Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:37 AM GMT

PDB ID	:	3PCI
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3-IODO-4-HYDROXYBENZOATE
Authors	:	Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-02
Resolution	:	2.21 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:

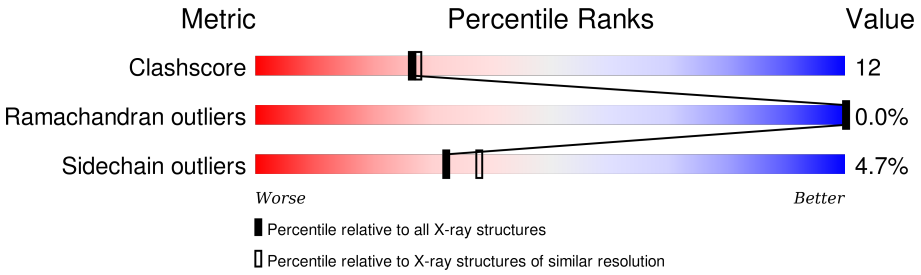
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.21 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	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)

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	200	75% 21% 5%
1	B	200	70% 27% •
1	C	200	77% 20% • •
1	D	200	73% 22% 5% •
1	E	200	67% 30% •
1	F	200	67% 28% 5% •
2	M	238	72% 21% • • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	238	
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22104 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 PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

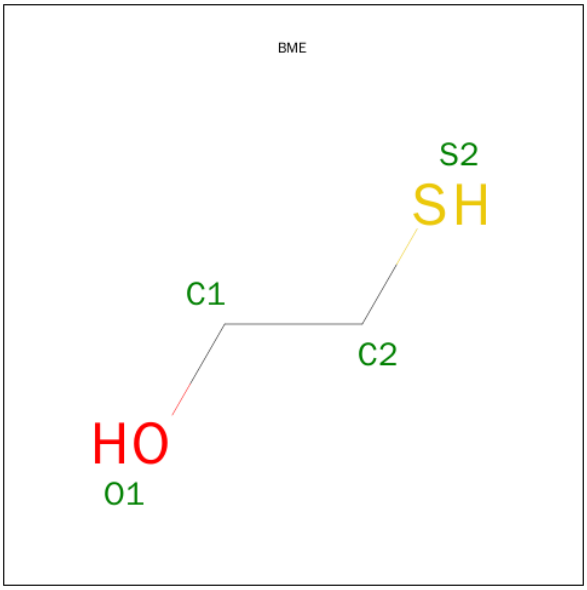
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	N	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	O	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	P	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	R	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

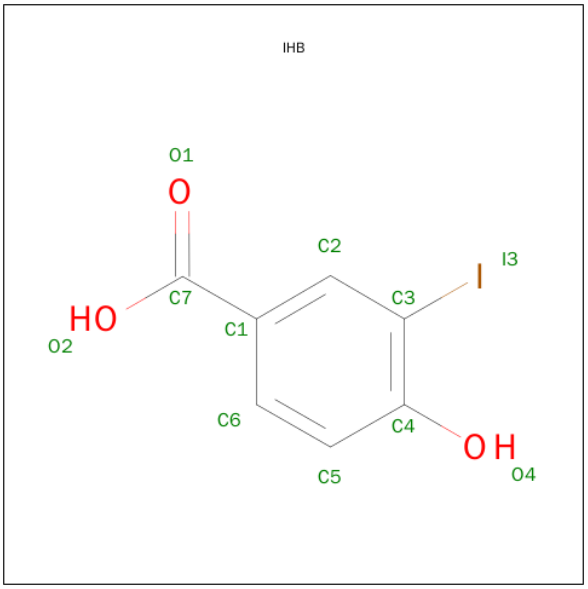
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 3-IODO-4-HYDROXYBENZOIC ACID (three-letter code: IHB) (formula: $C_7H_5IO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C I O 11 7 1 3	0	0
5	M	1	Total C I O 11 7 1 3	0	0
5	N	1	Total C I O 11 7 1 3	0	0
5	N	1	Total C I O 11 7 1 3	0	0
5	O	1	Total C I O 11 7 1 3	0	0
5	O	1	Total C I O 11 7 1 3	0	0
5	P	1	Total C I O 11 7 1 3	0	0
5	P	1	Total C I O 11 7 1 3	0	0
5	Q	1	Total C I O 11 7 1 3	0	0
5	Q	1	Total C I O 11 7 1 3	0	0
5	R	1	Total C I O 11 7 1 3	0	0
5	R	1	Total C I O 11 7 1 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	B	85	Total O 85 85	0	0
6	C	82	Total O 82 82	0	0
6	D	81	Total O 81 81	0	0
6	E	84	Total O 84 84	0	0
6	F	81	Total O 81 81	0	0
6	M	163	Total O 163 163	0	0
6	N	167	Total O 167 167	0	0
6	O	162	Total O 162 162	0	0
6	P	157	Total O 157 157	0	0
6	Q	165	Total O 165 165	0	0
6	R	167	Total O 167 167	0	0

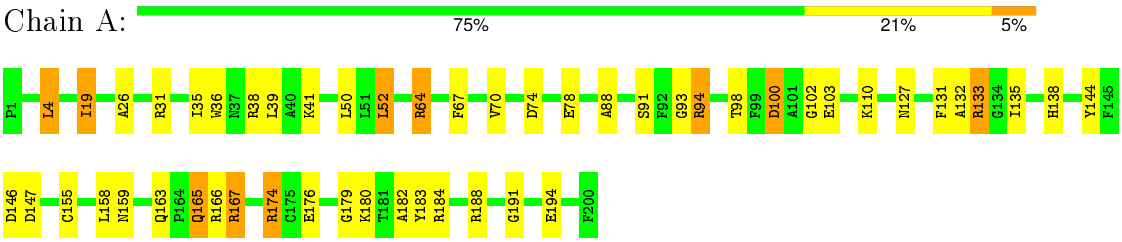
3 Residue-property plots (i)

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.

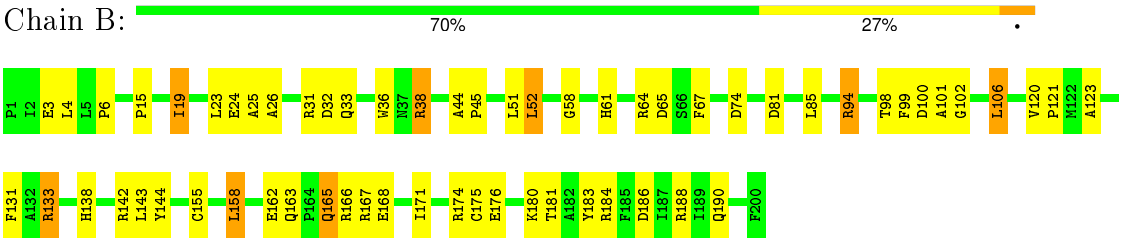
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



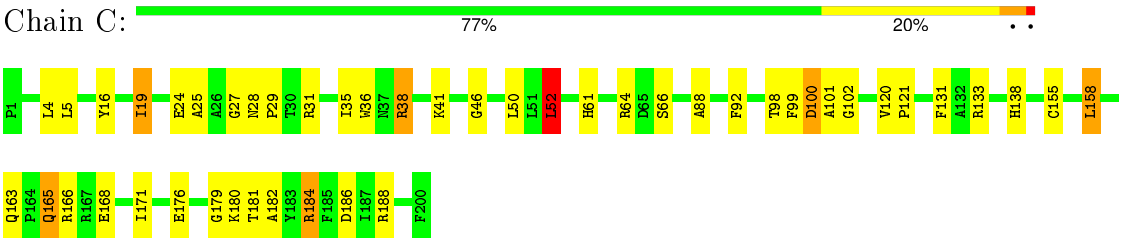
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



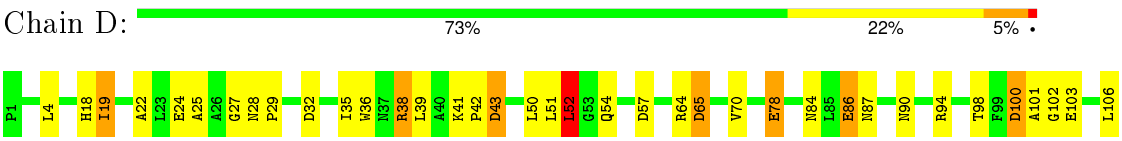
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C:



