Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 02:28 PM EDT

PDB ID	:	3PCH
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3-CHLORO-4-HYDROXYBENZOATE
Authors	:	Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-01
Resolution	:	2.05 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

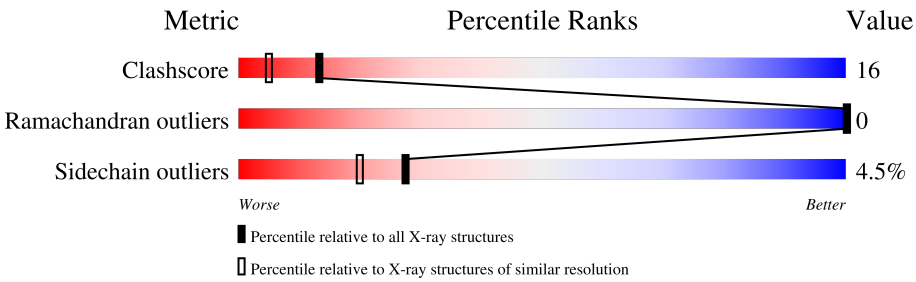
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.05 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	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	64% 30% • •
1	B	200	69% 26% • •
1	C	200	70% 26% • •
1	D	200	64% 31% •
1	E	200	60% 34% 5%
1	F	200	62% 32% • •
2	M	238	61% 31% 5% • •
2	N	238	70% 23% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	238	67% 26%
2	P	238	64% 29%
2	Q	238	63% 31%
2	R	238	68% 25% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22080 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
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

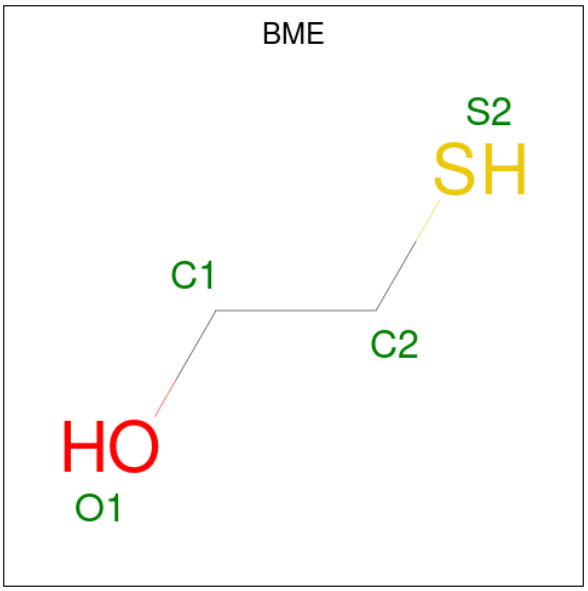
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

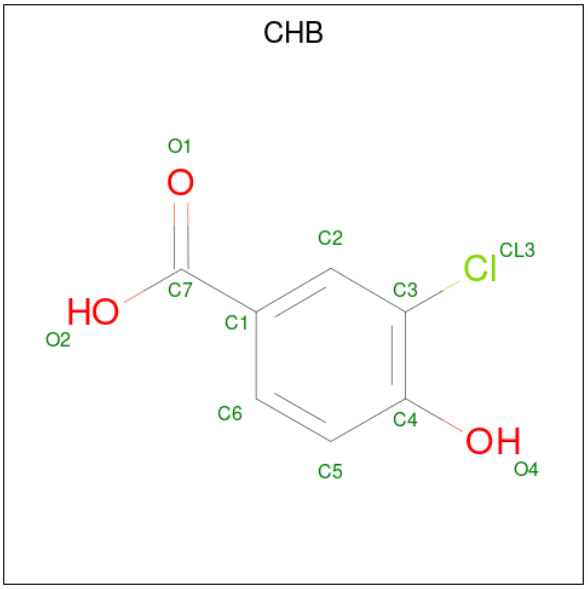
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	M	1	1	1	0	0
3	N	1	1	1	0	0
3	O	1	1	1	0	0
3	P	1	1	1	0	0
3	Q	1	1	1	0	0
3	R	1	1	1	0	0

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



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

- Molecule 5 is 3-CHLORO-4-HYDROXYBENZOIC ACID (three-letter code: CHB) (formula: $C_7H_5ClO_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	82	82	82	0	0
			Total	O		
6	M	160	160	160	0	0
			Total	O		
6	B	83	83	83	0	0
			Total	O		
6	N	164	164	164	0	0
			Total	O		
6	C	84	84	84	0	0
			Total	O		
6	O	155	155	155	0	0
			Total	O		
6	D	84	84	84	0	0
			Total	O		
6	P	153	153	153	0	0
			Total	O		
6	E	83	83	83	0	0
			Total	O		
6	Q	163	163	163	0	0
			Total	O		
6	F	83	83	83	0	0
			Total	O		
6	R	158	158	158	0	0

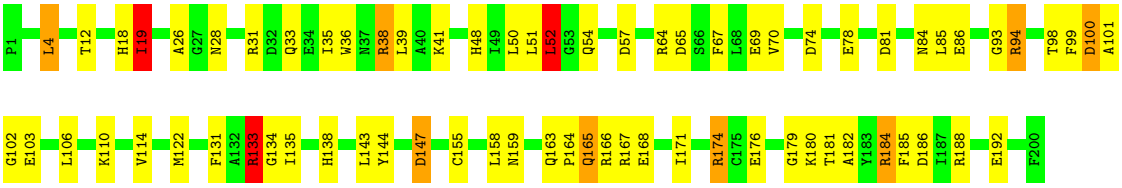
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

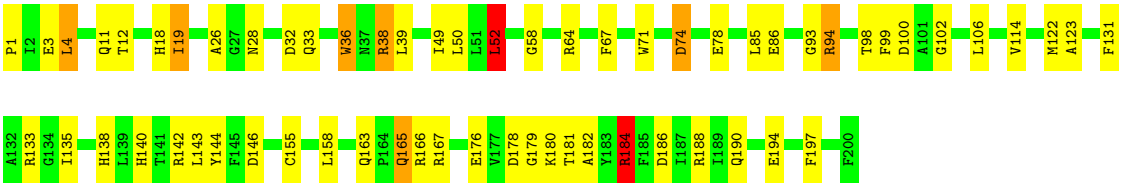
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



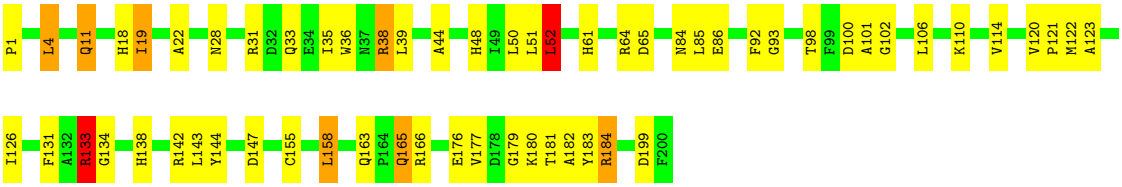
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



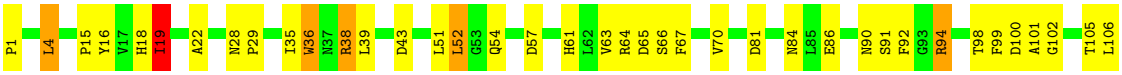
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C:



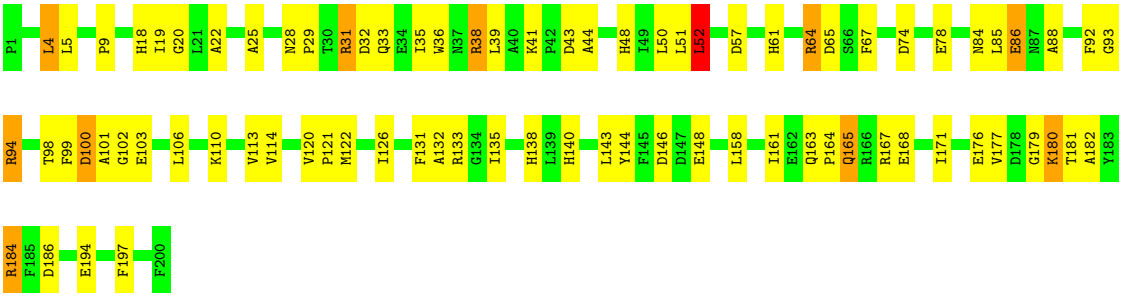
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D:



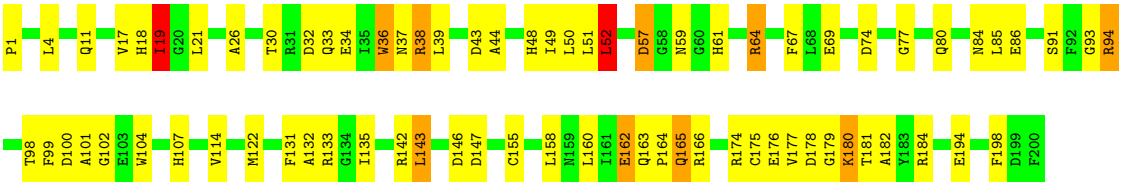
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



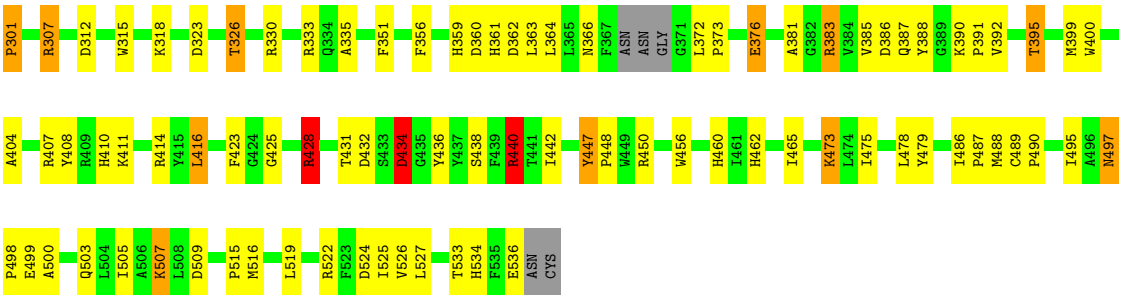
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:



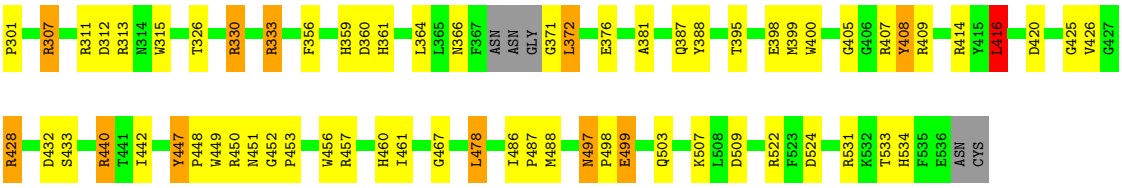
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:



