



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:26 AM UTC

PDB ID : 3PCC / pdb_00003pcc
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 4-HYDROXYBENZOATE
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-04-29
Resolution : 1.98 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

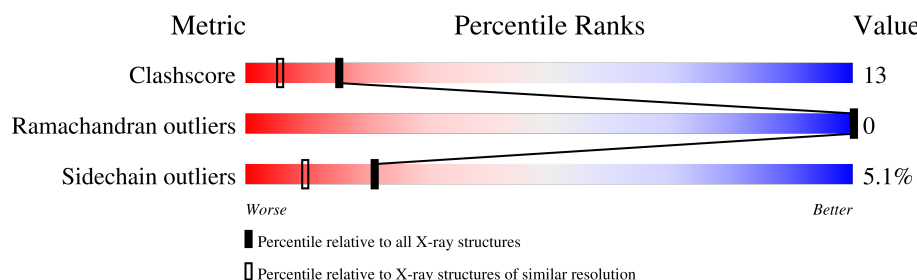
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	72% 23% . .
1	B	200	63% 30% 5% .
1	C	200	68% 26% 5% .
1	D	200	64% 28% 7%
1	E	200	62% 31% 6% .
1	F	200	60% 31% 8%
2	M	238	71% 21% 5% .
2	N	238	67% 27% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	238	 71% 21% 6% •
2	P	238	 71% 21% 6% ••
2	Q	238	 67% 25% 5% ••
2	R	238	 66% 26% 6% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22062 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			

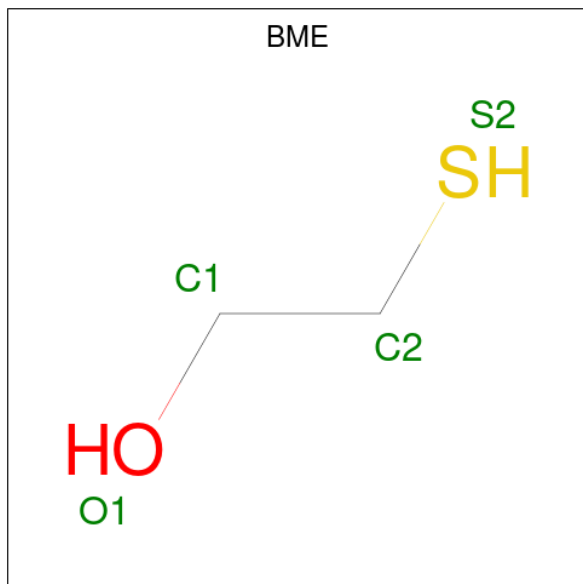
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 (CCD ID: FE) (formula: Fe).

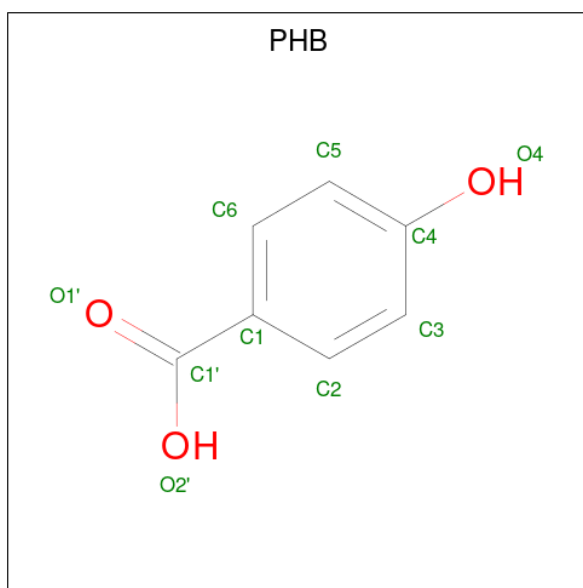
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: 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 P-HYDROXYBENZOIC ACID (CCD ID: PHB) (formula: $C_7H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	0
			10	7	3		
5	M	1	Total	C	O	0	0
			10	7	3		
5	N	1	Total	C	O	0	0
			10	7	3		
5	N	1	Total	C	O	0	0
			10	7	3		
5	O	1	Total	C	O	0	0
			10	7	3		
5	O	1	Total	C	O	0	0
			10	7	3		
5	P	1	Total	C	O	0	0
			10	7	3		
5	P	1	Total	C	O	0	0
			10	7	3		
5	Q	1	Total	C	O	0	0
			10	7	3		
5	Q	1	Total	C	O	0	0
			10	7	3		
5	R	1	Total	C	O	0	0
			10	7	3		
5	R	1	Total	C	O	0	0
			10	7	3		

- Molecule 6 is water.

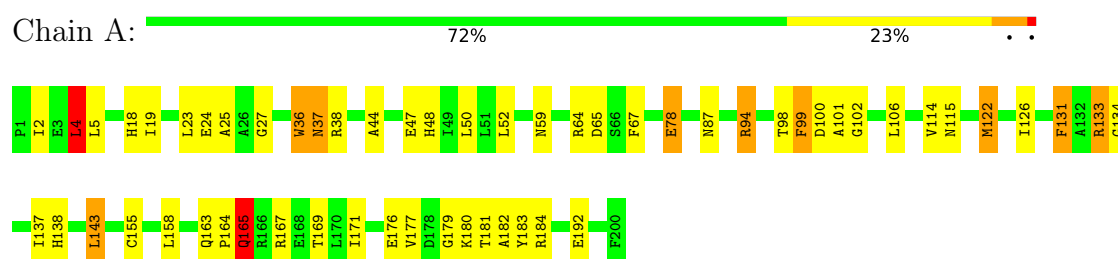
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total 81	O 81	0	0
6	M	160	Total 160	O 160	0	0
6	B	82	Total 82	O 82	0	0
6	N	162	Total 162	O 162	0	0
6	C	82	Total 82	O 82	0	0
6	O	159	Total 159	O 159	0	0
6	D	83	Total 83	O 83	0	0
6	P	151	Total 151	O 151	0	0
6	E	87	Total 87	O 87	0	0
6	Q	157	Total 157	O 157	0	0
6	F	74	Total 74	O 74	0	0
6	R	168	Total 168	O 168	0	0

3 Residue-property plots

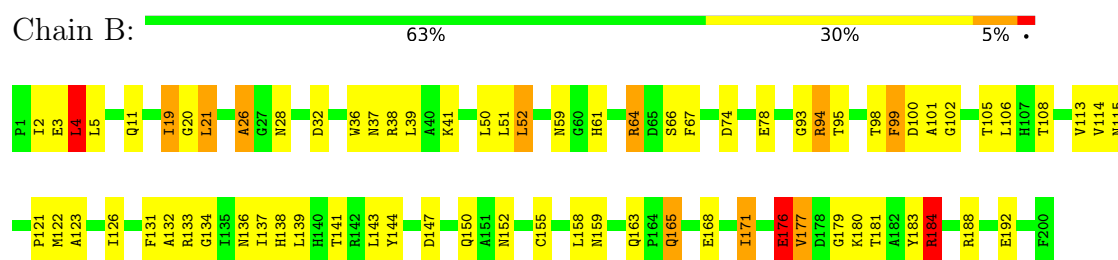
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