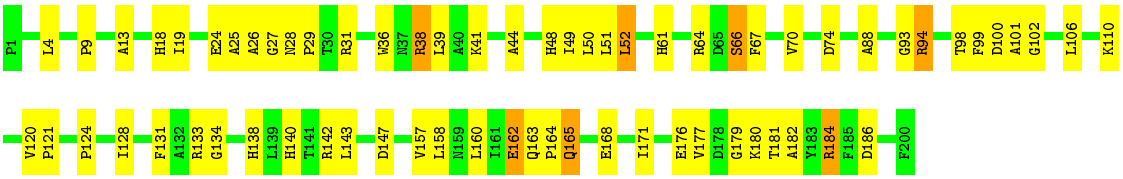
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D:



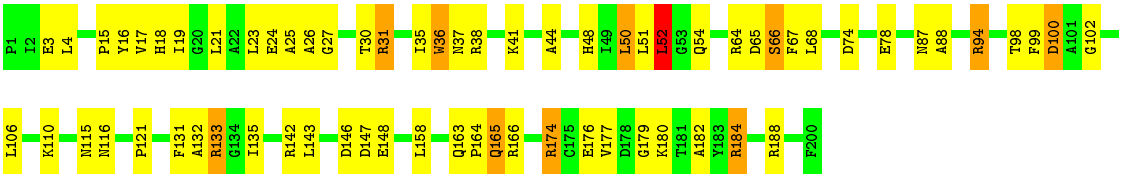
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



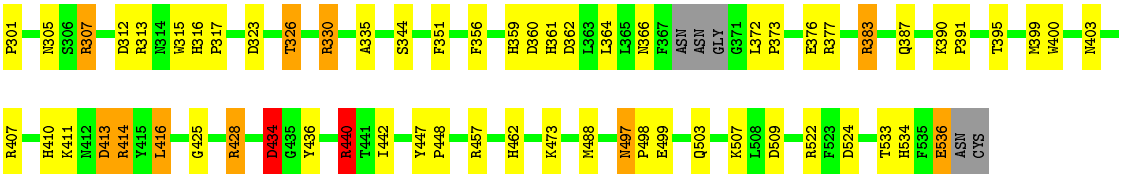
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:



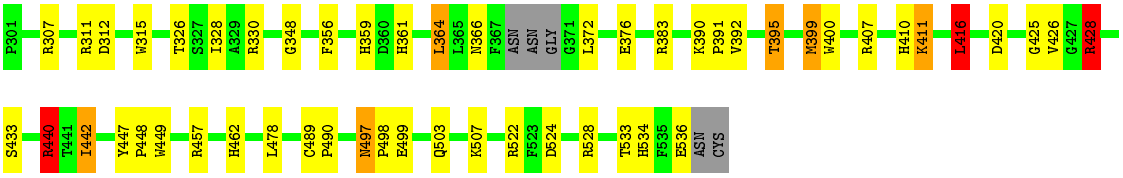
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:



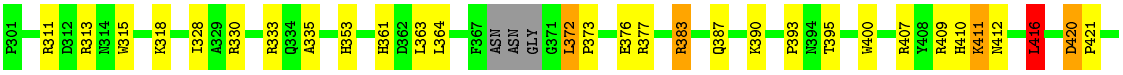
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

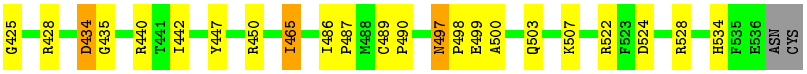
Chain N:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

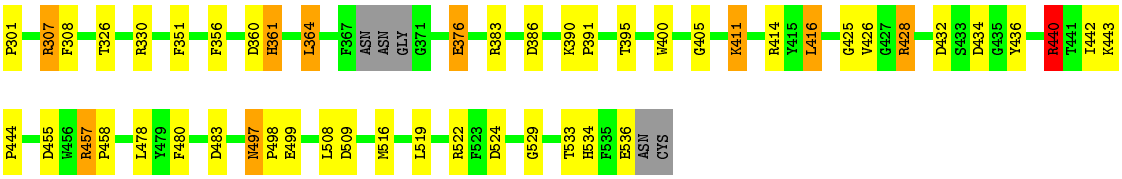
Chain O:





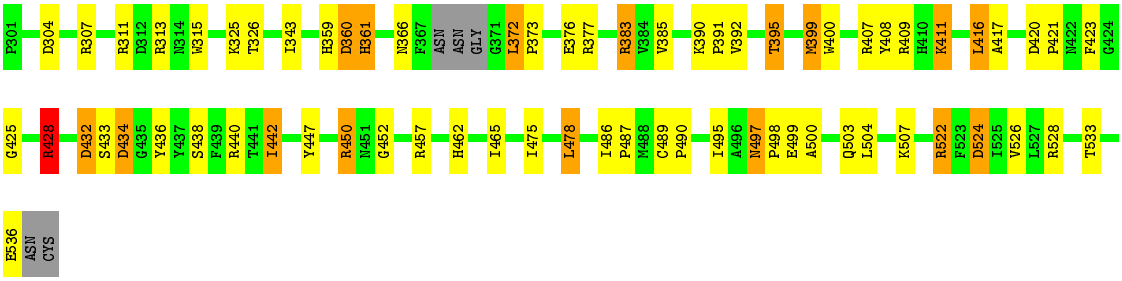
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



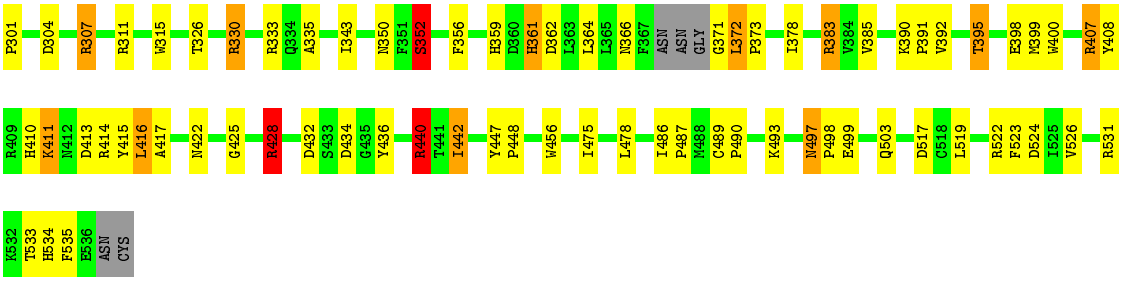
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	197.00Å 127.07Å 134.08Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	6.00 – 2.21	Depositor
% Data completeness (in resolution range)	83.0 (6.00-2.21)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22104	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: IHB, FE, BME

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	0.94	1/1611 (0.1%)	1.66	30/2195 (1.4%)
1	B	0.95	0/1611	1.66	33/2195 (1.5%)
1	C	0.95	1/1611 (0.1%)	1.50	14/2195 (0.6%)
1	D	0.92	0/1611	1.52	23/2195 (1.0%)
1	E	0.97	0/1611	1.52	23/2195 (1.0%)
1	F	0.98	0/1611	1.55	25/2195 (1.1%)
2	M	1.00	0/1895	1.54	25/2580 (1.0%)
2	N	0.98	0/1895	1.50	16/2580 (0.6%)
2	O	1.00	0/1895	1.55	24/2580 (0.9%)
2	P	0.97	0/1895	1.53	21/2580 (0.8%)
2	Q	1.02	1/1895 (0.1%)	1.54	24/2580 (0.9%)
2	R	1.00	1/1895 (0.1%)	1.56	24/2580 (0.9%)
All	All	0.98	4/21036 (0.0%)	1.55	282/28650 (1.0%)

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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-5.16	1.37	1.46
1	C	66	SER	CB-OG	-5.10	1.35	1.42
2	R	428	ARG	CD-NE	-5.07	1.37	1.46
2	Q	433	SER	CB-OG	5.05	1.48	1.42