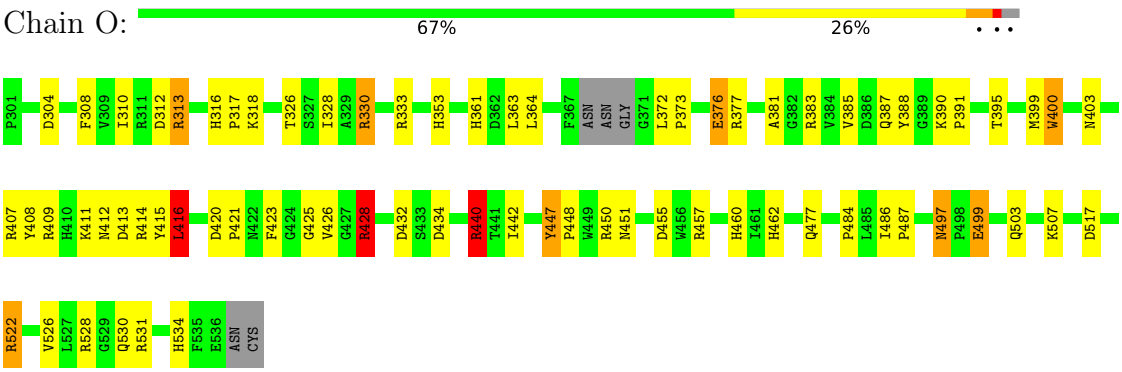
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N:



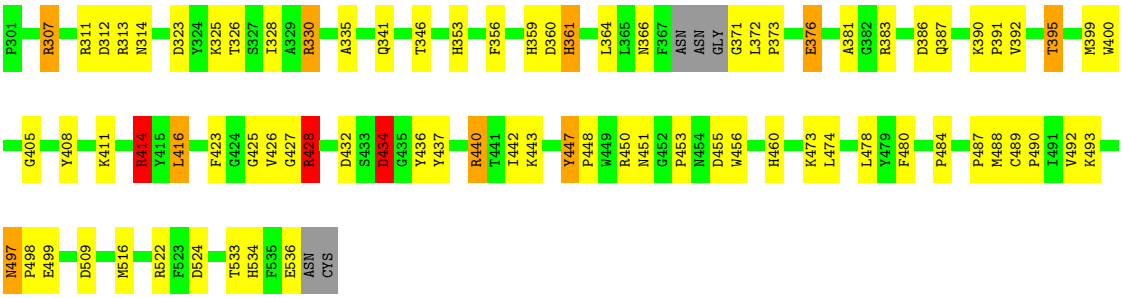
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:



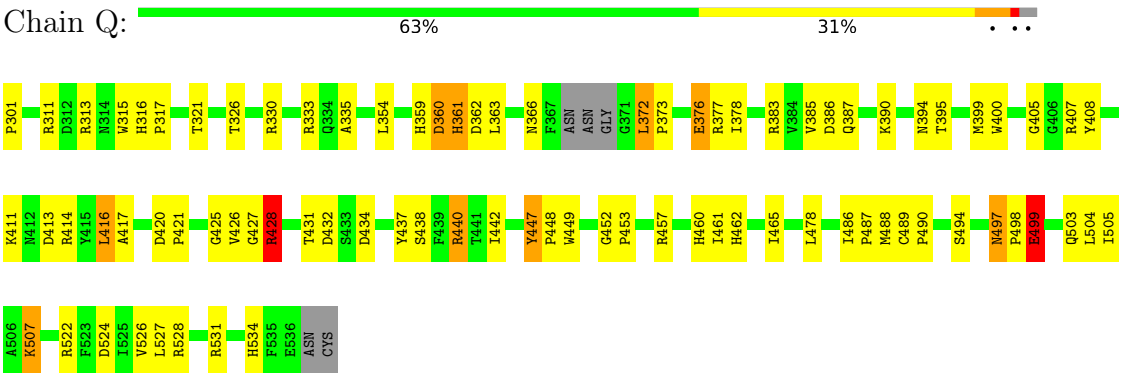
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



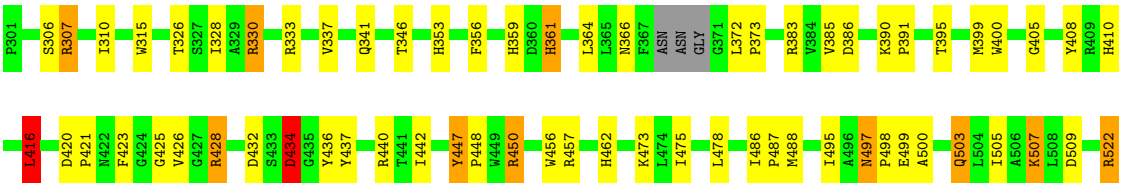
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



F523
D524
I525
V526
L527
R528
G529
Q530
R531
E536
ASN
CYS

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.39Å 126.52Å 133.33Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	6.00 – 2.05	Depositor
% Data completeness (in resolution range)	75.2 (6.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22080	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, FE, CHB

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	1.00	1/1611 (0.1%)	1.71	27/2195 (1.2%)
1	B	1.04	2/1611 (0.1%)	1.78	30/2195 (1.4%)
1	C	0.96	0/1611	1.53	16/2195 (0.7%)
1	D	1.03	0/1611	1.70	23/2195 (1.0%)
1	E	1.02	1/1611 (0.1%)	1.59	20/2195 (0.9%)
1	F	1.01	1/1611 (0.1%)	1.68	28/2195 (1.3%)
2	M	1.10	2/1895 (0.1%)	1.75	35/2580 (1.4%)
2	N	1.11	4/1895 (0.2%)	1.65	38/2580 (1.5%)
2	O	1.10	1/1895 (0.1%)	1.68	40/2580 (1.6%)
2	P	1.08	2/1895 (0.1%)	1.77	35/2580 (1.4%)
2	Q	1.13	3/1895 (0.2%)	1.73	38/2580 (1.5%)
2	R	1.08	2/1895 (0.1%)	1.72	33/2580 (1.3%)
All	All	1.06	19/21036 (0.1%)	1.69	363/28650 (1.3%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	428	ARG	CD-NE	-6.82	1.34	1.46
2	M	428	ARG	CD-NE	-6.53	1.35	1.46
2	Q	428	ARG	CD-NE	-6.52	1.35	1.46
1	B	94	ARG	CD-NE	-6.21	1.35	1.46
2	P	440	ARG	CD-NE	-5.93	1.36	1.46
2	Q	440	ARG	CD-NE	-5.79	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	440	ARG	CD-NE	-5.79	1.36	1.46
1	B	194	GLU	CD-OE2	-5.69	1.19	1.25
2	N	467	GLY	CA-C	5.63	1.60	1.51
2	R	428	ARG	CG-CD	-5.50	1.38	1.51
2	N	398	GLU	CD-OE1	-5.44	1.19	1.25
1	E	194	GLU	CD-OE2	-5.42	1.19	1.25
2	P	376	GLU	CD-OE1	-5.34	1.19	1.25
1	A	94	ARG	CD-NE	-5.29	1.37	1.46
2	Q	428	ARG	CG-CD	-5.14	1.39	1.51
2	M	376	GLU	CD-OE1	-5.07	1.20	1.25
2	N	428	ARG	CD-NE	-5.07	1.37	1.46
2	O	330	ARG	CZ-NH1	5.05	1.39	1.33
1	F	194	GLU	CD-OE2	-5.03	1.20	1.25