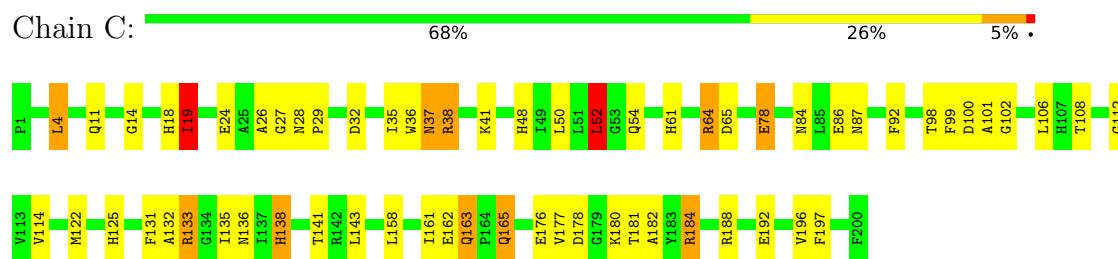
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



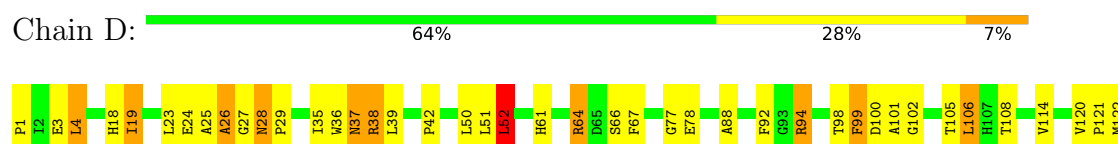
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

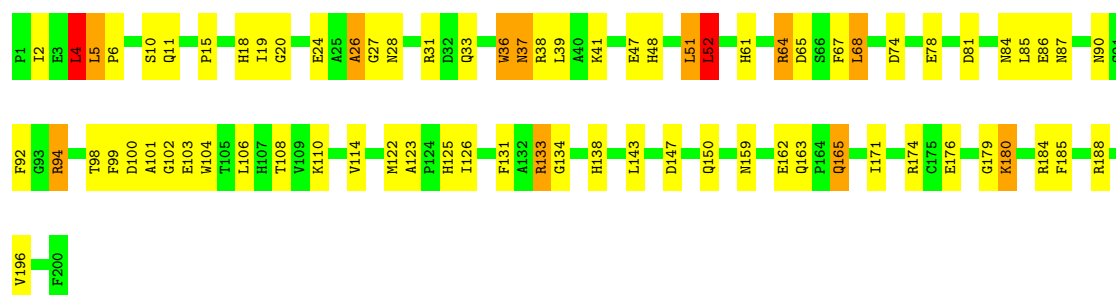


• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

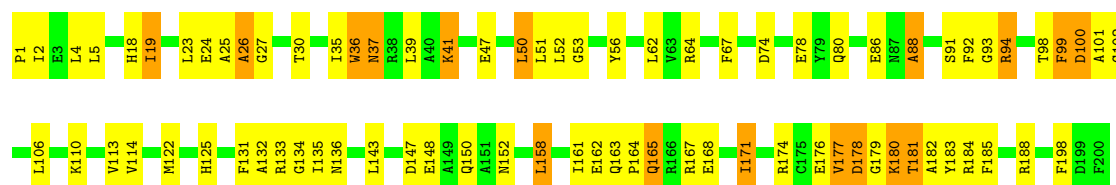




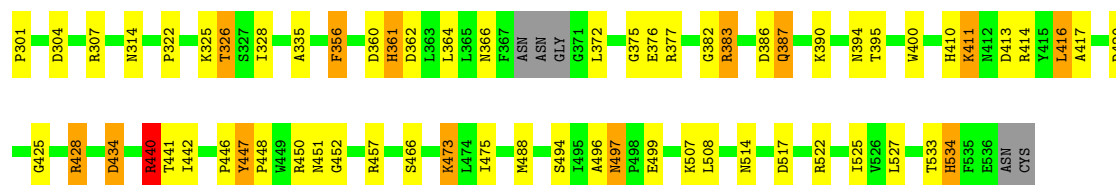
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



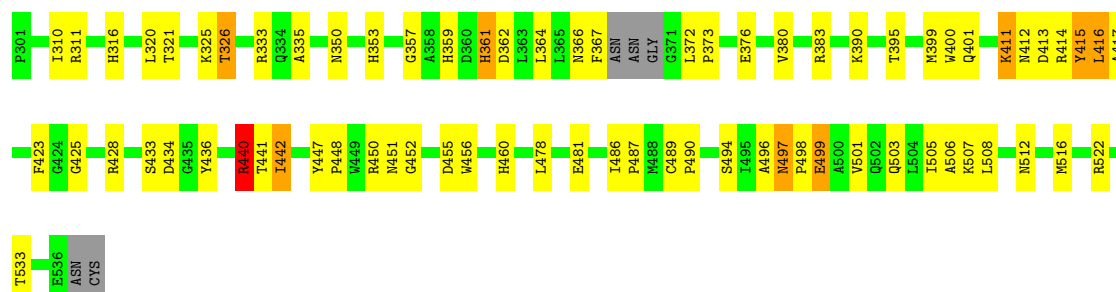
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



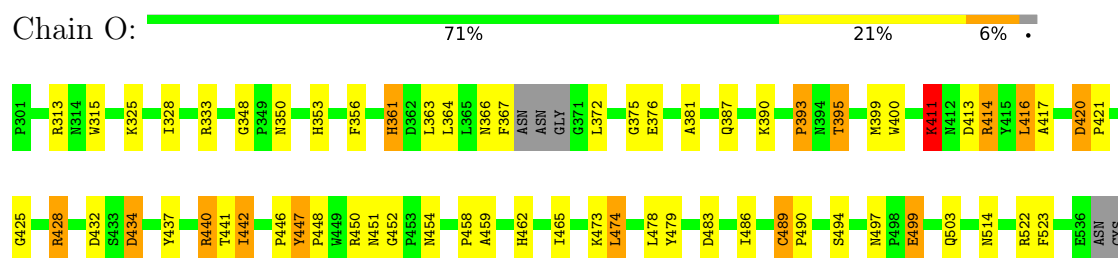
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



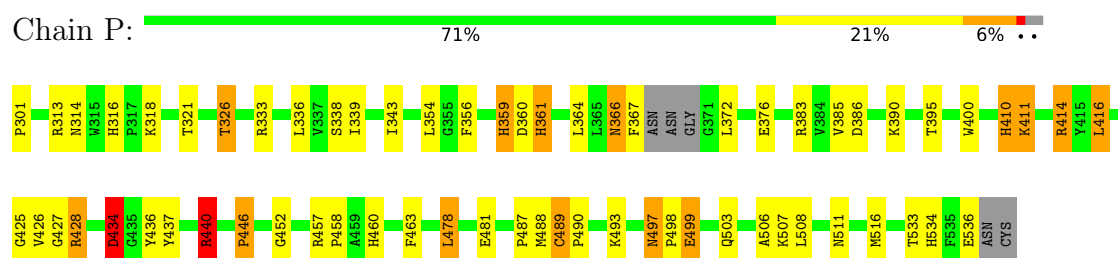
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