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	440	ARG	NE-CZ-NH2	-20.04	110.28	120.30
2	P	440	ARG	NE-CZ-NH2	-19.34	110.63	120.30
2	R	440	ARG	NE-CZ-NH2	-18.26	111.17	120.30
2	M	440	ARG	NE-CZ-NH2	-16.43	112.08	120.30
2	Q	440	ARG	NE-CZ-NH2	-15.94	112.33	120.30
2	P	440	ARG	NE-CZ-NH1	15.59	128.10	120.30
1	B	184	ARG	NE-CZ-NH2	-15.52	112.54	120.30
1	A	94	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	A	94	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	B	94	ARG	NE-CZ-NH1	13.71	127.16	120.30
1	A	133	ARG	NE-CZ-NH1	13.70	127.15	120.30
2	O	440	ARG	NE-CZ-NH2	-13.09	113.76	120.30
2	Q	457	ARG	NE-CZ-NH1	12.93	126.77	120.30
2	O	428	ARG	CD-NE-CZ	12.68	141.36	123.60
2	N	440	ARG	NE-CZ-NH1	10.82	125.71	120.30
2	M	457	ARG	CD-NE-CZ	10.76	138.67	123.60
2	O	528	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	B	188	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	188	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	C	188	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	B	94	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	B	38	ARG	NE-CZ-NH2	-10.34	115.13	120.30
2	Q	457	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	M	428	ARG	CD-NE-CZ	10.05	137.67	123.60
2	M	428	ARG	NE-CZ-NH2	-9.99	115.31	120.30
2	R	311	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	R	307	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	184	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	O	330	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	B	133	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	C	166	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	133	ARG	NE-CZ-NH2	-9.63	115.49	120.30
2	R	428	ARG	CD-NE-CZ	9.61	137.06	123.60
2	O	524	ASP	CB-CG-OD1	9.51	126.85	118.30
1	F	142	ARG	NE-CZ-NH1	9.49	125.04	120.30
2	Q	522	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	D	184	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	184	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	C	184	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	Q	440	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	B	133	ARG	CD-NE-CZ	9.09	136.32	123.60
1	F	166	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	E	184	ARG	NE-CZ-NH2	-8.98	115.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	457	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	188	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	P	307	ARG	NE-CZ-NH1	8.91	124.76	120.30
2	R	383	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	O	333	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	188	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	94	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	184	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	O	428	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	D	167	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	F	94	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	F	38	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	F	166	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	D	52	LEU	CB-CA-C	8.68	126.69	110.20
2	R	428	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	M	428	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	F	38	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	R	307	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	Q	428	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	C	166	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	E	184	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	O	528	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	65	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	133	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	174	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	166	ARG	NE-CZ-NH1	8.03	124.31	120.30
2	M	440	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	E	52	LEU	CB-CA-C	7.96	125.32	110.20
2	O	383	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	R	524	ASP	CB-CG-OD1	7.91	125.42	118.30
1	E	38	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	C	38	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	B	184	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	188	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	R	531	ARG	NE-CZ-NH2	-7.83	116.38	120.30
2	O	409	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	P	509	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	166	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	N	428	ARG	CG-CD-NE	7.71	127.98	111.80
1	E	31	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	M	414	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	Q	383	ARG	NE-CZ-NH2	-7.63	116.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	353	HIS	CA-CB-CG	-7.62	100.66	113.60
1	A	31	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	74	ASP	CB-CG-OD2	-7.60	111.46	118.30
2	N	528	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	74	ASP	CB-CG-OD1	7.48	125.03	118.30
2	Q	313	ARG	NE-CZ-NH1	7.47	124.04	120.30
2	M	312	ASP	CB-CG-OD1	7.47	125.02	118.30
2	M	383	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	M	407	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	38	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	R	428	ARG	CG-CD-NE	7.39	127.33	111.80
1	C	52	LEU	CB-CA-C	7.38	124.22	110.20
1	B	167	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	31	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	43	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	B	31	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	O	528	ARG	CD-NE-CZ	7.08	133.51	123.60
2	O	377	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	P	432	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	64	ARG	NE-CZ-NH1	-7.01	116.79	120.30
2	P	457	ARG	CD-NE-CZ	6.99	133.39	123.60
2	M	307	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	142	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	Q	528	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	F	38	ARG	CA-CB-CG	6.96	128.70	113.40
2	P	536	GLU	CA-C-O	6.96	134.71	120.10
1	D	133	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	C	133	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	P	414	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	F	142	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	133	ARG	CD-NE-CZ	6.88	133.22	123.60
1	B	133	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	E	74	ASP	CB-CG-OD2	-6.87	112.12	118.30
2	Q	428	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	Q	524	ASP	CB-CG-OD1	6.82	124.44	118.30
2	N	407	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	O	434	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	E	74	ASP	CB-CG-OD1	6.76	124.38	118.30
2	M	312	ASP	CB-CG-OD2	-6.75	112.22	118.30
2	N	312	ASP	CB-CG-OD1	6.72	124.35	118.30
1	B	31	ARG	CD-NE-CZ	6.68	132.95	123.60
1	E	94	ARG	NE-CZ-NH1	6.66	123.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	31	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	F	94	ARG	CD-NE-CZ	6.59	132.83	123.60
2	O	428	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	Q	432	ASP	CB-CG-OD1	6.57	124.21	118.30
2	O	420	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	186	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	162	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	94	ARG	CB-CG-CD	6.50	128.49	111.60
1	E	158	LEU	CB-CA-C	6.50	122.54	110.20
1	A	184	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	P	428	ARG	CG-CD-NE	6.44	125.32	111.80
1	A	52	LEU	CA-CB-CG	6.43	130.10	115.30
1	F	94	ARG	CG-CD-NE	6.42	125.28	111.80
1	E	94	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	186	ASP	CB-CG-OD1	6.38	124.04	118.30
2	M	536	GLU	CA-C-O	6.36	133.46	120.10
2	R	517	ASP	CB-CG-OD1	6.36	124.03	118.30
2	M	509	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	188	ARG	NE-CZ-NH2	-6.33	117.13	120.30
2	M	330	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	R	428	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	N	311	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	P	524	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	86	GLU	CG-CD-OE1	6.25	130.80	118.30
2	M	524	ASP	CB-CG-OD1	6.25	123.92	118.30
2	P	509	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	94	ARG	CB-CG-CD	6.24	127.83	111.60
2	R	333	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	N	428	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	N	524	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	142	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	166	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	R	383	ARG	NH1-CZ-NH2	6.19	126.21	119.40
2	O	333	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	P	414	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	O	407	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	F	106	LEU	CA-CB-CG	6.17	129.48	115.30
2	R	432	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	F	174	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	N	383	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	P	524	ASP	CB-CG-OD1	6.12	123.81	118.30
2	M	313	ARG	NE-CZ-NH1	6.11	123.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	386	ASP	CB-CA-C	6.10	122.59	110.40
1	D	166	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	F	31	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	P	483	ASP	CB-CG-OD2	6.07	123.76	118.30
2	Q	409	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	94	ARG	CG-CD-NE	6.05	124.51	111.80
1	A	52	LEU	CB-CA-C	6.04	121.67	110.20
1	B	94	ARG	CG-CD-NE	6.04	124.47	111.80
1	A	94	ARG	CD-NE-CZ	6.03	132.04	123.60
2	M	428	ARG	CG-CD-NE	6.03	124.45	111.80
2	Q	311	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	186	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	167	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	E	36	TRP	CB-CA-C	5.99	122.38	110.40
2	Q	361	HIS	CA-CB-CG	-5.98	103.44	113.60
2	R	362	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	188	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	Q	434	ASP	CB-CG-OD2	-5.97	112.93	118.30
2	Q	360	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	O	409	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	R	428	ARG	CB-CG-CD	5.91	126.96	111.60
1	F	94	ARG	CB-CG-CD	5.90	126.94	111.60
1	A	64	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	B	166	ARG	CD-NE-CZ	5.83	131.77	123.60
2	R	407	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	E	94	ARG	CG-CD-NE	5.83	124.03	111.80
1	F	31	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	R	440	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	142	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	186	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	Q	377	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	166	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	N	383	ARG	CD-NE-CZ	-5.75	115.55	123.60
2	O	311	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	52	LEU	CB-CA-C	5.73	121.09	110.20
1	F	184	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	N	457	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	133	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	31	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	36	TRP	CB-CA-C	5.68	121.75	110.40
1	B	186	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	M	313	ARG	CB-CA-C	5.62	121.64	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	440	ARG	NH1-CZ-NH2	5.62	125.58	119.40
2	Q	457	ARG	CA-CB-CG	5.61	125.73	113.40
1	B	52	LEU	CA-CB-CG	5.60	128.17	115.30
2	M	413	ASP	CB-CG-OD1	5.59	123.33	118.30
2	M	434	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	R	361	HIS	CA-CB-CG	-5.57	104.12	113.60
2	N	457	ARG	CA-CB-CG	5.57	125.66	113.40
1	B	133	ARG	CA-CB-CG	5.57	125.66	113.40
1	C	66	SER	N-CA-CB	5.56	118.84	110.50
1	D	38	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	P	361	HIS	CA-CB-CG	-5.52	104.22	113.60
1	F	74	ASP	CB-CG-OD1	5.49	123.24	118.30
2	P	519	LEU	CB-CA-C	5.48	120.61	110.20
1	F	52	LEU	CB-CA-C	5.48	120.61	110.20
1	F	66	SER	N-CA-CB	5.46	118.70	110.50
1	E	31	ARG	CD-NE-CZ	5.46	131.24	123.60
2	Q	360	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	133	ARG	CA-CB-CG	5.44	125.36	113.40
1	B	32	ASP	CB-CG-OD1	5.44	123.19	118.30
2	O	416	LEU	CB-CA-C	5.43	120.51	110.20
1	A	36	TRP	CB-CA-C	5.42	121.24	110.40
2	N	416	LEU	CB-CA-C	5.41	120.49	110.20
1	E	66	SER	N-CA-CB	5.41	118.62	110.50
1	A	103	GLU	CG-CD-OE1	-5.37	107.55	118.30
1	F	38	ARG	CB-CA-C	5.36	121.12	110.40
1	B	175	CYS	CA-CB-SG	5.36	123.64	114.00
1	F	36	TRP	CB-CA-C	5.36	121.11	110.40
1	F	158	LEU	CB-CA-C	5.35	120.37	110.20
2	R	434	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	E	140	HIS	CB-CA-C	-5.34	99.71	110.40
1	D	57	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	36	TRP	CB-CA-C	5.33	121.06	110.40
1	D	100	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	B	74	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	Q	407	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	O	440	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	F	146	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	133	ARG	CA-CB-CG	5.29	125.03	113.40
1	D	32	ASP	CB-CG-OD1	5.28	123.06	118.30
1	E	38	ARG	CD-NE-CZ	-5.28	116.22	123.60
1	D	32	ASP	CB-CG-OD2	-5.27	113.56	118.30
2	Q	452	GLY	N-CA-C	-5.26	99.94	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	103	GLU	CG-CD-OE1	-5.26	107.79	118.30
2	R	352	SER	N-CA-CB	5.24	118.36	110.50
2	O	500	ALA	CB-CA-C	5.23	117.95	110.10
1	A	146	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	P	307	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	R	330	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	36	TRP	CB-CA-C	5.21	120.83	110.40
1	A	183	TYR	N-CA-CB	5.18	119.93	110.60
2	P	376	GLU	CG-CD-OE1	5.17	128.64	118.30
2	M	323	ASP	CB-CG-OD1	5.16	122.94	118.30
2	M	524	ASP	CB-CG-OD2	-5.15	113.67	118.30
2	O	313	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	100	ASP	CB-CG-OD2	5.14	122.93	118.30
2	P	455	ASP	CB-CG-OD1	5.13	122.91	118.30
2	N	383	ARG	N-CA-CB	-5.12	101.39	110.60
2	Q	372	LEU	N-CA-CB	-5.11	100.19	110.40
1	B	24	GLU	CA-CB-CG	5.09	124.60	113.40
1	F	23	LEU	CB-CA-C	5.08	119.85	110.20
2	Q	383	ARG	N-CA-CB	-5.07	101.48	110.60
1	E	133	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	M	326	THR	CA-CB-OG1	-5.06	98.36	109.00
2	N	420	ASP	CB-CG-OD1	5.06	122.85	118.30
1	E	13	ALA	CB-CA-C	5.04	117.66	110.10
1	D	78	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	B	162	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	B	183	TYR	N-CA-CB	5.02	119.63	110.60
1	B	174	ARG	CD-NE-CZ	-5.01	116.58	123.60
2	P	478	LEU	CA-CB-CG	5.01	126.82	115.30
1	E	186	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	184	ARG	Sidechain