All (363) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	440	ARG	NE-CZ-NH2	-24.29	108.16	120.30
2	M	440	ARG	NE-CZ-NH2	-21.91	109.34	120.30
2	Q	440	ARG	NE-CZ-NH2	-21.30	109.65	120.30
2	P	440	ARG	NE-CZ-NH1	20.23	130.41	120.30
1	B	184	ARG	NE-CZ-NH2	-19.45	110.57	120.30
1	D	94	ARG	NE-CZ-NH2	-19.32	110.64	120.30
2	N	440	ARG	NE-CZ-NH2	-19.16	110.72	120.30
2	O	440	ARG	NE-CZ-NH2	-19.06	110.77	120.30
2	R	440	ARG	NE-CZ-NH2	-18.68	110.96	120.30
1	A	94	ARG	NE-CZ-NH1	18.26	129.43	120.30
1	D	133	ARG	CD-NE-CZ	18.05	148.88	123.60
2	Q	428	ARG	NE-CZ-NH2	-17.64	111.48	120.30
1	F	133	ARG	CD-NE-CZ	16.96	147.35	123.60
1	A	94	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	B	133	ARG	NE-CZ-NH1	16.04	128.32	120.30
1	B	133	ARG	CD-NE-CZ	15.85	145.78	123.60
2	O	428	ARG	NE-CZ-NH1	14.58	127.59	120.30
2	P	428	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	B	133	ARG	NE-CZ-NH2	-13.95	113.32	120.30
1	D	133	ARG	NE-CZ-NH1	13.85	127.22	120.30
2	M	450	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	A	94	ARG	CD-NE-CZ	13.32	142.25	123.60
1	B	94	ARG	NE-CZ-NH1	13.30	126.95	120.30
2	P	428	ARG	NE-CZ-NH2	-13.10	113.75	120.30
1	E	94	ARG	NE-CZ-NH1	13.02	126.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	428	ARG	CD-NE-CZ	12.97	141.76	123.60
2	R	428	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	B	184	ARG	NE-CZ-NH1	12.63	126.62	120.30
2	P	450	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	A	166	ARG	NE-CZ-NH1	11.98	126.29	120.30
2	O	428	ARG	CD-NE-CZ	11.75	140.04	123.60
2	R	428	ARG	CG-CD-NE	11.59	136.14	111.80
2	R	307	ARG	NE-CZ-NH1	11.59	126.09	120.30
2	M	428	ARG	NE-CZ-NH1	11.58	126.09	120.30
2	Q	428	ARG	CD-NE-CZ	11.32	139.45	123.60
1	B	38	ARG	NE-CZ-NH2	-11.30	114.65	120.30
2	Q	428	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	E	94	ARG	NE-CZ-NH2	-10.98	114.81	120.30
2	M	428	ARG	NE-CZ-NH2	-10.89	114.85	120.30
2	R	531	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	B	94	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	D	184	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	C	133	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	F	94	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	F	133	ARG	NE-CZ-NH2	10.51	125.55	120.30
2	Q	383	ARG	NE-CZ-NH2	-10.40	115.10	120.30
2	O	428	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	C	166	ARG	NE-CZ-NH2	-10.11	115.25	120.30
2	O	531	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	184	ARG	NE-CZ-NH2	-9.97	115.31	120.30
2	O	528	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	D	133	ARG	NE-CZ-NH2	-9.96	115.32	120.30
2	M	414	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	C	166	ARG	NE-CZ-NH1	9.87	125.23	120.30
2	P	524	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	B	166	ARG	NE-CZ-NH2	-9.61	115.50	120.30
2	R	524	ASP	CB-CG-OD2	-9.53	109.72	118.30
2	R	434	ASP	CB-CG-OD1	-9.49	109.75	118.30
2	M	434	ASP	CB-CG-OD2	-9.47	109.78	118.30
2	Q	531	ARG	NE-CZ-NH2	-9.40	115.60	120.30
2	N	428	ARG	NE-CZ-NH2	-9.37	115.62	120.30
2	N	407	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	E	186	ASP	CB-CG-OD1	9.34	126.71	118.30
1	F	94	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	N	447	TYR	CB-CG-CD1	-9.28	115.43	121.00
1	B	188	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	B	188	ARG	NE-CZ-NH1	9.03	124.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	186	ASP	CB-CG-OD2	-9.02	110.19	118.30
2	R	457	ARG	NE-CZ-NH2	-8.97	115.82	120.30
2	P	432	ASP	CB-CG-OD2	-8.95	110.24	118.30
2	N	428	ARG	NE-CZ-NH1	8.94	124.77	120.30
2	O	457	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	D	188	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	F	142	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	F	38	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	F	142	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	188	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	F	38	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	R	447	TYR	CB-CG-CD2	-8.67	115.80	121.00
1	C	133	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	C	184	ARG	NE-CZ-NH2	-8.61	116.00	120.30
2	R	428	ARG	NE-CZ-NH1	8.57	124.58	120.30
2	R	457	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	R	524	ASP	CB-CG-OD1	8.54	125.99	118.30
2	N	440	ARG	NE-CZ-NH1	8.51	124.56	120.30
2	P	383	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	F	64	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	94	ARG	CG-CD-NE	8.49	129.63	111.80
2	R	383	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	C	184	ARG	NE-CZ-NH1	8.45	124.53	120.30
2	P	434	ASP	CB-CG-OD2	-8.44	110.70	118.30
2	M	428	ARG	CG-CD-NE	8.36	129.35	111.80
2	P	450	ARG	CD-NE-CZ	8.28	135.19	123.60
2	N	524	ASP	CB-CG-OD2	-8.27	110.85	118.30
1	F	166	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	R	428	ARG	CD-NE-CZ	8.22	135.12	123.60
2	Q	313	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	D	38	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	M	407	ARG	NE-CZ-NH1	8.09	124.34	120.30
2	M	330	ARG	NE-CZ-NH2	-8.09	116.26	120.30
2	O	383	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	178	ASP	CB-CG-OD2	8.05	125.54	118.30
1	D	184	ARG	NE-CZ-NH2	-8.03	116.28	120.30
2	R	440	ARG	NH1-CZ-NH2	7.92	128.11	119.40
2	O	434	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	D	142	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	Q	428	ARG	CB-CG-CD	7.85	132.02	111.60
2	Q	432	ASP	CB-CG-OD1	7.84	125.36	118.30
1	E	31	ARG	NE-CZ-NH2	-7.81	116.39	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	94	ARG	CG-CD-NE	7.80	128.17	111.80
2	M	524	ASP	CB-CG-OD1	7.79	125.31	118.30
2	P	440	ARG	CD-NE-CZ	7.78	134.49	123.60
2	Q	524	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	186	ASP	CB-CG-OD2	-7.68	111.39	118.30
2	R	432	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	E	146	ASP	CB-CG-OD1	7.64	125.18	118.30
1	E	64	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	P	432	ASP	CB-CG-OD1	7.61	125.14	118.30
1	B	167	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	F	94	ARG	CD-NE-CZ	7.58	134.22	123.60
2	M	524	ASP	CB-CG-OD2	-7.53	111.53	118.30
2	N	307	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	N	524	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	166	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	O	517	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	199	ASP	CB-CG-OD2	7.30	124.87	118.30
2	Q	428	ARG	CG-CD-NE	7.29	127.10	111.80
2	O	353	HIS	CA-CB-CG	-7.28	101.22	113.60
2	Q	360	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	57	ASP	CB-CG-OD1	7.26	124.83	118.30
2	Q	447	TYR	CB-CG-CD1	-7.26	116.64	121.00
2	Q	407	ARG	NE-CZ-NH1	7.24	123.92	120.30
2	Q	377	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	F	133	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	100	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	147	ASP	CB-CG-OD2	-7.08	111.93	118.30
2	Q	311	ARG	CD-NE-CZ	7.03	133.44	123.60
1	D	166	ARG	NE-CZ-NH2	-7.01	116.79	120.30
2	P	386	ASP	CB-CG-OD2	7.01	124.61	118.30
2	Q	457	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	Q	440	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	O	312	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	F	57	ASP	CB-CG-OD2	-6.98	112.02	118.30
2	Q	333	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	N	432	ASP	CB-CG-OD1	6.96	124.56	118.30
2	N	428	ARG	CG-CD-NE	6.94	126.38	111.80
2	M	450	ARG	CD-NE-CZ	6.94	133.31	123.60
2	N	312	ASP	CB-CG-OD2	-6.93	112.06	118.30
2	N	313	ARG	NE-CZ-NH1	6.90	123.75	120.30
2	O	517	ASP	CB-CG-OD1	6.88	124.50	118.30
2	O	432	ASP	CB-CG-OD2	-6.85	112.13	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	52	LEU	CA-CB-CG	6.82	130.99	115.30
2	O	450	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	M	432	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	B	94	ARG	CD-NE-CZ	6.74	133.04	123.60
2	P	353	HIS	CA-CB-CG	-6.73	102.16	113.60
1	E	43	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	M	440	ARG	NH1-CZ-NH2	6.69	126.75	119.40
1	F	146	ASP	CB-CG-OD2	-6.67	112.29	118.30
2	R	522	ARG	NE-CZ-NH1	-6.67	116.96	120.30
2	R	428	ARG	CB-CG-CD	6.67	128.94	111.60
1	E	31	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	142	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	146	ASP	CB-CG-OD1	6.64	124.27	118.30
1	B	184	ARG	CD-NE-CZ	6.62	132.87	123.60
1	F	94	ARG	CG-CD-NE	6.61	125.68	111.80
1	B	38	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	F	94	ARG	CB-CG-CD	6.58	128.70	111.60
2	Q	376	GLU	OE1-CD-OE2	6.56	131.18	123.30
2	O	407	ARG	NE-CZ-NH2	-6.55	117.03	120.30
2	O	388	TYR	CB-CG-CD1	-6.54	117.07	121.00
1	A	36	TRP	CB-CA-C	6.54	123.48	110.40
1	D	94	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	M	376	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	B	94	ARG	CB-CG-CD	6.49	128.48	111.60
2	N	312	ASP	CB-CG-OD1	6.48	124.13	118.30
2	M	333	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	57	ASP	CB-CG-OD2	-6.43	112.51	118.30
2	O	313	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	E	52	LEU	CB-CA-C	6.42	122.39	110.20
2	O	377	ARG	NE-CZ-NH1	6.41	123.51	120.30
2	R	333	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	P	428	ARG	CD-NE-CZ	6.36	132.50	123.60
2	P	509	ASP	CB-CG-OD1	6.36	124.02	118.30
2	Q	457	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	81	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	167	ARG	CD-NE-CZ	-6.29	114.79	123.60
1	B	71	TRP	CA-CB-CG	6.28	125.62	113.70
2	R	434	ASP	OD1-CG-OD2	6.26	135.19	123.30
1	B	146	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	P	414	ARG	CD-NE-CZ	-6.21	114.91	123.60
2	N	408	TYR	CB-CG-CD2	-6.20	117.28	121.00
2	Q	499	GLU	OE1-CD-OE2	-6.19	115.87	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	432	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	D	65	ASP	CB-CG-OD1	6.18	123.86	118.30
2	Q	531	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	F	36	TRP	CB-CA-C	6.16	122.71	110.40
1	A	81	ASP	CB-CG-OD2	-6.15	112.76	118.30
2	M	307	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	R	457	ARG	CD-NE-CZ	6.15	132.21	123.60
2	R	361	HIS	CA-CB-CG	-6.15	103.15	113.60
2	M	312	ASP	CB-CG-OD2	-6.12	112.80	118.30
2	O	416	LEU	CB-CA-C	6.12	121.82	110.20
1	C	38	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	166	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	81	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	M	414	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	Q	449	TRP	CB-CA-C	6.07	122.54	110.40
2	Q	440	ARG	NH1-CZ-NH2	6.06	126.07	119.40
2	M	432	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	133	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	E	74	ASP	CB-CG-OD1	6.04	123.73	118.30
2	Q	311	ARG	NE-CZ-NH1	-6.01	117.30	120.30