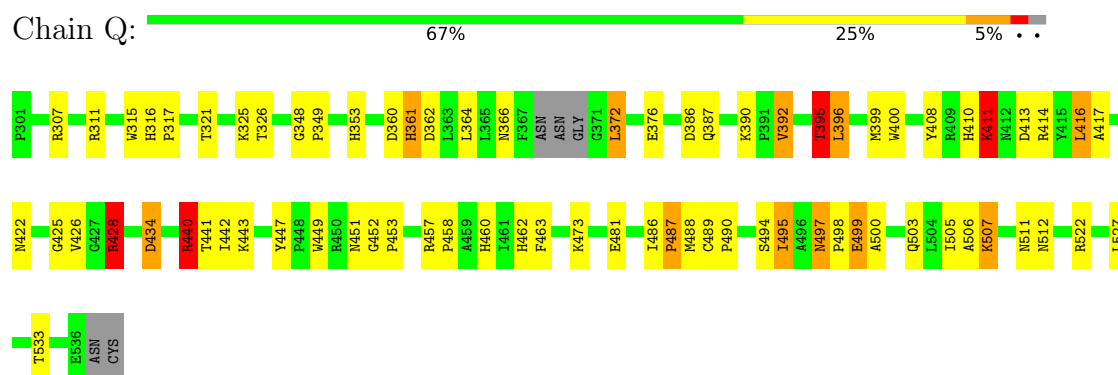
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



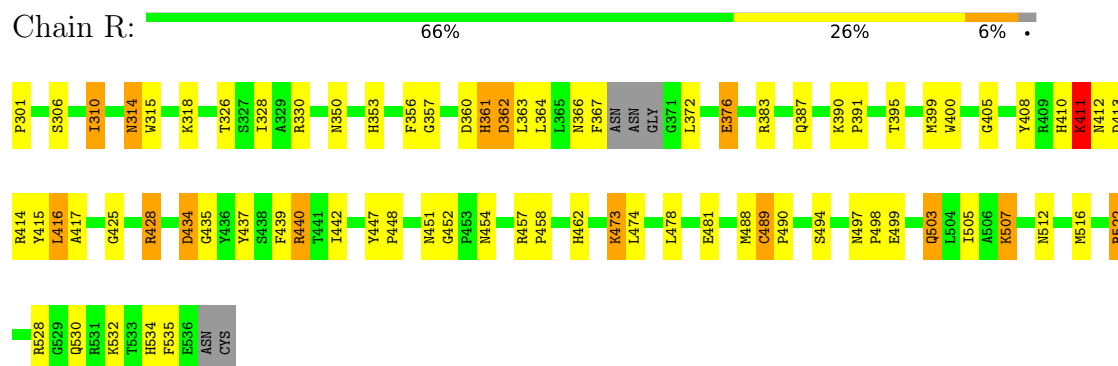
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



4 Data and refinement statistics

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	197.41 Å 127.97 Å 134.88 Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	6.00 – 1.98	Depositor
% Data completeness (in resolution range)	67.7 (6.00-1.98)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22062	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: PHB, BME, FE

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	1.32	2/1611 (0.1%)	1.89	27/2195 (1.2%)
1	B	1.34	4/1611 (0.2%)	1.81	33/2195 (1.5%)
1	C	1.34	6/1611 (0.4%)	1.76	26/2195 (1.2%)
1	D	1.37	5/1611 (0.3%)	1.82	28/2195 (1.3%)
1	E	1.43	8/1611 (0.5%)	1.84	30/2195 (1.4%)
1	F	1.39	3/1611 (0.2%)	1.88	36/2195 (1.6%)
2	M	1.47	10/1895 (0.5%)	1.89	41/2580 (1.6%)
2	N	1.52	13/1895 (0.7%)	1.88	35/2580 (1.4%)
2	O	1.48	11/1895 (0.6%)	1.88	45/2580 (1.7%)
2	P	1.45	8/1895 (0.4%)	1.85	39/2580 (1.5%)
2	Q	1.47	10/1895 (0.5%)	1.88	38/2580 (1.5%)
2	R	1.38	4/1895 (0.2%)	1.85	37/2580 (1.4%)
All	All	1.42	84/21036 (0.4%)	1.86	415/28650 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-11.60	1.30	1.46
1	E	94	ARG	CD-NE	-10.29	1.31	1.46
1	D	94	ARG	CD-NE	-8.75	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	8.45	1.56	1.52
2	M	451	ASN	CA-C	8.29	1.56	1.52
2	Q	428	ARG	CD-NE	-8.10	1.34	1.46
2	O	428	ARG	CD-NE	-7.52	1.35	1.46
2	R	428	ARG	CD-NE	-7.41	1.35	1.46
2	Q	451	ASN	CA-C	7.33	1.55	1.52
2	P	428	ARG	CD-NE	-7.13	1.36	1.46
2	N	428	ARG	CD-NE	-6.97	1.36	1.46
2	P	440	ARG	CD-NE	-6.97	1.36	1.46
2	N	321	THR	N-CA	6.76	1.53	1.46
1	D	108	THR	CA-CB	6.75	1.63	1.54
2	Q	441	THR	CA-CB	6.72	1.62	1.53
2	M	440	ARG	CD-NE	-6.63	1.36	1.46
2	M	452	GLY	CA-C	6.53	1.61	1.51
1	B	108	THR	CA-CB	6.49	1.63	1.54
1	F	94	ARG	CD-NE	-6.47	1.37	1.46
2	O	441	THR	CA-CB	6.35	1.62	1.53
2	P	460	HIS	ND1-CE1	6.33	1.38	1.32
1	C	188	ARG	N-CA	6.26	1.53	1.46
2	M	428	ARG	CD-NE	-6.12	1.37	1.46
1	E	108	THR	CA-CB	6.10	1.62	1.54
2	N	506	ALA	C-O	6.03	1.31	1.23
1	B	133	ARG	CD-NE	-5.98	1.37	1.46
2	N	401	GLN	N-CA	5.94	1.53	1.46
1	B	137	ILE	N-CA	5.90	1.53	1.46
2	O	375	GLY	N-CA	5.84	1.51	1.45
2	P	427	GLY	N-CA	5.76	1.51	1.45
1	E	123	ALA	N-CA	5.76	1.54	1.45
1	E	196	VAL	CA-C	5.74	1.58	1.52
1	D	188	ARG	N-CA	5.74	1.53	1.46
2	Q	458	PRO	C-O	5.69	1.30	1.23
2	N	441	THR	CA-CB	5.67	1.61	1.54
2	Q	495	ILE	CA-CB	5.66	1.60	1.53
2	R	451	ASN	CA-C	5.63	1.55	1.52
1	E	5	LEU	CA-C	5.62	1.59	1.53
2	O	440	ARG	CD-NE	-5.61	1.38	1.46
1	E	51	LEU	N-CA	5.57	1.52	1.46
2	M	382	GLY	N-CA	5.53	1.50	1.45
1	D	140	HIS	CG-CD2	5.53	1.42	1.35
2	N	455	ASP	N-CA	5.49	1.52	1.46
2	P	321	THR	CA-CB	5.49	1.60	1.53
1	C	14	GLY	N-CA	5.48	1.52	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	459	ALA	N-CA	5.46	1.53	1.46
1	F	135	ILE	N-CA	5.44	1.52	1.46
2	M	326	THR	CA-CB	5.42	1.62	1.53
2	O	451	ASN	N-CA	5.42	1.52	1.45
1	B	2	ILE	CA-CB	5.41	1.60	1.54
1	C	4	LEU	N-CA	5.41	1.52	1.45
2	N	452	GLY	N-CA	5.41	1.52	1.44
2	Q	321	THR	N-CA	5.40	1.53	1.46
2	P	339	ILE	C-O	5.40	1.28	1.24
1	A	126	ILE	CA-CB	5.38	1.61	1.54
2	Q	527	LEU	N-CA	5.38	1.52	1.45
2	N	505	ILE	CA-CB	5.37	1.60	1.53
2	R	452	GLY	N-CA	5.37	1.51	1.44
2	P	343	ILE	CA-CB	5.37	1.62	1.54
1	F	2	ILE	CA-CB	5.36	1.60	1.54
2	Q	440	ARG	CD-NE	-5.32	1.38	1.46
2	N	533	THR	CB-OG1	5.30	1.52	1.43
2	O	400	TRP	C-O	5.28	1.30	1.23
1	C	108	THR	CA-CB	5.26	1.61	1.54
2	O	458	PRO	CA-C	5.25	1.59	1.52
1	C	197	PHE	N-CA	5.21	1.52	1.45
2	N	451	ASN	N-CA	5.20	1.51	1.45
2	N	451	ASN	CA-C	5.20	1.54	1.52
2	M	375	GLY	N-CA	5.19	1.50	1.45
2	P	326	THR	CA-CB	5.18	1.62	1.53
2	Q	441	THR	C-O	5.17	1.29	1.23
1	E	171	ILE	CA-CB	5.16	1.60	1.54
2	O	395	THR	CA-CB	5.16	1.62	1.53
1	C	133	ARG	CA-C	5.15	1.59	1.52
2	N	508	LEU	CA-C	5.14	1.59	1.52
1	E	10	SER	CA-CB	5.09	1.61	1.53
1	D	135	ILE	CA-CB	5.08	1.60	1.53
2	M	441	THR	CA-CB	5.08	1.60	1.54
2	O	313	ARG	NE-CZ	5.08	1.38	1.33
2	M	527	LEU	CA-C	5.07	1.59	1.52
2	M	322	PRO	N-CA	-5.05	1.40	1.47
2	Q	449	TRP	N-CA	5.01	1.52	1.45
2	R	532	LYS	N-CA	5.01	1.51	1.45
2	N	310	ILE	CA-CB	5.01	1.59	1.54