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	1571	0	1499	37	0
1	B	1571	0	1499	40	0
1	C	1571	0	1499	29	1
1	D	1571	0	1499	35	1
1	E	1571	0	1499	47	0
1	F	1571	0	1499	66	0
2	M	1840	0	1792	57	0
2	N	1840	0	1792	39	0
2	O	1840	0	1792	36	0
2	P	1840	0	1792	41	0
2	Q	1840	0	1792	56	0
2	R	1840	0	1792	56	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	1	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	7	1	0
5	N	22	0	7	1	0
5	O	22	0	7	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	3	0
6	A	82	0	0	0	0
6	B	85	0	0	0	0
6	C	82	0	0	0	0
6	D	81	0	0	0	0
6	E	84	0	0	2	0
6	F	81	0	0	2	0
6	M	163	0	0	7	0
6	N	167	0	0	3	0
6	O	162	0	0	6	0
6	P	157	0	0	4	0
6	Q	165	0	0	8	1
6	R	167	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22104	0	19818	492	2

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 12.

All (492) 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:M:364:LEU:HD22	2:M:440:ARG:HD3	1.25	1.16
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.22	1.12
1:D:64:ARG:NH1	1:D:100:ASP:O	1.81	1.12
1:B:165:GLN:NE2	1:B:165:GLN:H	1.49	1.10
1:F:165:GLN:NE2	1:F:165:GLN:H	1.50	1.09
1:F:64:ARG:NH1	1:F:100:ASP:O	1.88	1.07
1:E:165:GLN:NE2	1:E:165:GLN:H	1.54	1.04
1:A:165:GLN:H	1:A:165:GLN:NE2	1.56	1.02
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.59	1.00
1:C:165:GLN:H	1:C:165:GLN:NE2	1.60	0.99
1:C:64:ARG:NH1	1:C:100:ASP:O	1.94	0.99
1:E:165:GLN:N	1:E:165:GLN:HE21	1.61	0.98
1:C:99:PHE:HE2	2:O:411:LYS:HZ3	1.11	0.92
2:R:361:HIS:H	2:R:361:HIS:CD2	1.87	0.92
1:B:165:GLN:HE21	1:B:165:GLN:H	1.05	0.92
1:D:165:GLN:H	1:D:165:GLN:HE21	1.05	0.92
1:F:165:GLN:HE21	1:F:165:GLN:H	1.16	0.91
2:M:497:ASN:ND2	2:M:499:GLU:H	1.69	0.90
1:A:165:GLN:H	1:A:165:GLN:HE21	1.11	0.90
1:C:165:GLN:H	1:C:165:GLN:HE21	1.12	0.90
1:C:25:ALA:O	2:O:411:LYS:NZ	2.03	0.89
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.00	0.89
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.38	0.89
2:M:522:ARG:NH1	6:M:665:HOH:O	2.07	0.88
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.71	0.88
1:D:165:GLN:H	1:D:165:GLN:NE2	1.73	0.86
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.05	0.86
2:R:497:ASN:ND2	2:R:499:GLU:H	1.73	0.86
2:N:390:LYS:HD2	6:N:649:HOH:O	1.75	0.86
1:A:64:ARG:NH1	1:A:100:ASP:O	2.09	0.85
1:B:25:ALA:O	2:N:411:LYS:NZ	2.10	0.84
1:D:176:GLU:OE2	1:D:179:GLY:HA2	1.76	0.84
2:M:390:LYS:HD2	6:M:642:HOH:O	1.78	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:361:HIS:H	2:Q:361:HIS:CD2	1.95	0.83
2:O:390:LYS:HD2	6:O:653:HOH:O	1.79	0.82
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.61	0.82
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.60	0.82
1:F:165:GLN:HE21	1:F:165:GLN:N	1.76	0.81
2:P:390:LYS:HD3	6:P:650:HOH:O	1.80	0.81
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.28	0.80
1:F:25:ALA:O	2:R:411:LYS:NZ	2.13	0.80
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.46	0.80
2:M:497:ASN:HD22	2:M:499:GLU:H	1.26	0.80
1:B:165:GLN:N	1:B:165:GLN:HE21	1.79	0.80
1:B:176:GLU:HG3	1:B:180:LYS:O	1.82	0.80
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.48	0.79
1:F:176:GLU:HG3	1:F:180:LYS:O	1.82	0.79
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.83	0.78
2:R:497:ASN:HD22	2:R:499:GLU:H	1.30	0.78
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.67	0.77
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.67	0.77
5:Q:550:IHB:H2	6:Q:1225:HOH:O	1.84	0.77
2:O:497:ASN:ND2	2:O:499:GLU:H	1.82	0.76
2:R:361:HIS:H	2:R:361:HIS:HD2	1.32	0.76
2:P:497:ASN:HD22	2:P:497:ASN:C	1.89	0.76
2:M:305:ASN:O	2:M:533:THR:HG23	1.84	0.76
1:C:165:GLN:N	1:C:165:GLN:HE21	1.83	0.76
2:P:361:HIS:CD2	2:P:361:HIS:H	2.04	0.75
2:P:497:ASN:ND2	2:P:499:GLU:H	1.85	0.75
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.68	0.73
1:A:165:GLN:N	1:A:165:GLN:HE21	1.85	0.73
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.35	0.73
1:C:98:THR:OG1	1:C:102:GLY:N	2.21	0.73
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.89	0.73
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.23	0.73
1:F:50:LEU:HD12	1:F:51:LEU:N	2.03	0.72
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.25	0.72
1:A:98:THR:OG1	1:A:102:GLY:N	2.22	0.72
2:N:522:ARG:NH1	6:N:671:HOH:O	2.22	0.72
1:E:64:ARG:NH1	1:E:100:ASP:O	2.22	0.71
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.22	0.70
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.15	0.70
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.73	0.69
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:NE2	1:F:165:GLN:N	2.31	0.69
1:A:98:THR:HB	1:A:100:ASP:OD1	1.93	0.69
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.56	0.69
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.75	0.69
2:R:304:ASP:HB2	2:R:343:ILE:HB	1.75	0.69
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.75	0.68
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	1.91	0.68
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.07	0.68
1:D:165:GLN:N	1:D:165:GLN:HE21	1.87	0.68
1:B:65:ASP:OD2	1:B:133:ARG:HD3	1.94	0.68
1:E:165:GLN:H	1:E:165:GLN:HE21	0.76	0.68
2:M:361:HIS:H	2:M:361:HIS:CD2	2.11	0.68
2:Q:497:ASN:HD22	2:Q:497:ASN:C	1.97	0.67
2:N:361:HIS:H	2:N:361:HIS:CD2	2.13	0.67
1:F:26:ALA:C	2:R:411:LYS:HZ2	1.98	0.67
1:F:188:ARG:HG3	1:F:188:ARG:HH11	1.60	0.67
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.77	0.66
1:E:98:THR:OG1	1:E:102:GLY:N	2.29	0.66
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.78	0.66
1:D:84:ASN:OD1	1:D:86:GLU:HB2	1.96	0.66
1:E:99:PHE:HE2	2:Q:411:LYS:NZ	1.93	0.66
2:P:390:LYS:HE2	6:P:726:HOH:O	1.95	0.65
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.31	0.65
1:F:98:THR:OG1	1:F:102:GLY:N	2.27	0.65
2:N:416:LEU:C	2:N:416:LEU:HD23	2.17	0.65
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.45	0.65
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.78	0.64
1:D:100:ASP:N	1:D:100:ASP:OD1	2.27	0.64
2:O:361:HIS:CD2	2:O:361:HIS:H	2.14	0.64
2:Q:536:GLU:HB2	6:Q:1142:HOH:O	1.97	0.64
1:B:99:PHE:HE2	2:N:411:LYS:NZ	1.96	0.64
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.98	0.64
2:R:522:ARG:NH1	6:R:1345:HOH:O	2.24	0.64
2:R:400:TRP:HA	2:R:425:GLY:O	1.98	0.63
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.32	0.63
2:Q:497:ASN:HD22	2:Q:498:PRO:N	1.96	0.63
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.96	0.63