2	P	323	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	166	ARG	CD-NE-CZ	6.00	132.00	123.60
1	B	36	TRP	CB-CA-C	5.98	122.36	110.40
2	O	432	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	31	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	O	440	ARG	O-C-N	5.94	132.21	122.70
2	Q	499	GLU	CG-CD-OE1	5.94	130.18	118.30
2	P	330	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	P	434	ASP	OD1-CG-OD2	5.92	134.56	123.30
2	N	330	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	R	353	HIS	CA-CB-CG	-5.92	103.54	113.60
1	F	166	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	19	ILE	CB-CA-C	5.91	123.42	111.60
2	O	304	ASP	CB-CG-OD1	5.90	123.61	118.30
2	P	307	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	D	65	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	O	522	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	94	ARG	CG-CD-NE	5.87	124.14	111.80
1	C	133	ARG	CD-NE-CZ	5.87	131.82	123.60
1	C	11	GLN	N-CA-CB	5.86	121.15	110.60
2	O	434	ASP	CA-CB-CG	-5.86	100.51	113.40
2	N	420	ASP	CB-CG-OD2	-5.86	113.03	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	330	ARG	NE-CZ-NH2	-5.85	117.37	120.30
2	P	312	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	M	411	LYS	CB-CA-C	-5.82	98.77	110.40
2	P	313	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	N	450	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	178	ASP	CB-CA-C	5.79	121.97	110.40
1	A	52	LEU	CA-CB-CG	5.78	128.58	115.30
2	N	311	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	D	94	ARG	NH1-CZ-NH2	5.77	125.74	119.40
1	D	186	ASP	CB-CG-OD2	-5.76	113.11	118.30
2	R	416	LEU	CB-CA-C	5.76	121.14	110.20
2	M	440	ARG	CB-CG-CD	-5.75	96.65	111.60
2	O	440	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	O	400	TRP	N-CA-CB	5.73	120.92	110.60
1	D	36	TRP	CB-CA-C	5.73	121.86	110.40
2	N	428	ARG	CB-CG-CD	5.72	126.48	111.60
2	O	388	TYR	CB-CG-CD2	5.72	124.44	121.00
2	R	432	ASP	CB-CG-OD1	5.72	123.45	118.30
2	R	434	ASP	CA-CB-CG	-5.72	100.81	113.40
2	O	440	ARG	NH1-CZ-NH2	5.70	125.67	119.40
1	F	166	ARG	CD-NE-CZ	5.69	131.56	123.60
1	B	38	ARG	CD-NE-CZ	5.69	131.56	123.60
1	A	65	ASP	CB-CG-OD1	5.68	123.41	118.30
2	O	440	ARG	CB-CG-CD	-5.68	96.84	111.60
2	O	447	TYR	CB-CG-CD1	-5.67	117.59	121.00
1	E	86	GLU	CG-CD-OE1	5.67	129.64	118.30
1	C	158	LEU	CB-CA-C	5.66	120.96	110.20
2	M	440	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	38	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	F	19	ILE	CB-CA-C	5.65	122.90	111.60
2	N	408	TYR	CB-CG-CD1	5.64	124.39	121.00
1	E	184	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	P	371	GLY	CA-C-O	5.64	130.75	120.60
2	N	452	GLY	N-CA-C	-5.63	99.03	113.10
1	B	74	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	57	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	O	428	ARG	N-CA-CB	5.62	120.71	110.60
2	N	457	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	N	457	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	F	52	LEU	CB-CA-C	5.59	120.82	110.20
2	N	409	ARG	NE-CZ-NH1	-5.59	117.51	120.30
2	M	434	ASP	OD1-CG-OD2	5.58	133.91	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	N	388	TYR	CB-CG-CD1	-5.58	117.65	121.00
2	Q	452	GLY	N-CA-C	-5.57	99.17	113.10
1	E	36	TRP	CB-CA-C	5.57	121.53	110.40
2	M	323	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	142	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	P	524	ASP	CB-CG-OD1	5.53	123.28	118.30
1	E	57	ASP	CB-CG-OD1	5.51	123.26	118.30
2	O	457	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	103	GLU	OE1-CD-OE2	5.51	129.91	123.30
2	R	522	ARG	CD-NE-CZ	-5.50	115.90	123.60
2	N	449	TRP	CB-CA-C	5.48	121.36	110.40
1	C	36	TRP	CB-CA-C	5.47	121.33	110.40
2	Q	333	ARG	CB-CA-C	5.46	121.33	110.40
2	P	447	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	M	434	ASP	CA-CB-CG	-5.44	101.44	113.40
2	N	333	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	174	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	M	407	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	N	409	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	P	313	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	Q	383	ARG	NH1-CZ-NH2	5.37	125.31	119.40
2	N	509	ASP	CB-CG-OD1	5.37	123.13	118.30
1	F	74	ASP	CB-CG-OD1	5.37	123.13	118.30
2	O	333	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	P	447	TYR	CA-CB-CG	-5.34	103.24	113.40
1	F	52	LEU	CA-CB-CG	5.33	127.56	115.30
1	F	162	GLU	CA-CB-CG	5.33	125.13	113.40
2	Q	372	LEU	N-CA-CB	-5.32	99.75	110.40
1	A	19	ILE	CB-CA-C	5.31	122.22	111.60
2	R	509	ASP	CB-CG-OD1	5.30	123.07	118.30
2	Q	361	HIS	CA-CB-CG	-5.29	104.60	113.60
1	F	175	CYS	CA-CB-SG	5.28	123.51	114.00
1	E	100	ASP	CB-CG-OD2	5.27	123.05	118.30
2	M	383	ARG	CD-NE-CZ	-5.26	116.23	123.60
2	N	531	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	43	ASP	CB-CG-OD2	-5.26	113.57	118.30
2	R	528	ARG	NE-CZ-NH1	-5.26	117.67	120.30
2	P	428	ARG	CG-CD-NE	5.25	122.83	111.80
2	N	371	GLY	CA-C-O	5.25	130.04	120.60
2	P	536	GLU	CG-CD-OE2	-5.24	107.82	118.30
2	R	450	ARG	NE-CZ-NH2	-5.21	117.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	65	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	11	GLN	N-CA-CB	5.21	119.98	110.60
1	A	74	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	M	388	TYR	CB-CG-CD1	-5.21	117.88	121.00
2	O	455	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	P	314	ASN	CB-CA-C	5.17	120.75	110.40
2	N	499	GLU	CG-CD-OE1	5.17	128.64	118.30
2	N	451	ASN	CB-CA-C	5.17	120.73	110.40
2	O	312	ASP	CB-CG-OD1	5.17	122.95	118.30
2	M	479	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	P	312	ASP	CB-CG-OD1	5.16	122.95	118.30
1	C	183	TYR	N-CA-CB	5.16	119.89	110.60
1	B	86	GLU	CG-CD-OE1	5.16	128.61	118.30
2	Q	524	ASP	CB-CG-OD1	5.15	122.94	118.30
2	Q	440	ARG	CB-CG-CD	-5.15	98.21	111.60
1	E	74	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	186	ASP	CB-CG-OD1	5.13	122.92	118.30
2	N	447	TYR	CA-CB-CG	-5.13	103.65	113.40
1	C	52	LEU	CB-CA-C	5.13	119.94	110.20
2	R	509	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	M	509	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	F	57	ASP	CB-CG-OD1	5.12	122.90	118.30
1	E	38	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	O	383	ARG	NH1-CZ-NH2	5.11	125.02	119.40
2	P	361	HIS	CA-CB-CG	-5.10	104.93	113.60
2	N	416	LEU	CB-CA-C	5.09	119.88	110.20
1	B	52	LEU	CB-CA-C	5.09	119.87	110.20
2	P	383	ARG	NH1-CZ-NH2	5.08	124.99	119.40
2	R	386	ASP	CB-CA-C	5.08	120.56	110.40
2	Q	428	ARG	N-CA-CB	5.08	119.74	110.60
2	M	326	THR	CA-CB-OG1	-5.08	98.33	109.00
2	O	376	GLU	OE1-CD-OE2	5.08	129.40	123.30
2	M	362	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	43	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	38	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	Q	461	ILE	O-C-N	5.06	130.79	122.70
2	N	461	ILE	O-C-N	5.06	130.79	122.70
2	P	311	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	11	GLN	N-CA-CB	5.04	119.66	110.60
2	N	372	LEU	N-CA-CB	-5.03	100.34	110.40
2	Q	528	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	O	451	ASN	CB-CA-C	5.02	120.44	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	499	GLU	CG-CD-OE1	5.01	128.33	118.30
2	M	447	TYR	CB-CG-CD1	-5.01	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	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	59	0
1	B	1571	0	1499	53	0
1	C	1571	0	1499	59	0
1	D	1571	0	1499	56	0
1	E	1571	0	1499	65	0
1	F	1571	0	1499	74	0
2	M	1840	0	1792	77	0
2	N	1840	0	1792	41	0
2	O	1840	0	1792	58	0
2	P	1840	0	1792	66	0
2	Q	1840	0	1792	61	0
2	R	1840	0	1792	54	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	3	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	22	0	7	1	0
5	N	22	0	7	2	0
5	O	22	0	6	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	2	0
6	A	82	0	0	3	0
6	B	83	0	0	4	0
6	C	84	0	0	4	0
6	D	84	0	0	2	0
6	E	83	0	0	3	0
6	F	83	0	0	3	0
6	M	160	0	0	4	0
6	N	164	0	0	2	0
6	O	155	0	0	6	0
6	P	153	0	0	4	0
6	Q	163	0	0	4	0
6	R	158	0	0	2	0
All	All	22080	0	19817	655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (655) 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:P:364:LEU:HD22	2:P:440:ARG:HD3	1.16	1.14
1:E:165:GLN:H	1:E:165:GLN:NE2	1.47	1.11
1:B:18:HIS:ND1	6:B:648:HOH:O	1.83	1.09
1:F:165:GLN:H	1:F:165:GLN:NE2	1.52	1.07
1:D:18:HIS:ND1	6:D:648:HOH:O	1.88	1.07
1:B:165:GLN:H	1:B:165:GLN:NE2	1.52	1.06
1:C:133:ARG:HD2	2:O:326:THR:HG21	1.33	1.05
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.22	1.02
1:E:165:GLN:HE21	1:E:165:GLN:N	1.56	1.02
1:F:18:HIS:ND1	6:F:648:HOH:O	1.93	0.99
1:C:18:HIS:ND1	6:C:648:HOH:O	1.74	0.97
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.79	0.96
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.29	0.96
1:E:18:HIS:ND1	6:E:648:HOH:O	1.99	0.95
1:F:64:ARG:NH1	1:F:100:ASP:O	2.03	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:GLN:H	1:C:165:GLN:NE2	1.67	0.90
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.54	0.89
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.86	0.89
1:C:133:ARG:HG3	1:C:133:ARG:O	1.71	0.89
2:R:361:HIS:H	2:R:361:HIS:CD2	1.86	0.89
1:E:78:GLU:OE1	6:E:692:HOH:O	1.91	0.87
2:R:361:HIS:H	2:R:361:HIS:HD2	1.22	0.86
1:A:69:GLU:OE1	2:M:473:LYS:HE2	1.75	0.85
1:C:134:GLY:HA3	2:O:326:THR:HG22	1.60	0.84
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.06	0.83
2:O:390:LYS:HD3	6:O:677:HOH:O	1.78	0.83
1:D:64:ARG:NH1	1:D:100:ASP:O	2.12	0.83
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.61	0.82
1:F:49:ILE:HA	1:F:180:LYS:HE3	1.61	0.82
2:P:390:LYS:HE2	6:P:756:HOH:O	1.78	0.82
1:C:133:ARG:CD	2:O:326:THR:HG21	2.10	0.81
1:C:177:VAL:O	1:C:180:LYS:HB3	1.79	0.81
2:Q:361:HIS:CD2	2:Q:361:HIS:H	1.98	0.81
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.15	0.81
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.62	0.81
2:M:390:LYS:HD2	6:M:642:HOH:O	1.80	0.81
1:B:165:GLN:NE2	1:B:165:GLN:N	2.27	0.80
2:P:361:HIS:H	2:P:361:HIS:CD2	2.00	0.80
1:F:98:THR:OG1	1:F:102:GLY:N	2.14	0.80
1:B:176:GLU:HG3	1:B:180:LYS:O	1.81	0.79
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.45	0.77
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.65	0.77
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.50	0.76
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.68	0.76
1:F:165:GLN:NE2	1:F:165:GLN:N	2.32	0.76
1:D:165:GLN:NE2	1:D:165:GLN:H	1.82	0.75
1:E:131:PHE:CE1	1:E:138:HIS:HB3	2.22	0.75
1:C:98:THR:OG1	1:C:102:GLY:N	2.21	0.74
1:D:177:VAL:O	1:D:180:LYS:HB3	1.88	0.74
2:P:361:HIS:H	2:P:361:HIS:HD2	1.34	0.73
1:C:133:ARG:HD2	2:O:326:THR:CG2	2.15	0.73
1:F:50:LEU:HD12	1:F:51:LEU:N	2.04	0.72
1:F:165:GLN:H	1:F:165:GLN:HE21	1.37	0.72
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.71	0.72
1:B:165:GLN:H	1:B:165:GLN:CD	1.92	0.72
1:C:64:ARG:NH1	1:C:100:ASP:O	2.22	0.72