All (415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	27.33	162.67	124.40
2	Q	428	ARG	CD-NE-CZ	16.70	147.79	124.40
1	D	94	ARG	CD-NE-CZ	14.70	144.99	124.40
2	O	428	ARG	CD-NE-CZ	14.68	144.95	124.40
1	E	94	ARG	CG-CD-NE	14.58	144.07	112.00
1	A	94	ARG	CG-CD-NE	14.52	143.94	112.00
2	R	428	ARG	CD-NE-CZ	14.09	144.12	124.40
1	E	94	ARG	CD-NE-CZ	14.05	144.07	124.40
1	F	94	ARG	CD-NE-CZ	13.99	143.98	124.40
2	M	440	ARG	NE-CZ-NH2	-12.47	107.97	119.20
2	N	440	ARG	NE-CZ-NH2	-12.15	108.26	119.20
2	P	440	ARG	NE-CZ-NH2	-11.77	108.61	119.20
1	B	94	ARG	CB-CG-CD	11.56	137.90	111.30
1	B	133	ARG	CD-NE-CZ	11.47	140.46	124.40
2	N	452	GLY	N-CA-C	-10.70	99.28	112.23
2	P	434	ASP	CA-CB-CG	-10.68	101.92	112.60
2	N	428	ARG	CD-NE-CZ	10.67	139.34	124.40
2	Q	440	ARG	NE-CZ-NH2	-10.59	109.67	119.20
2	O	440	ARG	NE-CZ-NH2	-10.43	109.81	119.20
2	R	451	ASN	O-C-N	10.33	128.47	120.83
2	N	428	ARG	CG-CD-NE	10.08	134.18	112.00
2	R	428	ARG	CG-CD-NE	9.81	133.59	112.00
2	M	452	GLY	N-CA-C	-9.80	100.37	112.23
2	O	353	HIS	CA-CB-CG	-9.58	104.22	113.80
2	Q	361	HIS	CA-CB-CG	-9.38	104.42	113.80
2	R	434	ASP	CA-CB-CG	-9.37	103.23	112.60
2	N	434	ASP	CA-CB-CG	-9.34	103.26	112.60
2	N	428	ARG	CB-CG-CD	9.25	132.58	111.30
1	A	94	ARG	CB-CG-CD	9.21	132.49	111.30
1	A	115	ASN	CA-CB-CG	9.14	121.74	112.60
2	O	428	ARG	CG-CD-NE	9.13	132.09	112.00
2	Q	452	GLY	N-CA-C	-9.07	101.25	112.23
2	M	428	ARG	CD-NE-CZ	8.96	136.94	124.40
2	Q	451	ASN	O-C-N	8.94	127.45	120.83
2	P	452	GLY	N-CA-C	-8.92	101.12	112.10
2	O	434	ASP	CA-CB-CG	-8.90	103.70	112.60
2	M	420	ASP	CA-CB-CG	8.79	121.39	112.60
1	D	94	ARG	CG-CD-NE	8.73	131.21	112.00
2	O	452	GLY	N-CA-C	-8.70	101.70	112.23
2	O	325	LYS	N-CA-C	8.66	121.51	111.11
2	P	386	ASP	CA-CB-CG	8.62	121.22	112.60
1	B	94	ARG	CG-CD-NE	8.46	130.60	112.00
2	Q	440	ARG	NE-CZ-NH1	8.44	129.94	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	353	HIS	CA-CB-CG	-8.40	105.40	113.80
1	F	177	VAL	CB-CA-C	8.40	120.72	110.73
2	R	361	HIS	CA-CB-CG	-8.39	105.41	113.80
2	M	457	ARG	CD-NE-CZ	8.28	135.99	124.40
2	N	428	ARG	NE-CZ-NH1	8.23	129.73	121.50
2	R	387	GLN	OE1-CD-NE2	8.14	130.74	122.60
2	O	451	ASN	O-C-N	8.10	126.82	120.83
1	C	37	ASN	N-CA-C	8.01	122.63	113.02
1	D	28	ASN	O-C-N	7.98	128.13	121.35
2	P	372	LEU	CB-CA-C	7.97	120.80	108.61
1	D	37	ASN	N-CA-C	7.96	122.36	113.21
2	P	428	ARG	CG-CD-NE	7.94	129.46	112.00
2	R	440	ARG	NE-CZ-NH2	-7.93	112.06	119.20
1	F	94	ARG	CG-CD-NE	7.93	129.45	112.00
1	E	133	ARG	CD-NE-CZ	-7.92	113.32	124.40
2	O	414	ARG	CD-NE-CZ	-7.81	113.46	124.40
2	P	361	HIS	CA-CB-CG	-7.68	106.12	113.80
1	B	94	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	F	94	ARG	CB-CG-CD	7.63	128.85	111.30
2	N	450	ARG	CD-NE-CZ	7.63	135.08	124.40
1	E	94	ARG	NE-CZ-NH1	7.61	129.11	121.50
2	Q	512	ASN	CA-CB-CG	-7.56	105.04	112.60
1	D	197	PHE	CA-CB-CG	7.52	121.32	113.80
2	Q	311	ARG	CD-NE-CZ	7.47	134.86	124.40
2	R	452	GLY	N-CA-C	-7.46	103.20	112.23
1	F	88	ALA	N-CA-C	-7.42	103.69	112.89
1	B	192	GLU	CA-CB-CG	7.40	128.91	114.10
1	A	131	PHE	CA-CB-CG	7.33	121.13	113.80
2	M	383	ARG	NE-CZ-NH1	-7.33	114.17	121.50
2	Q	434	ASP	CA-CB-CG	-7.33	105.27	112.60
2	O	451	ASN	CA-C-O	-7.32	115.60	119.77
2	O	414	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	C	38	ARG	CD-NE-CZ	-7.27	114.23	124.40
1	A	37	ASN	N-CA-C	7.25	121.06	112.93
1	D	99	PHE	CA-CB-CG	7.22	121.02	113.80
2	M	434	ASP	CA-CB-CG	-7.21	105.39	112.60
2	Q	411	LYS	CB-CA-C	-7.21	98.87	110.84
1	F	136	ASN	OD1-CG-ND2	7.06	129.66	122.60
2	Q	372	LEU	CB-CA-C	7.05	118.42	108.76
2	Q	428	ARG	CG-CD-NE	7.04	127.50	112.00
2	R	457	ARG	CA-CB-CG	7.03	128.16	114.10
1	F	167	ARG	CD-NE-CZ	-7.03	114.56	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	ASN	CA-CB-CG	7.02	119.62	112.60
2	N	357	GLY	N-CA-C	-7.00	103.57	112.54
2	M	420	ASP	CB-CA-C	6.99	118.19	110.15
2	O	428	ARG	CB-CG-CD	6.98	127.36	111.30
1	F	134	GLY	CA-C-N	-6.98	113.78	122.93
1	F	134	GLY	C-N-CA	-6.98	113.78	122.93
2	N	361	HIS	CA-CB-CG	-6.97	106.83	113.80
2	M	314	ASN	N-CA-C	-6.94	104.69	113.72
2	R	367	PHE	CA-C-O	-6.93	109.02	120.80
1	D	178	ASP	CA-CB-CG	-6.90	105.70	112.60
1	B	95	THR	CA-CB-CG2	6.89	122.21	110.50
1	D	23	LEU	CB-CA-C	6.88	121.85	110.92
1	B	4	LEU	N-CA-CB	-6.87	99.97	110.49
2	P	499	GLU	CA-CB-CG	6.85	127.79	114.10
1	E	37	ASN	N-CA-C	6.84	120.59	112.93
1	F	100	ASP	CA-CB-CG	-6.84	105.76	112.60
2	P	383	ARG	CD-NE-CZ	-6.82	114.85	124.40
2	O	440	ARG	O-C-N	6.82	131.29	123.31