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.29	0.63
1:B:165:GLN:N	1:B:165:GLN:NE2	2.34	0.63
1:F:99:PHE:HE2	2:R:411:LYS:HZ3	1.46	0.63
2:Q:376:GLU:OE1	6:Q:1049:HOH:O	2.15	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:416:LEU:C	2:O:416:LEU:HD23	2.19	0.62
1:F:100:ASP:N	1:F:100:ASP:OD1	2.32	0.62
2:O:497:ASN:HD22	2:O:498:PRO:N	1.97	0.62
2:O:497:ASN:HD22	2:O:499:GLU:H	1.47	0.61
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.80	0.61
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.68	0.61
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.83	0.61
1:B:176:GLU:HG3	1:B:180:LYS:C	2.20	0.61
2:Q:450:ARG:NE	6:Q:1470:HOH:O	2.18	0.61
2:Q:383:ARG:HG3	2:Q:436:TYR:CE1	2.36	0.61
1:F:110:LYS:NZ	1:F:148:GLU:OE2	2.25	0.61
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.81	0.60
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.83	0.60
2:O:497:ASN:HD22	2:O:497:ASN:C	2.05	0.60
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.82	0.60
1:F:188:ARG:HG3	1:F:188:ARG:NH1	2.17	0.60
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.44	0.60
2:M:400:TRP:HA	2:M:425:GLY:O	2.02	0.60
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.37	0.60
2:P:497:ASN:HD22	2:P:499:GLU:H	1.48	0.59
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.17	0.59
2:P:361:HIS:HD2	2:P:361:HIS:H	1.50	0.59
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.01	0.59
2:R:447:TYR:OH	5:R:550:IHB:O4	2.20	0.59
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.85	0.59
5:M:550:IHB:H2	6:M:742:HOH:O	2.03	0.59
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.03	0.59
1:D:176:GLU:HG3	1:D:180:LYS:O	2.02	0.59
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.68	0.59
1:B:98:THR:OG1	1:B:102:GLY:N	2.35	0.59
1:A:176:GLU:HA	1:A:180:LYS:O	2.03	0.58
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.36	0.58
1:C:100:ASP:OD1	1:C:100:ASP:N	2.36	0.58
1:A:165:GLN:N	1:A:165:GLN:NE2	2.41	0.58
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.83	0.58
2:P:497:ASN:HD22	2:P:498:PRO:N	2.00	0.58
2:O:376:GLU:O	2:O:442:ILE:HA	2.03	0.58
2:R:413:ASP:C	2:R:414:ARG:HD2	2.24	0.58
1:D:25:ALA:O	2:P:411:LYS:NZ	2.37	0.58
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.04	0.58
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:THR:O	1:E:102:GLY:HA2	2.04	0.57
1:F:41:LYS:HE3	1:F:87:ASN:O	2.04	0.57
1:E:99:PHE:CE2	2:Q:411:LYS:NZ	2.70	0.57
1:F:24:GLU:O	1:F:27:GLY:N	2.35	0.57
1:E:143:LEU:HD23	1:E:143:LEU:C	2.25	0.57
1:E:25:ALA:O	2:Q:411:LYS:NZ	2.37	0.57
1:E:176:GLU:HG3	1:E:180:LYS:O	2.04	0.57
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.34	0.57
2:P:416:LEU:HD23	2:P:416:LEU:C	2.25	0.57
1:F:50:LEU:O	1:F:182:ALA:HA	2.05	0.57
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.69	0.57
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.87	0.57
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.49	0.56
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.40	0.56
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.85	0.56
1:F:54:GLN:HG2	1:F:102:GLY:O	2.06	0.56
1:B:64:ARG:NH1	1:B:100:ASP:O	2.39	0.56
1:F:143:LEU:HD23	1:F:143:LEU:C	2.24	0.56
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.04	0.56
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.41	0.56
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.37	0.56
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.45	0.56
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.87	0.56
2:R:390:LYS:HD3	6:R:1425:HOH:O	2.05	0.56
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.21	0.55
1:F:165:GLN:CD	1:F:165:GLN:H	1.98	0.55
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.88	0.55
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.88	0.55
2:N:359:HIS:O	2:N:366:ASN:HB3	2.06	0.55
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.55
1:B:19:ILE:O	2:N:426:VAL:HG21	2.06	0.55
2:Q:465:ILE:N	2:Q:465:ILE:HD12	2.22	0.55
2:R:407:ARG:NH1	2:R:417:ALA:O	2.33	0.55
2:R:497:ASN:HD22	2:R:498:PRO:N	2.05	0.55
1:A:26:ALA:C	2:M:411:LYS:HZ2	2.10	0.55
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.42	0.55
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.42	0.55
1:A:50:LEU:O	1:A:182:ALA:HA	2.06	0.54
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.03	0.54
2:P:416:LEU:CD2	2:P:416:LEU:C	2.75	0.54
2:M:497:ASN:HD22	2:M:498:PRO:N	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:O	1:D:182:ALA:HA	2.08	0.54
2:M:361:HIS:HD2	2:M:361:HIS:H	1.55	0.54
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.54
1:F:121:PRO:O	6:F:1400:HOH:O	2.18	0.54
1:E:168:GLU:HA	1:E:171:ILE:CD1	2.37	0.54
2:M:376:GLU:OE1	6:M:637:HOH:O	2.18	0.54
2:O:315:TRP:HE1	2:O:503:GLN:HE22	1.56	0.54
2:N:497:ASN:ND2	2:N:499:GLU:H	2.06	0.54
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.90	0.54
1:C:16:TYR:O	1:C:19:ILE:HG23	2.09	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.09	0.53
1:A:176:GLU:HG3	1:A:180:LYS:O	2.09	0.53
1:D:78:GLU:HG2	2:P:301:PRO:HG2	1.91	0.53
2:O:522:ARG:NH1	6:O:676:HOH:O	2.42	0.53
2:M:536:GLU:HB2	6:M:697:HOH:O	2.08	0.53
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.91	0.52
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.44	0.52
1:B:180:LYS:HG2	1:B:181:THR:N	2.23	0.52
2:P:400:TRP:HA	2:P:425:GLY:O	2.10	0.52
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.44	0.52
2:R:361:HIS:N	2:R:361:HIS:CD2	2.62	0.52
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.91	0.52
2:M:434:ASP:HB3	2:M:436:TYR:CE2	2.45	0.52
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.45	0.52
1:F:78:GLU:OE2	2:R:301:PRO:HG3	2.09	0.52
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.40	0.52
2:N:376:GLU:O	2:N:442:ILE:HA	2.09	0.52
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.06	0.51
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.30	0.51
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.92	0.51
1:C:24:GLU:O	1:C:27:GLY:N	2.40	0.51
2:M:377:ARG:NH1	2:P:416:LEU:HD21	2.26	0.51
2:N:478:LEU:C	2:N:478:LEU:HD23	2.31	0.51
2:N:416:LEU:C	2:N:416:LEU:CD2	2.78	0.51
2:R:447:TYR:OH	5:R:550:IHB:C4	2.58	0.51
2:R:497:ASN:HD22	2:R:497:ASN:C	2.14	0.51
1:F:50:LEU:C	1:F:50:LEU:HD12	2.30	0.51
2:M:359:HIS:O	2:M:366:ASN:HB3	2.11	0.51
1:E:184:ARG:HG3	1:E:184:ARG:NH1	2.25	0.51
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.31	0.51
