	0.06	0.29	2,5,12,17	44
2	HDD	D	760[A]	44/44	0.99	0.06	0.10	2,4,10,15	44

6.5 Other polymers (i)

There are no such residues in this entry.