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:HD2	1.38	0.71
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.54	0.71
2:M:497:ASN:ND2	2:M:499:GLU:H	1.87	0.71
1:B:3:GLU:HA	1:B:3:GLU:OE1	1.90	0.71
2:O:361:HIS:H	2:O:361:HIS:CD2	2.09	0.71
1:B:98:THR:O	1:B:102:GLY:HA2	1.90	0.71
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.71	0.71
1:B:176:GLU:HG3	1:B:180:LYS:C	2.10	0.71
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.71	0.71
1:C:165:GLN:H	1:C:165:GLN:HE21	1.37	0.71
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.91	0.70
1:F:165:GLN:H	1:F:165:GLN:CD	1.94	0.70
2:R:497:ASN:HD22	2:R:499:GLU:H	1.38	0.69
1:A:98:THR:HB	1:A:100:ASP:OD1	1.91	0.69
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.39	0.69
1:A:134:GLY:CA	2:M:326:THR:HG22	2.23	0.69
2:N:361:HIS:CD2	2:N:361:HIS:H	2.11	0.69
1:E:99:PHE:HE2	2:Q:411:LYS:HE3	1.57	0.69
2:M:361:HIS:H	2:M:361:HIS:CD2	2.10	0.69
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.59	0.68
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.74	0.68
2:R:497:ASN:ND2	2:R:499:GLU:H	1.91	0.68
2:M:497:ASN:HD22	2:M:498:PRO:N	1.92	0.68
2:N:478:LEU:C	2:N:478:LEU:HD23	2.12	0.68
1:A:18:HIS:NE2	6:A:648:HOH:O	2.22	0.67
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.76	0.67
1:E:99:PHE:CE2	2:Q:411:LYS:HE3	2.29	0.67
2:R:361:HIS:CD2	2:R:361:HIS:N	2.58	0.67
2:N:497:ASN:HD22	2:N:499:GLU:H	1.43	0.67
2:Q:390:LYS:HD2	6:Q:670:HOH:O	1.95	0.66
2:O:497:ASN:HD22	2:O:499:GLU:H	1.41	0.66
2:P:497:ASN:C	2:P:497:ASN:HD22	1.99	0.66
1:B:49:ILE:HA	1:B:180:LYS:HE2	1.77	0.66
2:P:497:ASN:ND2	2:P:499:GLU:H	1.93	0.66
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.11	0.66
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.60	0.66
2:O:411:LYS:HG2	2:O:412:ASN:ND2	2.10	0.66
1:D:19:ILE:O	2:P:426:VAL:HG21	1.96	0.65
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.96	0.65
1:B:163:GLN:CB	1:B:165:GLN:HE22	2.04	0.65
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:TYR:CE1	1:B:158:LEU:HD13	2.31	0.65
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.12	0.65
1:E:131:PHE:CD1	1:E:138:HIS:HB3	2.31	0.65
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.62	0.65
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.96	0.65
1:A:100:ASP:OD1	1:A:100:ASP:N	2.27	0.65
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.61	0.65
2:Q:505:ILE:O	2:Q:507:LYS:HE3	1.97	0.65
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.78	0.65
2:N:356:PHE:HD2	2:N:428:ARG:HD3	1.61	0.64
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.33	0.64
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.45	0.64
1:D:165:GLN:H	1:D:165:GLN:HE21	1.44	0.64
2:Q:447:TYR:HE2	5:Q:550:CHB:H5	1.62	0.64
1:F:165:GLN:N	1:F:165:GLN:HE21	1.95	0.64
2:O:408:TYR:HE2	2:O:447:TYR:CZ	2.17	0.63
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.13	0.63
2:O:447:TYR:HE2	5:O:550:CHB:H5	1.64	0.63
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.33	0.63
2:O:390:LYS:HE2	6:O:800:HOH:O	1.98	0.63
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.12	0.63
1:A:165:GLN:CD	1:A:165:GLN:H	2.02	0.63
2:R:447:TYR:CE1	5:R:550:CHB:H5	2.33	0.63
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.80	0.62
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.34	0.62
1:E:98:THR:OG1	1:E:102:GLY:N	2.30	0.62
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.35	0.62
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.34	0.62
1:C:19:ILE:HG13	2:O:426:VAL:HG22	1.82	0.62
2:O:361:HIS:CG	4:O:601:BME:H21	2.34	0.62
2:N:453:PRO:HB2	2:O:310:ILE:HD12	1.81	0.62
1:E:98:THR:HB	1:E:100:ASP:OD1	1.99	0.62
2:N:448:PRO:HD3	2:N:456:TRP:CZ3	2.35	0.62
2:R:447:TYR:HE1	5:R:550:CHB:H5	1.65	0.62
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.81	0.61
1:F:98:THR:O	1:F:102:GLY:HA2	2.00	0.61
1:E:165:GLN:H	1:E:165:GLN:HE21	0.72	0.61
2:Q:390:LYS:HD3	6:Q:748:HOH:O	1.99	0.61
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.82	0.61
1:C:44:ALA:O	1:C:48:HIS:NE2	2.28	0.61
1:A:78:GLU:OE1	2:M:301:PRO:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:NH1	1:A:100:ASP:O	2.33	0.60
2:P:405:GLY:HA3	6:P:686:HOH:O	2.00	0.60
1:D:180:LYS:HG3	1:D:181:THR:N	2.14	0.60
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.01	0.60
2:M:364:LEU:HB2	2:M:440:ARG:HD3	1.83	0.60
2:N:497:ASN:ND2	2:N:499:GLU:H	1.99	0.60
2:O:497:ASN:ND2	2:O:499:GLU:H	2.00	0.60
1:F:98:THR:HB	1:F:100:ASP:OD1	2.01	0.60
1:F:143:LEU:C	1:F:143:LEU:HD23	2.20	0.60
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.16	0.60
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.84	0.60
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.36	0.60
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.65	0.60
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.02	0.60
2:R:405:GLY:HA3	6:R:682:HOH:O	2.02	0.60
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.82	0.59
2:Q:408:TYR:HE2	2:Q:447:TYR:CZ	2.20	0.59
2:P:448:PRO:HD3	2:P:456:TRP:CZ3	2.38	0.59
1:F:100:ASP:CG	1:F:101:ALA:H	2.06	0.59
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.84	0.59
1:D:99:PHE:HE2	2:P:411:LYS:HE3	1.68	0.59
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.18	0.59
1:E:177:VAL:O	1:E:180:LYS:HB3	2.02	0.59
1:A:176:GLU:HA	1:A:180:LYS:O	2.03	0.59
2:N:522:ARG:NH1	6:N:762:HOH:O	2.29	0.58
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.84	0.58
1:B:165:GLN:N	1:B:165:GLN:HE21	2.01	0.58
2:N:447:TYR:HB2	2:N:448:PRO:HD2	1.86	0.58
2:O:486:ILE:N	2:O:487:PRO:HD2	2.19	0.58
1:B:18:HIS:CG	6:B:648:HOH:O	2.43	0.57
1:F:19:ILE:HG21	2:R:410:HIS:HB2	1.85	0.57
2:O:361:HIS:H	2:O:361:HIS:HD2	1.53	0.57
1:F:18:HIS:CG	6:F:648:HOH:O	2.50	0.57
2:M:361:HIS:H	2:M:361:HIS:HD2	1.52	0.57
1:A:133:ARG:HG3	2:M:326:THR:HG21	1.86	0.57
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.39	0.57
2:M:497:ASN:HD22	2:M:497:ASN:C	2.07	0.57
2:N:361:HIS:H	2:N:361:HIS:HD2	1.49	0.57
2:O:376:GLU:O	2:O:442:ILE:HA	2.04	0.57
1:F:19:ILE:HD11	2:R:408:TYR:HD2	1.70	0.57
2:P:497:ASN:HD22	2:P:499:GLU:H	1.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:GLN:O	1:F:91:SER:HB2	2.04	0.57
1:D:110:LYS:NZ	1:D:147:ASP:OD1	2.30	0.57
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.40	0.57
2:R:408:TYR:HE1	2:R:447:TYR:CZ	2.23	0.57
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.40	0.57
1:D:100:ASP:CG	1:D:101:ALA:H	2.07	0.57
1:D:51:LEU:O	1:D:105:THR:HA	2.05	0.57
1:E:143:LEU:HD23	1:E:143:LEU:C	2.25	0.57
1:C:176:GLU:HG2	1:C:179:GLY:HA2	1.85	0.56
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.20	0.56
1:D:176:GLU:HA	1:D:180:LYS:O	2.05	0.56
2:Q:447:TYR:HB2	2:Q:448:PRO:HD2	1.86	0.56
1:C:98:THR:O	1:C:102:GLY:HA2	2.05	0.56
1:F:177:VAL:O	1:F:180:LYS:HB3	2.05	0.56
2:M:447:TYR:HB2	2:M:448:PRO:HD2	1.88	0.56
1:C:98:THR:HB	1:C:100:ASP:OD1	2.04	0.56
1:E:164:PRO:HD2	1:E:165:GLN:HE22	1.70	0.56
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.21	0.56
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	1.87	0.56
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.26	0.56
2:R:447:TYR:HB2	2:R:448:PRO:HD2	1.87	0.56
2:M:408:TYR:HE2	2:M:447:TYR:CZ	2.23	0.56
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.26	0.56
1:A:155:CYS:HB3	1:A:158:LEU:HB2	1.86	0.56
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.06	0.56
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.88	0.55
1:E:100:ASP:CG	1:E:101:ALA:H	2.09	0.55
2:O:447:TYR:CE2	5:O:550:CHB:H5	2.41	0.55
2:P:307:ARG:CG	2:P:533:THR:HG22	2.34	0.55
1:C:143:LEU:HD23	1:C:143:LEU:C	2.27	0.55
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.21	0.55
2:O:416:LEU:C	2:O:416:LEU:HD23	2.26	0.55
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.36	0.55
1:C:52:LEU:C	1:C:52:LEU:HD22	2.27	0.55
1:B:114:VAL:HG23	1:B:122:MET:HE2	1.89	0.55
2:P:442:ILE:C	2:P:442:ILE:HD12	2.27	0.55
1:E:98:THR:O	1:E:102:GLY:HA2	2.06	0.55
1:A:176:GLU:HG3	1:A:180:LYS:N	2.21	0.55
2:M:448:PRO:HB2	2:P:516:MET:HA	1.89	0.55
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.88	0.55
1:D:155:CYS:HB3	1:D:158:LEU:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.88	0.55
1:B:64:ARG:NH1	1:B:100:ASP:O	2.40	0.54
2:P:390:LYS:HD3	6:P:683:HOH:O	2.07	0.54
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.70	0.54
1:D:1:PRO:HG2	2:R:488:MET:HE1	1.88	0.54
1:D:98:THR:HB	1:D:100:ASP:OD1	2.08	0.54
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.39	0.54
1:B:176:GLU:OE2	1:B:179:GLY:O	2.24	0.54
2:P:408:TYR:HE2	2:P:447:TYR:CZ	2.26	0.54
2:R:400:TRP:HA	2:R:425:GLY:O	2.08	0.54
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.53	0.54
2:N:447:TYR:CE1	2:N:460:HIS:HE1	2.26	0.54
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.08	0.54
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.41	0.54
1:B:52:LEU:C	1:B:52:LEU:HD22	2.29	0.53
1:B:140:HIS:O	1:B:197:PHE:HA	2.08	0.53
2:O:316:HIS:HB3	2:O:317:PRO:HD2	1.90	0.53
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.08	0.53
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.72	0.53
2:P:497:ASN:HD22	2:P:498:PRO:N	2.06	0.53
1:C:100:ASP:OD1	1:C:100:ASP:N	2.42	0.53
2:Q:447:TYR:CE1	2:Q:460:HIS:HE1	2.26	0.53
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.44	0.53
2:R:522:ARG:NH1	6:R:716:HOH:O	2.40	0.53
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.91	0.52
1:B:33:GLN:CG	1:B:85:LEU:HD12	2.39	0.52
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.90	0.52
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.42	0.52
1:F:176:GLU:HA	1:F:180:LYS:O	2.09	0.52
2:N:359:HIS:O	2:N:366:ASN:HB3	2.09	0.52
1:C:84:ASN:OD1	1:C:86:GLU:HB2	2.09	0.52
1:D:98:THR:O	1:D:102:GLY:HA2	2.08	0.52
2:O:486:ILE:N	2:O:487:PRO:CD	2.73	0.52
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.24	0.52
2:R:505:ILE:HG22	2:R:507:LYS:HE2	1.91	0.52
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.92	0.52
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.40	0.52
1:F:131:PHE:O	1:F:132:ALA:HB2	2.10	0.52
1:B:50:LEU:O	1:B:182:ALA:HA	2.10	0.52