2	P	536	GLU	CA-C-O	6.82	132.40	120.80
1	C	163	GLN	CA-C-O	6.82	124.71	119.46
2	O	387	GLN	OE1-CD-NE2	6.82	129.41	122.60
2	M	494	SER	N-CA-C	-6.81	104.23	112.54
2	R	458	PRO	CB-CA-C	-6.81	102.52	111.23
2	P	533	THR	O-C-N	6.76	130.50	122.79
2	R	439	PHE	CA-CB-CG	6.76	120.56	113.80
2	O	447	TYR	O-C-N	6.76	127.10	121.83
2	Q	366	ASN	N-CA-C	6.68	121.26	113.18
1	F	94	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	D	64	ARG	CD-NE-CZ	-6.66	115.07	124.40
1	D	159	ASN	CA-CB-CG	-6.64	105.96	112.60
1	B	176	GLU	CB-CG-CD	6.63	123.88	112.60
1	F	41	LYS	N-CA-C	-6.63	101.72	110.07
2	M	525	ILE	O-C-N	6.62	130.33	123.18
2	M	428	ARG	CG-CD-NE	6.62	126.55	112.00
2	P	314	ASN	N-CA-C	-6.61	105.37	113.50
1	D	94	ARG	NE-CZ-NH2	-6.60	113.26	119.20
2	N	451	ASN	O-C-N	6.58	125.70	120.83
1	D	94	ARG	NE-CZ-NH1	6.58	128.08	121.50
1	C	87	ASN	CA-CB-CG	6.57	119.17	112.60
1	E	64	ARG	CD-NE-CZ	-6.57	115.21	124.40
1	C	99	PHE	CA-CB-CG	6.54	120.34	113.80
2	Q	348	GLY	O-C-N	6.53	128.30	121.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	361	HIS	CA-CB-CG	-6.53	107.27	113.80
1	F	133	ARG	CD-NE-CZ	6.53	133.54	124.40
2	M	411	LYS	CB-CA-C	-6.49	99.64	110.68
2	Q	473	LYS	CB-CA-C	6.49	120.15	109.70
1	A	122	MET	CA-C-O	-6.46	113.65	121.28
1	E	185	PHE	CA-CB-CG	6.46	120.26	113.80
2	Q	325	LYS	N-CA-C	6.45	118.85	111.11
2	Q	494	SER	N-CA-C	-6.42	104.70	112.54
2	N	333	ARG	N-CA-C	-6.41	105.77	113.97
2	R	481	GLU	CB-CG-CD	6.36	123.42	112.60
2	P	326	THR	CA-CB-OG1	-6.36	100.06	109.60
2	Q	481	GLU	CB-CG-CD	6.36	123.40	112.60
1	B	184	ARG	NE-CZ-NH2	-6.34	113.50	119.20
1	B	37	ASN	N-CA-C	6.33	120.61	113.02
1	F	150	GLN	N-CA-CB	6.31	119.41	109.82
2	M	451	ASN	O-C-N	6.31	125.50	120.83
2	M	386	ASP	CA-CB-CG	6.29	118.89	112.60
2	O	494	SER	N-CA-C	-6.29	104.71	112.38
1	F	150	GLN	O-C-N	6.29	128.81	122.08
2	M	361	HIS	CA-CB-CG	-6.28	107.52	113.80
1	E	196	VAL	O-C-N	6.28	129.52	122.67
2	O	395	THR	CA-CB-OG1	-6.28	100.18	109.60
1	B	36	TRP	CB-CA-C	6.25	122.86	110.42
2	M	496	ALA	CA-C-O	-6.25	113.80	120.42
2	N	440	ARG	NH1-CZ-NH2	6.25	127.42	119.30
1	F	181	THR	N-CA-CB	6.25	119.16	109.85
2	N	508	LEU	O-C-N	6.23	130.67	122.95
2	N	353	HIS	CA-CB-CG	-6.22	107.58	113.80
2	N	367	PHE	CA-C-O	-6.21	110.24	120.80
2	M	447	TYR	O-C-N	6.21	126.67	121.83
1	E	81	ASP	N-CA-C	6.21	119.02	111.82
1	D	4	LEU	CA-C-O	-6.20	113.73	121.55
2	R	454	ASN	CA-CB-CG	6.18	118.78	112.60
1	E	171	ILE	N-CA-CB	-6.18	103.98	111.21
1	F	37	ASN	N-CA-C	6.18	119.85	112.93
1	F	198	PHE	CA-CB-CG	6.18	119.98	113.80
1	B	28	ASN	O-C-N	6.17	126.59	121.35
2	M	366	ASN	N-CA-C	6.17	120.66	113.20
1	F	36	TRP	CB-CA-C	6.14	122.65	110.42
1	B	38	ARG	CD-NE-CZ	-6.13	115.81	124.40
1	B	152	ASN	CA-CB-CG	6.12	118.72	112.60
1	F	5	LEU	N-CA-C	-6.11	102.07	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	ARG	CD-NE-CZ	-6.09	115.87	124.40
1	C	158	LEU	CB-CA-C	6.09	121.90	110.63
1	E	2	ILE	N-CA-CB	-6.09	103.89	110.53
2	P	367	PHE	CA-C-O	-6.09	110.45	120.80
1	D	171	ILE	N-CA-CB	-6.09	104.09	111.21
2	P	410	HIS	CA-C-N	6.06	129.91	120.82
2	P	410	HIS	C-N-CA	6.06	129.91	120.82
2	P	533	THR	N-CA-C	-6.06	102.53	110.53
1	F	99	PHE	CA-CB-CG	6.06	119.86	113.80
1	D	99	PHE	N-CA-C	-6.04	105.02	112.38
2	O	366	ASN	N-CA-C	6.03	120.49	113.20
2	M	428	ARG	CB-CG-CD	6.01	125.12	111.30
1	C	178	ASP	CA-CB-CG	-5.98	106.62	112.60
1	E	28	ASN	O-C-N	5.98	126.44	121.35
2	N	512	ASN	CA-CB-CG	-5.98	106.62	112.60
1	C	78	GLU	CB-CG-CD	5.97	122.75	112.60
2	Q	395	THR	CA-CB-OG1	-5.97	100.64	109.60
2	N	412	ASN	CA-CB-CG	5.95	118.55	112.60
2	R	411	LYS	CB-CA-C	-5.95	101.28	110.81
2	O	440	ARG	CA-C-O	-5.94	113.73	120.32
2	R	454	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	F	30	THR	CA-CB-OG1	-5.93	100.71	109.60
2	R	376	GLU	CG-CD-OE2	-5.92	104.78	118.40
2	O	440	ARG	CB-CG-CD	-5.92	97.69	111.30
2	M	514	ASN	O-C-N	5.91	127.85	121.12
2	R	522	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	E	94	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	C	141	THR	CA-CB-CG2	5.88	120.50	110.50
2	M	383	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	E	5	LEU	N-CA-C	-5.87	101.98	110.08
1	B	137	ILE	CB-CA-C	5.87	119.55	110.28
1	B	139	LEU	O-C-N	5.87	129.90	123.27
1	D	171	ILE	N-CA-C	5.86	116.54	107.99
2	M	356	PHE	CA-CB-CG	5.85	119.65	113.80
1	C	48	HIS	CA-CB-CG	-5.85	107.95	113.80
2	P	463	PHE	CA-CB-CG	5.84	119.64	113.80
2	N	503	GLN	OE1-CD-NE2	5.84	128.44	122.60
2	P	316	HIS	CA-CB-CG	-5.84	107.96	113.80