1:B:51:LEU:HD12	1:B:106:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.27	0.50
2:Q:390:LYS:HE2	6:Q:1179:HOH:O	2.11	0.50
2:M:497:ASN:ND2	2:M:499:GLU:N	2.50	0.50
2:Q:522:ARG:NH1	6:Q:1099:HOH:O	2.43	0.50
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.27	0.50
2:P:326:THR:HG22	2:P:330:ARG:HD2	1.93	0.50
1:B:6:PRO:HB2	2:N:503:GLN:HE22	1.76	0.50
2:Q:447:TYR:CE1	5:Q:550:IHB:C5	2.95	0.50
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.93	0.50
1:F:131:PHE:O	1:F:132:ALA:HB2	2.11	0.50
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.50
1:D:98:THR:OG1	1:D:102:GLY:N	2.39	0.50
1:B:165:GLN:CD	1:B:165:GLN:H	2.14	0.50
2:M:416:LEU:C	2:M:416:LEU:HD23	2.32	0.50
1:B:99:PHE:HE2	2:N:411:LYS:HZ3	1.58	0.49
2:N:364:LEU:CD2	2:N:440:ARG:HD3	2.36	0.49
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.94	0.49
2:M:497:ASN:HD22	2:M:497:ASN:C	2.16	0.49
2:N:410:HIS:CE1	2:N:411:LYS:HG3	2.47	0.49
1:F:44:ALA:O	1:F:48:HIS:NE2	2.30	0.49
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.47	0.49
5:O:550:IHB:H2	6:O:760:HOH:O	2.11	0.49
2:R:410:HIS:CE1	2:R:411:LYS:HG3	2.47	0.49
1:A:26:ALA:C	2:M:411:LYS:NZ	2.65	0.49
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.13	0.49
1:B:98:THR:O	1:B:102:GLY:HA2	2.13	0.49
2:R:371:GLY:N	2:R:422:ASN:ND2	2.61	0.49
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.30	0.49
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.94	0.49
1:D:24:GLU:O	1:D:27:GLY:N	2.45	0.49
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.76	0.49
1:A:133:ARG:HG2	2:M:326:THR:HG21	1.95	0.49
2:N:497:ASN:HD22	2:N:499:GLU:H	1.61	0.49
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.49
2:Q:450:ARG:NH2	6:Q:1470:HOH:O	2.42	0.48
2:R:385:VAL:O	2:R:526:VAL:HA	2.14	0.48
1:F:115:ASN:HA	1:F:121:PRO:HA	1.95	0.48
1:E:70:VAL:HG12	1:E:128:ILE:HG12	1.96	0.48
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.78	0.48
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.48	0.48
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:497:ASN:C	2:P:497:ASN:ND2	2.63	0.48
1:F:52:LEU:O	1:F:184:ARG:HA	2.14	0.48
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.72	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.49	0.48
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.96	0.48
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.72	0.47
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.35	0.47
1:B:51:LEU:HD12	1:B:106:LEU:CD2	2.44	0.47
2:N:536:GLU:HB2	6:N:704:HOH:O	2.14	0.47
2:N:447:TYR:OH	5:N:550:IHB:C5	2.62	0.47
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.96	0.47
1:D:100:ASP:CG	1:D:101:ALA:H	2.17	0.47
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.71	0.47
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.97	0.47
2:O:465:ILE:N	2:O:465:ILE:HD12	2.30	0.47
1:C:98:THR:HG1	1:C:101:ALA:HB3	1.80	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.72	0.47
2:M:383:ARG:HG3	2:M:436:TYR:CE1	2.49	0.47
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.50	0.47
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.96	0.47
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.79	0.47
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.30	0.47
1:D:143:LEU:HD23	1:D:143:LEU:C	2.35	0.47
1:F:26:ALA:C	2:R:411:LYS:NZ	2.68	0.47
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.77	0.47
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.30	0.47
2:O:447:TYR:OH	5:O:550:IHB:C5	2.63	0.47
1:E:165:GLN:NE2	1:E:165:GLN:N	2.38	0.46
2:M:403:ASN:HB2	6:M:610:HOH:O	2.15	0.46
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.63	0.46
2:Q:325:LYS:HG2	2:R:335:ALA:HB1	1.96	0.46
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.50	0.46
1:D:98:THR:O	1:D:102:GLY:HA2	2.14	0.46
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.97	0.46
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.50	0.46
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.15	0.46
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.15	0.46
2:Q:432:ASP:OD1	2:Q:434:ASP:N	2.38	0.46
1:D:176:GLU:OE2	1:D:179:GLY:CA	2.56	0.46
2:R:414:ARG:N	2:R:414:ARG:HD2	2.30	0.46
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:GLU:HA	1:E:180:LYS:O	2.16	0.46
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.86	0.46
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.50	0.46
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.97	0.46
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.97	0.46
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.30	0.46
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.98	0.46
1:D:24:GLU:O	1:D:27:GLY:HA2	2.16	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.46
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.98	0.46
1:D:39:LEU:HB3	1:D:90:ASN:O	2.15	0.46
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.82	0.45
1:C:98:THR:O	1:C:102:GLY:HA2	2.16	0.45
2:Q:522:ARG:NE	2:Q:524:ASP:OD1	2.49	0.45
1:F:94:ARG:HH22	2:R:398:GLU:CD	2.20	0.45
1:F:68:LEU:HD12	1:F:68:LEU:N	2.31	0.45
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.78	0.45
2:Q:399:MET:HA	2:Q:462:HIS:O	2.17	0.45
2:M:448:PRO:CB	2:P:516:MET:HA	2.46	0.45
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.99	0.45
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.51	0.45
2:P:308:PHE:HA	2:P:529:GLY:O	2.16	0.45
2:O:410:HIS:ND1	2:O:412:ASN:N	2.52	0.45
2:O:383:ARG:HA	2:O:435:GLY:O	2.17	0.45
1:F:16:TYR:O	1:F:19:ILE:HG12	2.17	0.45
1:E:100:ASP:N	1:E:100:ASP:OD1	2.49	0.45
2:M:361:HIS:CG	4:M:601:BME:H21	2.52	0.45
2:N:361:HIS:HD2	2:N:361:HIS:H	1.62	0.45
2:Q:450:ARG:CZ	6:Q:1470:HOH:O	2.63	0.45
2:Q:522:ARG:HD3	2:Q:522:ARG:HH11	1.52	0.45
1:D:54:GLN:HG3	1:D:184:ARG:HH22	1.82	0.45
2:O:410:HIS:CE1	2:O:412:ASN:HB2	2.52	0.44
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.99	0.44
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.32	0.44
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.18	0.44
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.98	0.44
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.16	0.44
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.98	0.44
2:M:376:GLU:O	2:M:442:ILE:HA	2.16	0.44
2:R:383:ARG:NH2	2:R:391:PRO:HG3	2.32	0.44
1:C:98:THR:OG1	1:C:101:ALA:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LEU:O	1:E:182:ALA:HA	2.18	0.44