2:O:373:PRO:HB3	2:O:423:PHE:HB2	1.90	0.52
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD12	1:A:106:LEU:HD23	1.91	0.51
2:N:315:TRP:HZ2	2:N:503:GLN:NE2	2.08	0.51
1:D:54:GLN:HG3	1:D:184:ARG:NH2	2.25	0.51
1:C:100:ASP:CG	1:C:101:ALA:H	2.13	0.51
1:E:144:TYR:CE1	1:E:158:LEU:HD13	2.45	0.51
2:P:376:GLU:O	2:P:442:ILE:HA	2.11	0.51
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.91	0.51
2:Q:326:THR:HG22	2:Q:330:ARG:HD2	1.91	0.51
1:F:100:ASP:OD1	1:F:100:ASP:N	2.40	0.51
1:D:165:GLN:HE21	1:D:165:GLN:N	2.09	0.51
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.46	0.51
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.76	0.51
2:P:359:HIS:O	2:P:366:ASN:HB3	2.11	0.51
2:P:416:LEU:C	2:P:416:LEU:HD23	2.30	0.51
2:M:376:GLU:O	2:M:442:ILE:HA	2.11	0.51
2:P:326:THR:CG2	2:P:330:ARG:HD2	2.41	0.51
1:E:165:GLN:NE2	1:E:165:GLN:N	2.33	0.51
1:C:18:HIS:HA	1:C:22:ALA:HB3	1.93	0.51
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.41	0.51
2:O:308:PHE:CE2	2:O:530:GLN:HB2	2.45	0.51
1:E:52:LEU:HD23	1:E:103:GLU:CD	2.31	0.51
2:M:383:ARG:HD2	2:M:436:TYR:CZ	2.46	0.51
1:D:99:PHE:CE2	2:P:411:LYS:HE3	2.44	0.51
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	1.92	0.51
1:C:28:ASN:HB3	6:C:817:HOH:O	2.10	0.51
1:D:16:TYR:O	1:D:19:ILE:HG23	2.11	0.51
1:D:98:THR:OG1	1:D:102:GLY:N	2.40	0.51
2:M:495:ILE:HG21	2:M:500:ALA:HB3	1.93	0.50
2:P:447:TYR:HB2	2:P:448:PRO:HD2	1.92	0.50
2:P:478:LEU:C	2:P:478:LEU:HD23	2.31	0.50
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.92	0.50
1:A:100:ASP:CG	1:A:101:ALA:H	2.13	0.50
1:F:38:ARG:HA	1:F:107:HIS:HB2	1.93	0.50
1:C:19:ILE:O	2:O:426:VAL:HG21	2.11	0.50
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.45	0.50
2:P:442:ILE:HD12	2:P:442:ILE:O	2.11	0.50
1:E:161:ILE:O	1:E:167:ARG:NH2	2.44	0.50
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.11	0.50
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.14	0.50
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.50
2:P:400:TRP:HA	2:P:425:GLY:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.09	0.50
1:F:44:ALA:O	1:F:48:HIS:NE2	2.31	0.50
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.94	0.50
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.41	0.50
2:M:505:ILE:HG22	2:M:507:LYS:HE2	1.94	0.50
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.42	0.50
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.27	0.49
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.93	0.49
1:B:143:LEU:C	1:B:143:LEU:HD23	2.32	0.49
2:N:376:GLU:O	2:N:442:ILE:HA	2.12	0.49
2:O:408:TYR:CE2	2:O:447:TYR:CZ	3.00	0.49
1:E:35:ILE:HG21	1:E:92:PHE:HE1	1.76	0.49
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.94	0.49
1:A:28:ASN:HB3	6:A:817:HOH:O	2.12	0.49
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.95	0.49
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.93	0.49
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.49
1:A:78:GLU:HG2	2:M:301:PRO:HG3	1.94	0.49
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.47	0.49
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.47	0.49
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.93	0.49
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.95	0.49
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.94	0.49
2:N:447:TYR:HE2	5:N:550:CHB:H5	1.78	0.49
1:C:19:ILE:HG12	2:O:400:TRP:HB2	1.93	0.49
1:D:18:HIS:CG	6:D:648:HOH:O	2.48	0.49
2:P:414:ARG:NE	2:P:414:ARG:HA	2.28	0.49
2:Q:405:GLY:HA3	6:Q:673:HOH:O	2.13	0.49
2:P:325:LYS:HG2	2:Q:335:ALA:HB1	1.94	0.49
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.13	0.49
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.95	0.49
1:E:131:PHE:O	1:E:132:ALA:HB2	2.12	0.49
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.95	0.49
2:N:447:TYR:CE2	5:N:550:CHB:H5	2.48	0.48
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.12	0.48
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.42	0.48
1:A:50:LEU:O	1:A:182:ALA:HA	2.13	0.48
1:A:98:THR:O	1:A:102:GLY:HA2	2.13	0.48
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.95	0.48
2:M:361:HIS:CG	4:M:601:BME:H21	2.48	0.48
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:416:LEU:HD23	2:N:416:LEU:C	2.32	0.48
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.95	0.48
1:F:176:GLU:HG3	1:F:180:LYS:N	2.28	0.48
1:A:176:GLU:HG3	1:A:180:LYS:O	2.13	0.48
2:M:318:LYS:HD3	2:M:318:LYS:HA	1.50	0.48
1:B:98:THR:HB	1:B:100:ASP:OD1	2.14	0.48
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.96	0.48
2:N:360:ASP:OD2	2:N:428:ARG:HD2	2.14	0.48
2:O:364:LEU:HB2	2:O:440:ARG:HD3	1.96	0.48
2:P:411:LYS:O	2:P:414:ARG:NH1	2.46	0.48
2:P:489:CYS:HB3	2:P:492:VAL:HB	1.96	0.48
1:E:61:HIS:CE1	1:F:163:GLN:HG3	2.49	0.48
1:E:64:ARG:NH1	1:E:100:ASP:O	2.45	0.48
1:E:131:PHE:CE1	1:E:138:HIS:CB	2.95	0.48
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.48	0.48
1:C:165:GLN:HE21	1:C:165:GLN:N	2.07	0.48
2:O:447:TYR:CE1	2:O:460:HIS:HE1	2.32	0.48
1:D:54:GLN:HG3	1:D:184:ARG:HH22	1.79	0.48
1:E:52:LEU:O	1:E:184:ARG:HA	2.14	0.48
1:F:50:LEU:O	1:F:182:ALA:HA	2.14	0.48
1:A:52:LEU:O	1:A:184:ARG:HA	2.14	0.47
1:A:180:LYS:HG3	1:A:181:THR:N	2.29	0.47
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.79	0.47
1:B:176:GLU:HA	1:B:180:LYS:O	2.12	0.47
2:P:473:LYS:HD2	2:P:474:LEU:N	2.29	0.47
2:Q:438:SER:O	4:Q:601:BME:H22	2.14	0.47
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.34	0.47
2:M:522:ARG:NH1	6:M:666:HOH:O	2.31	0.47
1:D:134:GLY:HA3	2:P:326:THR:CG2	2.40	0.47
1:D:143:LEU:C	1:D:143:LEU:HD23	2.35	0.47
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.75	0.47
1:E:114:VAL:HG23	1:E:122:MET:CE	2.44	0.47
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.96	0.47
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.29	0.47
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.50	0.47
2:O:403:ASN:HB2	6:O:620:HOH:O	2.15	0.47
1:D:191:GLY:O	1:D:194:GLU:HB2	2.13	0.47
2:R:437:TYR:CD1	2:R:437:TYR:C	2.87	0.47
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.50	0.47
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.96	0.47
1:F:49:ILE:CA	1:F:180:LYS:HE3	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:356:PHE:HD2	2:P:428:ARG:HD3	1.79	0.47
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.95	0.47
2:Q:447:TYR:CE2	5:Q:550:CHB:H5	2.46	0.47
2:R:359:HIS:O	2:R:366:ASN:HB3	2.15	0.47
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.80	0.47
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.45	0.47
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.15	0.47
2:M:416:LEU:C	2:M:416:LEU:HD23	2.35	0.47
1:F:69:GLU:OE2	1:F:94:ARG:HD3	2.15	0.47
1:F:114:VAL:HG23	1:F:122:MET:CE	2.45	0.47
2:M:399:MET:HA	2:M:462:HIS:O	2.15	0.47
2:M:465:ILE:HG12	2:M:525:ILE:HD13	1.96	0.47
1:D:52:LEU:C	1:D:52:LEU:HD22	2.35	0.47
1:E:140:HIS:O	1:E:197:PHE:HA	2.14	0.47
2:M:473:LYS:NZ	6:M:652:HOH:O	2.48	0.46
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.97	0.46
2:Q:447:TYR:OH	2:Q:460:HIS:CE1	2.67	0.46
2:Q:488:MET:CE	1:F:1:PRO:HG2	2.45	0.46
2:R:306:SER:CB	2:R:530:GLN:HE21	2.28	0.46
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.96	0.46
1:E:176:GLU:HA	1:E:180:LYS:O	2.16	0.46
2:M:381:ALA:O	2:M:522:ARG:HA	2.15	0.46
2:M:488:MET:HE2	1:B:1:PRO:HG2	1.96	0.46
2:P:392:VAL:HG12	2:P:395:THR:HB	1.95	0.46
2:Q:447:TYR:CE1	2:Q:460:HIS:CE1	3.03	0.46
2:M:438:SER:O	4:M:601:BME:H22	2.15	0.46
2:M:448:PRO:CB	2:P:516:MET:HA	2.46	0.46
1:B:74:ASP:HB2	6:B:690:HOH:O	2.16	0.46
1:B:180:LYS:HD2	1:B:181:THR:H	1.81	0.46
2:Q:465:ILE:HD12	2:Q:465:ILE:N	2.29	0.46
2:M:361:HIS:CD2	2:M:361:HIS:N	2.81	0.46
1:C:11:GLN:HB2	2:O:477:GLN:HG3	1.97	0.46
2:N:497:ASN:HD22	2:N:497:ASN:C	2.18	0.46
2:R:341:GLN:HB3	2:R:346:THR:CG2	2.46	0.46
2:N:414:ARG:NE	2:N:414:ARG:HA	2.30	0.46
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.16	0.46
2:M:519:LEU:HD21	2:P:456:TRP:CG	2.50	0.46
2:P:484:PRO:O	2:P:487:PRO:HD2	2.16	0.46
1:E:51:LEU:HD12	1:E:106:LEU:CD2	2.45	0.46
2:M:386:ASP:HA	2:M:527:LEU:O	2.16	0.46
2:R:497:ASN:HD22	2:R:497:ASN:C	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:505:ILE:O	2:R:507:LYS:HE3	2.16	0.46
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.78	0.45
1:E:50:LEU:O	1:E:182:ALA:HA	2.16	0.45
1:F:162:GLU:O	1:F:164:PRO:HD3	2.15	0.45
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.64	0.45
2:R:522:ARG:HE	2:R:524:ASP:CG	2.20	0.45
2:M:361:HIS:ND1	4:M:601:BME:H21	2.32	0.45
2:M:385:VAL:O	2:M:526:VAL:HA	2.16	0.45
1:B:180:LYS:HD2	1:B:181:THR:N	2.31	0.45
2:R:385:VAL:O	2:R:526:VAL:HA	2.15	0.45
1:C:110:LYS:NZ	1:C:147:ASP:OD1	2.49	0.45
1:D:39:LEU:HB3	1:D:90:ASN:O	2.17	0.45
2:R:408:TYR:HE1	2:R:447:TYR:CE2	2.34	0.45
2:M:516:MET:HA	2:P:448:PRO:HB2	1.98	0.45
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.52	0.45
1:D:15:PRO:HB3	1:D:133:ARG:HD3	1.99	0.45
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.99	0.45
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.47	0.45
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.31	0.45
2:N:381:ALA:O	2:N:522:ARG:HA	2.17	0.45
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.51	0.45
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.81	0.45
1:F:77:GLY:O	1:F:114:VAL:HG12	2.16	0.45
2:R:416:LEU:C	2:R:416:LEU:HD23	2.37	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.81	0.45
2:P:443:LYS:HE2	2:P:480:PHE:CG	2.52	0.45
1:E:180:LYS:HD2	1:E:181:THR:O	2.17	0.45
1:B:165:GLN:N	1:B:165:GLN:CD	2.67	0.45
1:A:19:ILE:HD11	2:M:408:TYR:HD1	1.81	0.45
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.99	0.45
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.98	0.45
1:D:164:PRO:O	1:D:167:ARG:HB2	2.17	0.45
2:Q:522:ARG:HD3	6:Q:694:HOH:O	2.16	0.45
2:O:361:HIS:CD2	6:O:866:HOH:O	2.70	0.44
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.47	0.44
2:M:515:PRO:HB3	2:P:453:PRO:O	2.17	0.44
1:D:176:GLU:CG	1:D:179:GLY:HA2	2.48	0.44
2:P:360:ASP:O	2:P:427:GLY:HA2	2.18	0.44
1:E:51:LEU:HB2	1:E:106:LEU:HB3	2.00	0.44