1	F	94	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	B	136	ASN	O-C-N	5.82	128.78	122.15
2	R	366	ASN	N-CA-C	5.81	120.23	113.20
1	A	87	ASN	CA-CB-CG	5.80	118.40	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	152	ASN	CA-CB-CG	5.78	118.38	112.60
2	P	440	ARG	CD-NE-CZ	5.78	132.49	124.40
2	O	454	ASN	CA-C-O	-5.77	115.32	121.78
1	F	19	ILE	CB-CA-C	5.77	121.10	112.16
2	R	503	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	E	4	LEU	CA-C-O	-5.74	114.32	121.50
2	M	522	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	B	11	GLN	CA-C-O	-5.73	115.14	121.33
2	M	473	LYS	CB-CA-C	5.72	118.91	109.70
1	A	133	ARG	N-CA-C	-5.72	102.44	110.50
2	N	316	HIS	CA-CB-CG	-5.71	108.09	113.80
1	E	150	GLN	CB-CG-CD	-5.71	102.90	112.60
1	D	52	LEU	CB-CA-C	5.69	121.21	110.62
2	O	417	ALA	CB-CA-C	5.69	117.62	109.26
2	R	494	SER	N-CA-C	-5.69	105.60	112.54
1	D	177	VAL	CB-CA-C	5.68	117.49	110.73
1	E	36	TRP	CB-CA-C	5.67	121.71	110.42
1	C	136	ASN	O-C-N	5.67	128.62	122.15
2	M	387	GLN	N-CA-CB	5.67	119.95	110.32
2	P	497	ASN	CB-CG-ND2	5.67	124.90	116.40
2	O	451	ASN	N-CA-C	-5.66	99.47	108.30
2	Q	392	VAL	O-C-N	5.66	127.55	121.10
2	Q	458	PRO	N-CA-C	-5.66	102.93	111.41
1	A	94	ARG	NE-CZ-NH1	5.65	127.15	121.50
2	O	428	ARG	NE-CZ-NH1	5.63	127.13	121.50
2	R	310	ILE	CA-C-O	5.63	127.55	121.36
2	N	311	ARG	CD-NE-CZ	5.63	132.28	124.40
2	P	366	ASN	N-CA-C	5.62	120.01	113.20
2	R	451	ASN	N-CA-C	-5.62	99.54	108.30
1	A	36	TRP	CB-CA-C	5.61	121.59	110.42
2	M	304	ASP	CA-CB-CG	5.61	118.21	112.60
2	P	385	VAL	CA-C-O	-5.61	116.14	121.64
2	Q	422	ASN	OD1-CG-ND2	5.60	128.20	122.60
2	P	497	ASN	OD1-CG-ND2	-5.59	117.01	122.60
2	M	387	GLN	CA-C-O	-5.58	112.73	119.49
1	E	26	ALA	N-CA-C	-5.58	106.32	113.01
2	N	325	LYS	N-CA-C	5.57	120.55	111.37
2	P	458	PRO	CB-CA-C	-5.56	103.66	110.95
1	A	171	ILE	N-CA-C	5.55	116.09	107.99
2	R	328	ILE	N-CA-C	5.55	115.75	110.42
2	Q	512	ASN	OD1-CG-ND2	5.55	128.15	122.60
2	N	533	THR	CA-CB-OG1	-5.54	101.29	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH2	-5.53	114.22	119.20
2	P	481	GLU	CB-CG-CD	5.52	121.99	112.60
1	C	192	GLU	CB-CG-CD	5.52	121.98	112.60
2	O	483	ASP	O-C-N	5.52	126.21	121.30
1	D	99	PHE	N-CA-CB	5.50	119.67	110.32
1	E	5	LEU	O-C-N	5.50	127.58	121.53
1	E	99	PHE	N-CA-C	-5.49	105.68	112.38
1	C	41	LYS	N-CA-C	-5.48	102.23	110.24
1	B	99	PHE	N-CA-C	-5.47	105.70	112.38
2	R	412	ASN	CA-CB-CG	5.47	118.07	112.60
2	O	486	ILE	O-C-N	5.46	123.92	120.42
2	N	428	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	E	11	GLN	OE1-CD-NE2	-5.46	117.14	122.60
1	B	26	ALA	N-CA-C	-5.46	106.46	113.01
2	N	481	GLU	CB-CA-C	-5.46	103.09	109.80
1	D	38	ARG	NE-CZ-NH2	-5.45	114.29	119.20
2	Q	457	ARG	NE-CZ-NH2	-5.45	114.29	119.20
1	A	177	VAL	O-C-N	5.45	127.88	122.97
2	O	350	ASN	CA-C-O	-5.45	114.44	120.38
2	R	362	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	59	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	B	177	VAL	O-C-N	5.45	128.97	123.20
2	R	350	ASN	CA-C-O	-5.44	114.48	120.36
1	A	2	ILE	N-CA-CB	-5.44	104.60	110.53
1	B	59	ASN	OD1-CG-ND2	5.43	128.03	122.60
2	O	479	TYR	CA-C-O	-5.43	115.28	121.68
1	E	133	ARG	N-CA-C	-5.42	102.37	110.23
2	P	336	LEU	CA-C-O	-5.42	115.65	121.56
1	D	66	SER	CA-C-N	5.42	130.41	122.77
1	D	66	SER	C-N-CA	5.42	130.41	122.77
1	F	158	LEU	CB-CA-C	5.41	120.64	110.63
1	A	183	TYR	N-CA-CB	5.41	119.90	110.81
1	B	78	GLU	N-CA-C	5.41	117.78	109.07
1	D	94	ARG	CB-CG-CD	5.40	123.73	111.30
2	O	450	ARG	CD-NE-CZ	5.40	131.96	124.40
2	N	494	SER	N-CA-C	-5.39	105.80	112.38
1	A	5	LEU	N-CA-C	-5.39	102.99	109.83
2	M	394	ASN	CB-CG-ND2	5.38	124.47	116.40
1	E	162	GLU	CB-CG-CD	5.38	121.74	112.60
1	B	41	LYS	N-CA-C	-5.37	102.41	110.24
1	D	199	ASP	O-C-N	5.37	129.82	123.27
2	O	350	ASN	CA-CB-CG	-5.37	107.23	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	357	GLY	N-CA-C	-5.37	105.67	112.54
2	N	326	THR	CA-CB-OG1	-5.36	101.55	109.60
2	Q	360	ASP	CA-CB-CG	5.36	117.96	112.60
2	Q	497	ASN	CA-C-N	5.36	125.69	119.47
2	Q	497	ASN	C-N-CA	5.36	125.69	119.47
2	Q	440	ARG	CD-NE-CZ	5.36	131.90	124.40
2	P	489	CYS	CA-C-O	5.35	123.58	119.46
1	F	162	GLU	N-CA-CB	5.35	117.95	109.82
2	O	348	GLY	O-C-N	5.35	127.12	121.77
1	C	52	LEU	CB-CA-C	5.35	121.33	109.94
2	P	533	THR	CA-C-O	-5.34	115.67	121.87
1	F	47	GLU	CB-CG-CD	5.34	121.68	112.60
2	M	325	LYS	N-CA-C	5.33	120.17	111.37
1	A	137	ILE	CB-CA-C	5.33	119.94	110.71
1	A	167	ARG	CD-NE-CZ	-5.33	116.94	124.40
2	N	320	LEU	CA-C-O	-5.32	115.38	120.92