5:R:550:IHB:H2	6:R:1471:HOH:O	2.16	0.44
2:R:359:HIS:O	2:R:366:ASN:HB3	2.17	0.44
1:F:19:ILE:HD11	2:R:408:TYR:HD1	1.83	0.44
2:P:360:ASP:HB3	2:P:428:ARG:HG3	2.00	0.44
1:A:147:ASP:OD2	1:A:174:ARG:HD2	2.18	0.44
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.89	0.44
2:R:486:ILE:HB	2:R:487:PRO:HD3	2.00	0.44
1:F:36:TRP:CG	1:F:37:ASN:N	2.86	0.44
1:E:177:VAL:O	1:E:180:LYS:HB3	2.18	0.44
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.72	0.44
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.79	0.43
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.88	0.43
2:R:390:LYS:HD2	6:R:1307:HOH:O	2.17	0.43
1:D:41:LYS:HD2	1:D:87:ASN:O	2.18	0.43
2:O:318:LYS:HA	2:O:318:LYS:HD3	1.88	0.43
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.48	0.43
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.85	0.43
1:B:58:GLY:CA	1:B:190:GLN:HB3	2.48	0.43
2:O:410:HIS:CE1	2:O:412:ASN:H	2.31	0.43
1:D:176:GLU:HA	1:D:180:LYS:O	2.18	0.43
1:D:132:ALA:HB3	1:D:135:ILE:HD12	2.00	0.43
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.54	0.43
2:Q:522:ARG:HE	2:Q:524:ASP:CG	2.20	0.43
2:M:448:PRO:HB2	2:P:516:MET:HA	2.00	0.43
1:A:191:GLY:O	1:A:194:GLU:HB2	2.19	0.43
1:A:167:ARG:HD2	1:A:167:ARG:HH11	1.56	0.43
1:B:81:ASP:HB2	2:N:348:GLY:O	2.19	0.43
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.83	0.43
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.34	0.43
1:A:98:THR:O	1:A:102:GLY:HA2	2.19	0.43
2:Q:497:ASN:ND2	2:Q:497:ASN:C	2.70	0.43
1:D:133:ARG:NH2	1:E:162:GLU:OE2	2.52	0.43
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.86	0.43
2:M:413:ASP:C	2:M:414:ARG:HD2	2.39	0.43
2:Q:373:PRO:HB3	2:Q:423:PHE:HB2	1.99	0.43
2:P:497:ASN:ND2	2:P:499:GLU:N	2.61	0.43
1:D:162:GLU:OE2	1:F:133:ARG:NH2	2.51	0.43
2:R:378:ILE:HA	2:R:519:LEU:O	2.19	0.43
1:A:155:CYS:O	1:A:159:ASN:ND2	2.32	0.43
2:O:361:HIS:CG	4:O:601:BME:H21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:383:ARG:NE	2:P:434:ASP:O	2.38	0.43
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.70	0.43
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.16	0.42
2:N:497:ASN:HD22	2:N:498:PRO:N	2.17	0.42
1:E:163:GLN:HA	1:E:164:PRO:HD3	1.91	0.42
1:B:23:LEU:N	1:B:23:LEU:HD12	2.34	0.42
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.53	0.42
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.67	0.42
1:E:124:PRO:HA	6:E:220:HOH:O	2.19	0.42
1:E:44:ALA:O	1:E:48:HIS:NE2	2.37	0.42
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.19	0.42
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.54	0.42
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.39	0.42
1:F:176:GLU:HA	1:F:180:LYS:O	2.19	0.42
2:N:328:ILE:HD12	2:O:335:ALA:HB2	2.01	0.42
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.82	0.42
1:E:168:GLU:CA	1:E:171:ILE:HD12	2.44	0.42
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.71	0.42
1:F:15:PRO:HB3	1:F:133:ARG:HD2	2.00	0.42
2:N:399:MET:HA	2:N:462:HIS:O	2.19	0.42
1:E:18:HIS:CE1	6:E:221:HOH:O	2.73	0.42
1:F:177:VAL:O	1:F:180:LYS:HB3	2.19	0.42
2:Q:438:SER:O	4:Q:601:BME:H22	2.20	0.42
2:O:361:HIS:HD2	6:O:711:HOH:O	2.02	0.42
1:E:19:ILE:HG21	1:E:19:ILE:HD13	1.76	0.42
2:R:489:CYS:O	2:R:493:LYS:HE3	2.19	0.42
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.78	0.42
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.34	0.42
2:R:372:LEU:HA	2:R:373:PRO:HD3	1.84	0.42
2:P:443:LYS:HA	2:P:444:PRO:HD2	1.94	0.42
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.35	0.42
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.88	0.42
1:F:116:ASN:C	1:F:116:ASN:OD1	2.58	0.42
1:F:176:GLU:HG3	1:F:180:LYS:C	2.39	0.41
1:F:18:HIS:CE1	6:F:1278:HOH:O	2.72	0.41
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.54	0.41
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	2.01	0.41
2:R:392:VAL:HG12	2:R:395:THR:HB	2.02	0.41
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.41
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.19	0.41
2:N:497:ASN:HD22	2:N:497:ASN:C	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.79	0.41
2:O:390:LYS:HD3	6:O:732:HOH:O	2.20	0.41
2:P:390:LYS:HA	2:P:391:PRO:HD3	1.88	0.41
1:E:100:ASP:CG	1:E:101:ALA:H	2.23	0.41
1:D:51:LEU:HD12	1:D:106:LEU:HD23	2.03	0.41
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	2.01	0.41
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	2.02	0.41
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.82	0.41
2:M:473:LYS:NZ	6:M:651:HOH:O	2.44	0.41
1:B:44:ALA:HA	1:B:45:PRO:HD2	1.88	0.41
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.56	0.41
2:N:392:VAL:HG12	2:N:395:THR:HB	2.02	0.41
1:E:24:GLU:O	1:E:27:GLY:N	2.50	0.41
2:O:416:LEU:CD2	2:O:416:LEU:C	2.87	0.41
2:M:447:TYR:HB2	2:M:448:PRO:HD2	2.02	0.41
2:Q:304:ASP:HB2	2:Q:343:ILE:HB	2.02	0.41
1:C:5:LEU:O	2:O:387:GLN:HG2	2.20	0.41
1:D:98:THR:OG1	1:D:101:ALA:HB3	2.20	0.41
2:P:522:ARG:NH1	6:P:673:HOH:O	2.24	0.41
2:M:488:MET:CE	2:P:508:LEU:HD23	2.50	0.41
2:O:450:ARG:HG3	6:O:642:HOH:O	2.21	0.41
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.21	0.41
1:C:180:LYS:HG2	1:C:181:THR:N	2.36	0.41
1:D:51:LEU:O	1:D:52:LEU:HB3	2.21	0.41
1:B:143:LEU:C	1:B:143:LEU:HD23	2.41	0.41
2:M:335:ALA:HB2	2:O:328:ILE:HD12	2.02	0.41
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.74	0.41
2:M:326:THR:HG22	2:M:330:ARG:HD2	2.03	0.41
1:D:18:HIS:HA	1:D:22:ALA:HB3	2.03	0.41
1:A:70:VAL:HA	1:A:127:ASN:O	2.21	0.41
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.39	0.40
2:Q:392:VAL:HG12	2:Q:395:THR:HB	2.03	0.40
2:P:405:GLY:HA3	6:P:653:HOH:O	2.20	0.40
2:M:399:MET:HA	2:M:462:HIS:O	2.21	0.40
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.80	0.40
1:B:100:ASP:CG	1:B:101:ALA:H	2.24	0.40
1:A:39:LEU:HD11	1:A:93:GLY:HA3	2.02	0.40
1:D:35:ILE:HD13	2:P:351:PHE:CE1	2.56	0.40
2:R:407:ARG:HG2	2:R:407:ARG:NH1	2.37	0.40
1:E:157:VAL:O	1:E:160:LEU:HB2	2.21	0.40
2:P:457:ARG:HA	2:P:458:PRO:HD3	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ILE:O	2:P:426:VAL:HG21	2.20	0.40
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.87	0.40
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.40	0.40
1:D:24:GLU:O	1:D:27:GLY:CA	2.69	0.40
1:F:52:LEU:HD22	1:F:52:LEU:C	2.42	0.40
2:P:443:LYS:HE2	2:P:480:PHE:CG	2.57	0.40
2:N:449:TRP:CD1	2:N:449:TRP:N	2.89	0.40
2:N:447:TYR:HB2	2:N:448:PRO:HD2	2.03	0.40