2:Q:408:TYR:CE2	2:Q:447:TYR:CZ	3.04	0.44
1:F:50:LEU:HD12	1:F:51:LEU:H	1.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:373:PRO:HB3	2:R:423:PHE:HB2	2.00	0.44
2:M:478:LEU:HD23	2:M:478:LEU:C	2.37	0.44
1:D:63:VAL:HG12	1:D:66:SER:HB3	1.98	0.44
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.32	0.44
2:P:381:ALA:O	2:P:522:ARG:HA	2.17	0.44
1:B:114:VAL:HG23	1:B:122:MET:CE	2.48	0.44
2:O:313:ARG:O	2:O:318:LYS:HE2	2.17	0.44
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.17	0.44
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.99	0.44
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.82	0.44
1:E:44:ALA:O	1:E:48:HIS:NE2	2.32	0.44
1:F:174:ARG:HE	1:F:181:THR:HG23	1.83	0.44
1:B:28:ASN:HB3	6:B:817:HOH:O	2.17	0.44
1:D:84:ASN:OD1	1:D:86:GLU:HB2	2.18	0.44
2:P:373:PRO:HB3	2:P:423:PHE:HB2	1.99	0.44
1:F:57:ASP:OD1	1:F:59:ASN:N	2.48	0.44
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.47	0.44
2:M:447:TYR:CE1	2:M:460:HIS:HE1	2.36	0.44
2:M:497:ASN:HD22	2:M:498:PRO:CD	2.31	0.44
2:O:484:PRO:O	2:O:487:PRO:HD2	2.18	0.44
2:P:356:PHE:CD2	2:P:428:ARG:HD3	2.52	0.44
2:Q:486:ILE:N	2:Q:487:PRO:HD2	2.33	0.44
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.48	0.44
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.98	0.44
1:E:22:ALA:O	1:E:25:ALA:HB3	2.18	0.44
1:F:155:CYS:HB3	1:F:158:LEU:HB2	2.00	0.44
1:C:134:GLY:CA	2:O:326:THR:HG22	2.41	0.43
1:C:180:LYS:HD2	1:C:181:THR:N	2.33	0.43
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.52	0.43
2:M:400:TRP:HA	2:M:425:GLY:O	2.18	0.43
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.66	0.43
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.53	0.43
1:B:19:ILE:O	2:N:426:VAL:HG21	2.17	0.43
2:O:415:TYR:CE1	2:O:416:LEU:HD22	2.52	0.43
1:D:172:ALA:HB1	1:D:183:TYR:HB3	1.99	0.43
2:P:484:PRO:O	2:P:488:MET:CE	2.66	0.43
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.77	0.43
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.72	0.43
1:F:184:ARG:NH1	1:F:184:ARG:HG3	2.33	0.43
1:C:19:ILE:HG21	1:C:19:ILE:HD13	1.78	0.43
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:335:ALA:HB2	2:R:328:ILE:HD12	2.01	0.43
2:P:341:GLN:HB3	2:P:346:THR:CG2	2.49	0.43
2:P:437:TYR:CD1	2:P:437:TYR:C	2.92	0.43
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.66	0.43
2:R:486:ILE:N	2:R:487:PRO:HD2	2.33	0.43
2:N:405:GLY:HA3	6:N:742:HOH:O	2.18	0.43
1:F:30:THR:HB	1:F:34:GLU:HG3	2.01	0.43
1:A:12:THR:HA	1:A:135:ILE:O	2.18	0.43
1:A:54:GLN:HG3	1:A:184:ARG:HH22	1.83	0.43
1:C:176:GLU:HG2	1:C:179:GLY:CA	2.49	0.43
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.53	0.43
2:R:505:ILE:HG22	2:R:507:LYS:CE	2.48	0.43
1:A:41:LYS:O	1:A:48:HIS:HE1	2.02	0.43
1:B:64:ARG:HD3	1:B:99:PHE:O	2.18	0.43
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.54	0.43
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.77	0.43
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.88	0.43
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.92	0.43
2:M:400:TRP:CZ2	2:M:462:HIS:HB3	2.53	0.43
2:M:497:ASN:ND2	2:M:497:ASN:C	2.72	0.43
2:P:307:ARG:HD2	6:P:695:HOH:O	2.19	0.43
1:A:54:GLN:HG3	1:A:184:ARG:NH2	2.34	0.42
2:N:488:MET:HE1	1:C:1:PRO:CG	2.49	0.42
1:D:19:ILE:HG21	1:D:19:ILE:HD13	1.53	0.42
2:Q:447:TYR:CZ	2:Q:460:HIS:HE1	2.37	0.42
1:F:32:ASP:HB2	6:F:820:HOH:O	2.19	0.42
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.92	0.42
1:C:19:ILE:O	2:O:426:VAL:CG2	2.67	0.42
1:E:18:HIS:CG	6:E:648:HOH:O	2.60	0.42
1:E:113:VAL:HG13	1:E:122:MET:O	2.19	0.42
2:R:450:ARG:HH11	2:R:450:ARG:HD2	1.65	0.42
1:A:114:VAL:HG23	1:A:122:MET:CE	2.49	0.42
1:A:165:GLN:NE2	1:A:165:GLN:H	2.17	0.42
1:B:12:THR:HA	1:B:135:ILE:O	2.20	0.42
2:O:409:ARG:HD3	6:O:864:HOH:O	2.20	0.42
1:A:114:VAL:HG23	1:A:122:MET:HE2	2.01	0.42
1:A:143:LEU:HD12	1:A:185:PHE:CG	2.55	0.42
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.89	0.42
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.79	0.42
1:C:165:GLN:H	1:C:165:GLN:CD	2.19	0.42
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:399:MET:HA	2:Q:462:HIS:O	2.19	0.42
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.71	0.42
1:D:4:LEU:HB3	2:P:387:GLN:HB3	2.01	0.42
2:N:478:LEU:C	2:N:478:LEU:CD2	2.85	0.42
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.00	0.42
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.20	0.42
1:B:58:GLY:CA	1:B:190:GLN:HB3	2.49	0.42
1:C:18:HIS:CD2	1:C:22:ALA:HB3	2.55	0.42
1:C:39:LEU:HD11	1:C:93:GLY:HA3	2.02	0.42
1:C:180:LYS:HD2	1:C:181:THR:H	1.85	0.42
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.35	0.42
1:D:18:HIS:HD2	1:D:22:ALA:HB3	1.85	0.42
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	2.02	0.42
1:F:198:PHE:HA	2:R:337:VAL:O	2.20	0.42
2:M:497:ASN:HD22	2:M:499:GLU:H	1.63	0.42
2:M:505:ILE:O	2:M:507:LYS:HE3	2.20	0.42
2:N:333:ARG:HD3	2:N:333:ARG:HA	1.99	0.42
2:O:413:ASP:C	2:O:414:ARG:HD2	2.40	0.42
1:D:176:GLU:HG3	1:D:179:GLY:HA2	2.02	0.42
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.84	0.42
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.55	0.42
2:R:434:ASP:HB3	2:R:436:TYR:CE2	2.55	0.42
2:M:307:ARG:NE	2:M:536:GLU:OE2	2.48	0.42
2:N:315:TRP:CZ2	2:N:503:GLN:NE2	2.85	0.42
2:P:443:LYS:HE2	2:P:480:PHE:CD2	2.55	0.42
2:R:399:MET:HA	2:R:462:HIS:O	2.19	0.42
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.88	0.41
1:C:176:GLU:CG	1:C:179:GLY:HA2	2.48	0.41
2:O:381:ALA:O	2:O:522:ARG:HA	2.20	0.41
2:Q:363:LEU:N	2:Q:363:LEU:HD12	2.35	0.41
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.17	0.41
1:F:52:LEU:HA	1:F:104:TRP:O	2.20	0.41
1:A:168:GLU:HA	1:A:171:ILE:HD12	2.00	0.41
1:D:114:VAL:HG23	1:D:122:MET:CE	2.50	0.41
1:E:35:ILE:HG21	1:E:92:PHE:CE1	2.54	0.41
1:F:19:ILE:O	2:R:426:VAL:HG21	2.20	0.41
1:F:158:LEU:HA	1:F:158:LEU:HD12	1.75	0.41
1:F:176:GLU:HG3	1:F:180:LYS:H	1.84	0.41
1:F:177:VAL:N	1:F:180:LYS:O	2.46	0.41
1:C:19:ILE:CG1	2:O:400:TRP:HB2	2.49	0.41
1:C:114:VAL:HG23	1:C:122:MET:HE2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ALA:HB3	1:C:144:TYR:CE2	2.55	0.41
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.90	0.41
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.77	0.41
5:M:550:CHB:C4	6:M:742:HOH:O	2.68	0.41
1:D:132:ALA:HB3	1:D:135:ILE:HD12	2.01	0.41
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.88	0.41
1:B:100:ASP:OD1	1:B:100:ASP:N	2.49	0.41
6:C:697:HOH:O	2:O:426:VAL:HG21	2.20	0.41
2:O:326:THR:CG2	2:O:330:ARG:HD2	2.50	0.41
2:P:447:TYR:CE2	2:P:460:HIS:HE1	2.38	0.41
1:F:114:VAL:HG23	1:F:122:MET:HE2	2.02	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.90	0.41
1:A:147:ASP:OD2	1:A:174:ARG:HD2	2.21	0.41
2:M:404:ALA:HB2	2:M:442:ILE:HD13	2.02	0.41
1:C:4:LEU:HB3	2:O:387:GLN:HB3	2.03	0.41
1:D:165:GLN:H	1:D:165:GLN:CD	2.24	0.41
1:E:5:LEU:O	2:Q:387:GLN:HG2	2.20	0.41
2:R:364:LEU:CD1	2:R:442:ILE:HG23	2.50	0.41
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.55	0.41
1:A:18:HIS:CE1	1:A:99:PHE:CE1	3.09	0.41
2:N:486:ILE:N	2:N:487:PRO:HD2	2.36	0.41
1:C:51:LEU:HB2	1:C:106:LEU:HB3	2.02	0.41
1:A:18:HIS:CE1	6:A:648:HOH:O	2.70	0.41
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.16	0.41
2:M:359:HIS:O	2:M:366:ASN:HB3	2.21	0.41
2:O:399:MET:HA	2:O:462:HIS:O	2.20	0.41
1:D:36:TRP:HA	1:D:36:TRP:CE3	2.56	0.41
2:P:489:CYS:C	2:P:493:LYS:HE3	2.41	0.41
2:P:497:ASN:C	2:P:497:ASN:ND2	2.71	0.41
1:E:33:GLN:HG2	1:E:85:LEU:HD12	2.03	0.41
2:Q:321:THR:HG21	2:Q:494:SER:HB2	2.03	0.41
2:Q:378:ILE:O	2:Q:378:ILE:HG13	2.21	0.41
1:F:180:LYS:HD2	1:F:181:THR:H	1.85	0.41
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.51	0.41
1:C:18:HIS:HD2	1:C:22:ALA:HB3	1.86	0.41
1:C:50:LEU:O	1:C:182:ALA:HA	2.21	0.41
2:O:390:LYS:CE	6:O:800:HOH:O	2.65	0.41
1:D:18:HIS:CD2	1:D:22:ALA:HB3	2.56	0.41
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.56	0.41
1:E:51:LEU:HD11	1:E:126:ILE:HD12	2.02	0.41
2:R:361:HIS:CG	4:R:601:BME:H21	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:OD1	1:A:86:GLU:HB2	2.21	0.40
1:C:18:HIS:CG	6:C:648:HOH:O	2.51	0.40
1:E:61:HIS:CG	1:F:163:GLN:HG3	2.55	0.40
1:E:65:ASP:OD2	1:E:133:ARG:NH1	2.45	0.40
1:E:84:ASN:OD1	1:E:86:GLU:HB2	2.22	0.40
1:F:19:ILE:HG22	1:F:26:ALA:HB1	2.03	0.40
1:B:36:TRP:CE3	1:B:36:TRP:HA	2.56	0.40
2:O:361:HIS:CD2	2:O:361:HIS:N	2.81	0.40
1:D:70:VAL:HG12	1:D:128:ILE:HG12	2.03	0.40
1:F:180:LYS:HD2	1:F:181:THR:N	2.36	0.40
1:A:33:GLN:HG2	1:A:85:LEU:HD12	2.02	0.40
2:M:400:TRP:CE2	2:M:462:HIS:CB	3.05	0.40
2:M:431:THR:HA	2:M:436:TYR:O	2.21	0.40
1:B:78:GLU:HB3	2:N:301:PRO:HB3	2.02	0.40
1:A:155:CYS:O	1:A:159:ASN:ND2	2.30	0.40
1:E:33:GLN:OE1	2:Q:354:LEU:HD12	2.21	0.40
2:Q:394:ASN:HD22	2:Q:394:ASN:HA	1.61	0.40
1:F:18:HIS:ND1	1:F:99:PHE:HZ	2.19	0.40
1:F:36:TRP:CG	1:F:37:ASN:N	2.90	0.40
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.89	0.40
2:M:392:VAL:HG12	2:M:395:THR:HB	2.04	0.40
2:O:385:VAL:O	2:O:526:VAL:HA	2.21	0.40
2:P:390:LYS:HA	2:P:391:PRO:HD3	1.98	0.40
1:E:110:LYS:HE2	1:E:148:GLU:OE2	2.22	0.40
2:R:420:ASP:HA	2:R:421:PRO:HD2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	198/200 (99%)	193 (98%)	5 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	D	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	E	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	M	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	R	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
All	All	2562/2628 (98%)	2480 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	34	27
1	B	162/163 (99%)	154 (95%)	8 (5%)	25	17
1	C	162/163 (99%)	156 (96%)	6 (4%)	34	27
1	D	162/163 (99%)	154 (95%)	8 (5%)	25	17
1	E	162/163 (99%)	155 (96%)	7 (4%)	29	22
1	F	162/163 (99%)	156 (96%)	6 (4%)	34	27
2	M	196/202 (97%)	185 (94%)	11 (6%)	21	12
2	N	196/202 (97%)	187 (95%)	9 (5%)	27	19
2	O	196/202 (97%)	187 (95%)	9 (5%)	27	19
2	P	196/202 (97%)	187 (95%)	9 (5%)	27	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	196/202 (97%)	187 (95%)	9 (5%)	27	19
2	R	196/202 (97%)	188 (96%)	8 (4%)	30	23
All	All	2148/2190 (98%)	2052 (96%)	96 (4%)	27	20