2	O	420	ASP	CB-CA-C	5.32	115.44	110.17
1	B	21	LEU	N-CA-CB	-5.32	102.88	110.80
1	A	133	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	Q	396	LEU	N-CA-C	5.31	117.40	108.96
2	N	350	ASN	CA-C-O	-5.30	114.60	120.38
1	E	52	LEU	CB-CA-C	5.30	121.85	110.45
2	Q	362	ASP	CA-CB-CG	5.30	117.90	112.60
2	P	354	LEU	N-CA-C	-5.30	102.44	110.28
2	P	446	PRO	N-CA-C	-5.29	103.81	111.22
1	E	159	ASN	CA-CB-CG	-5.29	107.31	112.60
1	C	125	HIS	CA-CB-CG	-5.29	108.51	113.80
1	F	23	LEU	CB-CA-C	5.29	119.33	110.92
2	M	441	THR	N-CA-CB	-5.29	103.00	110.51
1	C	112	GLY	N-CA-C	-5.28	104.35	112.85
2	O	489	CYS	CA-C-N	5.28	124.78	119.19
2	O	489	CYS	C-N-CA	5.28	124.78	119.19
1	F	133	ARG	N-CA-C	-5.28	102.58	110.23
2	R	512	ASN	CA-CB-CG	-5.28	107.32	112.60
1	F	188	ARG	CD-NE-CZ	-5.27	117.02	124.40
2	O	432	ASP	CA-CB-CG	5.27	117.87	112.60
2	Q	353	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	64	ARG	CD-NE-CZ	-5.26	117.03	124.40
2	Q	506	ALA	CB-CA-C	5.26	118.42	109.53
1	C	19	ILE	CB-CA-C	5.25	120.30	112.16
1	D	88	ALA	N-CA-C	-5.25	106.72	113.23
2	P	497	ASN	CA-CB-CG	5.25	117.85	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	THR	CA-CB-CG2	5.25	119.42	110.50
1	A	47	GLU	CB-CG-CD	5.25	121.52	112.60
2	R	428	ARG	CB-CG-CD	5.25	123.37	111.30
2	M	387	GLN	O-C-N	5.24	129.21	122.39
2	O	514	ASN	CA-CB-CG	5.24	117.84	112.60
1	D	158	LEU	CB-CA-C	5.24	119.49	110.79
1	D	162	GLU	N-CA-C	5.24	117.40	111.11
2	P	338	SER	O-C-N	5.24	129.19	123.01
2	Q	511	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	F	171	ILE	N-CA-C	5.24	116.25	108.23
2	N	501	VAL	N-CA-CB	5.23	116.67	110.55
2	Q	463	PHE	O-C-N	5.23	129.67	123.24
2	R	314	ASN	N-CA-C	-5.23	106.94	113.38
1	F	26	ALA	N-CA-C	-5.23	106.97	113.19
2	Q	386	ASP	CB-CA-C	5.22	119.48	110.45
1	C	162	GLU	CA-CB-CG	5.22	124.54	114.10
2	P	338	SER	CA-C-O	-5.21	115.11	121.05
2	P	457	ARG	CD-NE-CZ	5.21	131.70	124.40
2	M	450	ARG	CA-C-N	5.21	128.82	121.79
2	M	450	ARG	C-N-CA	5.21	128.82	121.79
1	A	192	GLU	CA-C-O	-5.21	115.18	120.80
1	E	171	ILE	N-CA-C	5.20	115.59	107.99
2	R	411	LYS	N-CA-C	5.20	117.35	111.11
2	Q	533	THR	N-CA-C	-5.20	103.67	110.53
1	C	138	HIS	N-CA-C	5.19	116.99	110.24
2	O	499	GLU	CG-CD-OE1	5.19	130.34	118.40
1	C	11	GLN	N-CA-CB	5.19	121.18	111.53
1	F	171	ILE	N-CA-CB	-5.19	105.08	111.00
2	R	489	CYS	N-CA-C	5.19	117.09	109.42
2	Q	428	ARG	NE-CZ-NH2	-5.18	114.53	119.20
2	O	440	ARG	NH1-CZ-NH2	5.18	126.04	119.30
2	R	528	ARG	NE-CZ-NH1	-5.18	116.32	121.50
2	N	380	VAL	CA-C-O	-5.17	115.02	120.39
1	A	4	LEU	N-CA-CB	-5.17	102.18	110.39
2	O	333	ARG	CB-CA-C	5.16	117.74	109.07
1	C	135	ILE	CB-CA-C	5.16	118.53	111.31
1	B	66	SER	N-CA-CB	5.16	118.29	110.45
1	A	23	LEU	CB-CA-C	5.15	119.11	110.92
1	E	47	GLU	CB-CG-CD	5.15	121.36	112.60
2	P	333	ARG	CB-CA-C	5.15	117.72	109.07
1	B	113	VAL	N-CA-C	5.15	116.22	109.58
2	N	415	TYR	CB-CA-C	5.15	118.27	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	HIS	N-CA-CB	5.14	117.51	109.85
1	D	26	ALA	N-CA-C	-5.14	106.71	112.87
2	P	452	GLY	CA-C-O	-5.13	117.48	122.46
2	M	466	SER	CA-C-O	-5.13	115.06	120.55
1	A	99	PHE	N-CA-C	-5.12	106.13	112.38
2	P	506	ALA	O-C-N	5.12	129.05	123.01
1	C	181	THR	N-CA-CB	5.11	117.47	109.85
1	A	165	GLN	OE1-CD-NE2	-5.11	117.49	122.60
2	O	367	PHE	CA-C-O	-5.10	112.13	120.80
1	B	132	ALA	O-C-N	5.10	128.00	123.41
2	O	454	ASN	CA-CB-CG	5.10	117.70	112.60
2	R	448	PRO	CB-CA-C	5.09	117.91	110.63
2	O	474	LEU	N-CA-CB	-5.09	102.06	111.53
2	M	314	ASN	CA-CB-CG	5.09	117.69	112.60
1	F	86	GLU	CB-CG-CD	5.08	121.23	112.60
2	M	326	THR	CA-CB-OG1	-5.07	101.99	109.60
2	M	508	LEU	CB-CA-C	5.07	117.81	109.90
1	C	158	LEU	N-CA-CB	-5.07	102.42	110.22
1	B	5	LEU	N-CA-C	-5.07	103.09	110.08
1	B	171	ILE	N-CA-C	5.07	115.06	107.51
1	E	125	HIS	CA-CB-CG	-5.06	108.74	113.80
2	R	440	ARG	CB-CG-CD	-5.04	99.70	111.30
2	N	496	ALA	N-CA-C	5.04	117.67	111.82
1	B	133	ARG	N-CA-C	-5.04	102.92	110.23
2	N	325	LYS	CA-C-N	5.04	127.53	120.28
2	N	325	LYS	C-N-CA	5.04	127.53	120.28
2	M	417	ALA	CB-CA-C	5.04	116.66	109.26
2	Q	487	PRO	CB-CA-C	5.03	118.96	111.62
2	P	359	HIS	CA-CB-CG	-5.02	108.78	113.80
1	F	99	PHE	N-CA-C	-5.02	105.94	111.71
2	O	446	PRO	N-CA-C	-5.02	104.19	111.22
1	C	192	GLU	CA-C-O	-5.02	115.38	120.80
1	C	32	ASP	O-C-N	5.02	127.24	122.07
2	O	411	LYS	CB-CA-C	-5.01	102.42	110.74
2	M	410	HIS	CA-C-N	5.00	127.24	120.38
2	M	410	HIS	C-N-CA	5.00	127.24	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	184	ARG	Sidechain
1	F	184	ARG	Sidechain