All (2) 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)
1:C:46:GLY:O	1:D:150:GLN:OE1[3_554]	1.84	0.36
6:Q:1200:HOH:O	6:Q:1200:HOH:O[2_555]	2.10	0.10

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	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	229/238 (96%)	222 (97%)	7 (3%)	0	100 100
2	Q	229/238 (96%)	218 (95%)	11 (5%)	0	100 100
2	R	229/238 (96%)	221 (96%)	7 (3%)	1 (0%)	39 41
All	All	2562/2628 (98%)	2475 (97%)	86 (3%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	535	PHE

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	162/163 (99%)	156 (96%)	6 (4%)	41 50
1	B	162/163 (99%)	155 (96%)	7 (4%)	35 42
1	C	162/163 (99%)	155 (96%)	7 (4%)	35 42
1	D	162/163 (99%)	155 (96%)	7 (4%)	35 42
1	E	162/163 (99%)	155 (96%)	7 (4%)	35 42
1	F	162/163 (99%)	155 (96%)	7 (4%)	35 42
2	M	196/202 (97%)	188 (96%)	8 (4%)	37 45
2	N	196/202 (97%)	183 (93%)	13 (7%)	21 21
2	O	196/202 (97%)	186 (95%)	10 (5%)	29 33
2	P	196/202 (97%)	189 (96%)	7 (4%)	42 51
2	Q	196/202 (97%)	185 (94%)	11 (6%)	26 29
2	R	196/202 (97%)	185 (94%)	11 (6%)	26 29
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	32 38

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	52	LEU
1	A	91	SER
1	A	165	GLN
2	M	344	SER
2	M	395	THR
2	M	416	LEU
2	M	434	ASP
2	M	440	ARG
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	38	ARG
1	B	52	LEU
1	B	106	LEU
1	B	158	LEU
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	411	LYS
2	N	416	LEU
2	N	428	ARG
2	N	433	SER
2	N	440	ARG
2	N	442	ILE
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	100	ASP
1	C	158	LEU
1	C	165	GLN
2	O	372	LEU
2	O	393	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	434	ASP
2	O	465	ILE
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	42	PRO
1	D	43	ASP
1	D	52	LEU
1	D	165	GLN
2	P	364	LEU
2	P	395	THR
2	P	411	LYS
2	P	416	LEU
2	P	440	ARG
2	P	497	ASN
2	P	534	HIS
1	E	4	LEU
1	E	38	ARG
1	E	49	ILE
1	E	52	LEU
1	E	66	SER
1	E	165	GLN
1	E	181	THR
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	411	LYS
2	Q	416	LEU
2	Q	428	ARG
2	Q	442	ILE
2	Q	450	ARG
2	Q	478	LEU
2	Q	497	ASN
2	Q	507	LYS
1	F	4	LEU
1	F	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	50	LEU
1	F	52	LEU
1	F	66	SER
1	F	100	ASP
1	F	165	GLN
2	R	352	SER
2	R	372	LEU
2	R	395	THR
2	R	399	MET
2	R	411	LYS
2	R	416	LEU
2	R	428	ARG
2	R	440	ARG
2	R	442	ILE
2	R	497	ASN
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	165	GLN
2	N	361	HIS
2	N	497	ASN
2	N	503	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	107	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	IHB	M	550	3	8,11,11	1.33	1 (12%)	10,15,15	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	IHB	M	551	-	8,11,11	1.20	1 (12%)	10,15,15	0.55	0
4	BME	M	601	2	3,3,3	0.55	0	2,2,2	0.12	0
5	IHB	N	550	3	8,11,11	1.22	1 (12%)	10,15,15	0.99	0
5	IHB	N	551	-	8,11,11	0.89	0	10,15,15	0.68	0
4	BME	N	601	2	3,3,3	0.50	0	2,2,2	0.07	0
5	IHB	O	550	3	8,11,11	1.00	1 (12%)	10,15,15	0.53	0
5	IHB	O	551	-	8,11,11	1.28	1 (12%)	10,15,15	0.89	0
4	BME	O	601	2	3,3,3	0.66	0	2,2,2	0.29	0
5	IHB	P	550	3	8,11,11	1.18	1 (12%)	10,15,15	0.57	0
5	IHB	P	551	-	8,11,11	1.21	1 (12%)	10,15,15	0.82	0
4	BME	P	601	2	3,3,3	0.54	0	2,2,2	0.56	0
5	IHB	Q	550	3	8,11,11	1.16	1 (12%)	10,15,15	0.53	0
5	IHB	Q	551	-	8,11,11	0.87	1 (12%)	10,15,15	0.65	0
4	BME	Q	601	2	3,3,3	0.35	0	2,2,2	0.55	0
5	IHB	R	550	3	8,11,11	1.28	1 (12%)	10,15,15	0.55	0
5	IHB	R	551	-	8,11,11	1.13	1 (12%)	10,15,15	0.84	0
4	BME	R	601	2	3,3,3	0.52	0	2,2,2	0.41	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
5	IHB	M	550	3	-	0/0/4/4	0/1/1/1
5	IHB	M	551	-	-	0/0/4/4	0/1/1/1
4	BME	M	601	2	-	0/1/1/1	0/0/0/0
5	IHB	N	550	3	-	0/0/4/4	0/1/1/1
5	IHB	N	551	-	-	0/0/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	0/0/0/0
5	IHB	O	550	3	-	0/0/4/4	0/1/1/1
5	IHB	O	551	-	-	0/0/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	0/0/0/0
5	IHB	P	550	3	-	0/0/4/4	0/1/1/1
5	IHB	P	551	-	-	0/0/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	0/0/0/0
5	IHB	Q	550	3	-	0/0/4/4	0/1/1/1
5	IHB	Q	551	-	-	0/0/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	0/0/0/0
5	IHB	R	550	3	-	0/0/4/4	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IHB	R	551	-	-	0/0/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550	IHB	C3-I3	-3.43	2.01	2.10
5	R	550	IHB	C3-I3	-3.23	2.01	2.10
5	O	551	IHB	C3-I3	-3.18	2.01	2.10
5	N	550	IHB	C3-I3	-3.01	2.02	2.10
5	P	551	IHB	C3-I3	-2.92	2.02	2.10
5	Q	550	IHB	C3-I3	-2.89	2.02	2.10
5	M	551	IHB	C3-I3	-2.88	2.02	2.10
5	P	550	IHB	C3-I3	-2.85	2.02	2.10
5	R	551	IHB	C3-I3	-2.52	2.03	2.10
5	O	550	IHB	C3-I3	-2.47	2.03	2.10
5	Q	551	IHB	C3-I3	-2.00	2.04	2.10

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550	IHB	1	0
4	M	601	BME	1	0
5	N	550	IHB	1	0
5	O	550	IHB	2	0
4	O	601	BME	1	0
5	Q	550	IHB	2	0
4	Q	601	BME	2	0
5	R	550	IHB	3	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.