All (96) 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	165	GLN
1	A	192	GLU
2	M	301	PRO
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	428	ARG
2	M	434	ASP
2	M	440	ARG
2	M	473	LYS
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	106	LEU
1	B	165	GLN
1	B	184	ARG
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	433	SER
2	N	478	LEU
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	133	ARG
1	C	165	GLN
2	O	372	LEU
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	440	ARG
2	O	497	ASN
2	O	503	GLN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	91	SER
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	372	LEU
2	P	395	THR
2	P	399	MET
2	P	414	ARG
2	P	416	LEU
2	P	428	ARG
2	P	434	ASP
2	P	497	ASN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	32	ASP
1	E	38	ARG
1	E	52	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	301	PRO
2	Q	395	THR
2	Q	416	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	428	ARG
2	Q	434	ASP
2	Q	497	ASN
2	Q	499	GLU
2	Q	507	LYS
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	143	LEU
1	F	165	GLN
1	F	180	LYS
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	434	ASP
2	R	473	LYS
2	R	497	ASN
2	R	503	GLN
2	R	507	LYS

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	163	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	394	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	534	HIS
1	F	80	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	497	ASN
2	R	503	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	CHB	N	550	2,3	11,11,11	1.06	1 (9%)	15,15,15	0.99	1 (6%)
4	BME	N	601	2	3,3,3	0.16	0	1,2,2	0.30	0
4	BME	O	601	2	3,3,3	0.43	0	1,2,2	0.30	0
4	BME	R	601	2	3,3,3	0.65	0	1,2,2	1.64	0
5	CHB	O	550	3	11,11,11	1.18	2 (18%)	15,15,15	1.08	1 (6%)
5	CHB	Q	551	-	11,11,11	1.27	2 (18%)	15,15,15	1.01	0
4	BME	P	601	2	3,3,3	0.83	0	1,2,2	1.42	0
5	CHB	P	550	3	11,11,11	1.34	2 (18%)	15,15,15	1.00	0
5	CHB	P	551	-	11,11,11	1.30	2 (18%)	15,15,15	0.98	1 (6%)
5	CHB	M	551	-	11,11,11	1.13	2 (18%)	15,15,15	1.04	1 (6%)
5	CHB	N	551	-	11,11,11	1.25	1 (9%)	15,15,15	1.27	2 (13%)
5	CHB	O	551	-	11,11,11	1.26	2 (18%)	15,15,15	1.16	2 (13%)
5	CHB	R	550	2,3	11,11,11	1.14	1 (9%)	15,15,15	0.81	0
5	CHB	R	551	-	11,11,11	1.15	1 (9%)	15,15,15	0.96	1 (6%)
4	BME	Q	601	2	3,3,3	0.63	0	1,2,2	0.47	0
4	BME	M	601	2	3,3,3	0.32	0	1,2,2	0.33	0
5	CHB	Q	550	3	11,11,11	1.22	2 (18%)	15,15,15	1.13	2 (13%)
5	CHB	M	550	3	11,11,11	1.13	1 (9%)	15,15,15	0.85	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	CHB	N	550	2,3	-	0/4/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	-
4	BME	O	601	2	-	1/1/1/1	-
4	BME	R	601	2	-	0/1/1/1	-
5	CHB	O	550	3	-	0/4/4/4	0/1/1/1
5	CHB	Q	551	-	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
5	CHB	P	550	3	-	0/4/4/4	0/1/1/1
5	CHB	P	551	-	-	0/4/4/4	0/1/1/1
5	CHB	M	551	-	-	0/4/4/4	0/1/1/1
5	CHB	N	551	-	-	0/4/4/4	0/1/1/1
5	CHB	O	551	-	-	0/4/4/4	0/1/1/1
5	CHB	R	550	2,3	-	0/4/4/4	0/1/1/1
5	CHB	R	551	-	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	M	601	2	-	0/1/1/1	-
5	CHB	Q	550	3	-	0/4/4/4	0/1/1/1
5	CHB	M	550	3	-	0/4/4/4	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	CHB	O2-C7	-2.84	1.21	1.30
5	R	551	CHB	C1-C7	2.69	1.55	1.49
5	R	550	CHB	C1-C7	2.65	1.55	1.49
5	Q	551	CHB	C1-C7	2.62	1.55	1.49
5	Q	550	CHB	C1-C7	2.55	1.54	1.49
5	P	551	CHB	C1-C7	2.53	1.54	1.49
5	O	550	CHB	O2-C7	-2.51	1.22	1.30
5	P	550	CHB	C1-C7	2.48	1.54	1.49
5	N	550	CHB	C1-C7	2.32	1.54	1.49
5	N	551	CHB	C1-C7	2.31	1.54	1.49
5	O	551	CHB	C1-C7	2.20	1.54	1.49
5	Q	551	CHB	O2-C7	-2.18	1.23	1.30
5	M	551	CHB	C1-C7	2.18	1.54	1.49
5	O	551	CHB	O2-C7	-2.18	1.23	1.30
5	O	550	CHB	C1-C7	2.18	1.54	1.49
5	M	550	CHB	C2-C1	2.04	1.42	1.39
5	Q	550	CHB	O2-C7	-2.02	1.24	1.30
5	M	551	CHB	O2-C7	-2.01	1.24	1.30
5	P	551	CHB	O2-C7	-2.01	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	551	CHB	O2-C7-O1	-3.10	116.47	123.35
5	N	551	CHB	O2-C7-C1	2.88	122.32	114.85
5	O	550	CHB	C5-C4-C3	2.62	121.09	118.55
5	Q	550	CHB	C5-C4-C3	2.48	120.96	118.55
5	P	551	CHB	O2-C7-C1	2.40	121.08	114.85
5	R	551	CHB	O2-C7-C1	2.30	120.81	114.85
5	O	551	CHB	O2-C7-C1	2.26	120.72	114.85
5	O	551	CHB	C5-C4-C3	2.15	120.64	118.55
5	N	550	CHB	C5-C4-C3	2.02	120.52	118.55
5	M	551	CHB	O2-C7-C1	2.02	120.08	114.85
5	Q	550	CHB	C2-C3-C4	-2.01	119.75	120.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	601	BME	O1-C1-C2-S2

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	550	CHB	2	0
4	O	601	BME	1	0
4	R	601	BME	1	0
5	O	550	CHB	2	0
5	R	550	CHB	2	0
4	Q	601	BME	2	0
4	M	601	BME	3	0
5	Q	550	CHB	2	0
5	M	550	CHB	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.