5.2 Too-close contacts

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	45	0
1	B	1571	0	1499	49	0
1	C	1571	0	1499	46	0
1	D	1571	0	1499	55	0
1	E	1571	0	1499	55	0
1	F	1571	0	1499	68	0
2	M	1840	0	1792	40	0
2	N	1840	0	1792	39	0
2	O	1840	0	1792	37	0
2	P	1840	0	1792	46	0
2	Q	1840	0	1792	55	0
2	R	1840	0	1792	57	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	0	0
4	N	4	0	5	0	0
4	O	4	0	5	0	0
4	P	4	0	5	0	0
4	Q	4	0	5	0	0
4	R	4	0	5	0	0
5	M	20	0	9	0	0
5	N	20	0	9	1	0
5	O	20	0	9	0	0
5	P	20	0	8	0	0
5	Q	20	0	9	0	0
5	R	20	0	9	1	0
6	A	81	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	82	0	0	1	0
6	C	82	0	0	1	0
6	D	83	0	0	1	0
6	E	87	0	0	1	0
6	F	74	0	0	1	0
6	M	160	0	0	2	0
6	N	162	0	0	3	0
6	O	159	0	0	3	0
6	P	151	0	0	2	0
6	Q	157	0	0	4	0
6	R	168	0	0	4	0
All	All	22062	0	19829	545	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 13.

All (545) 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:N:411:LYS:HE2	2:N:411:LYS:N	1.31	1.39
1:C:26:ALA:O	2:O:411:LYS:NZ	1.61	1.31
2:N:411:LYS:H	2:N:411:LYS:CE	1.43	1.30
2:P:411:LYS:HE2	2:P:411:LYS:N	1.49	1.27
2:P:411:LYS:H	2:P:411:LYS:CE	1.56	1.18
1:F:64:ARG:NH1	1:F:100:ASP:O	1.77	1.17
1:C:64:ARG:NH1	1:C:100:ASP:O	1.83	1.10
1:E:26:ALA:O	2:Q:411:LYS:NZ	1.86	1.09
1:E:64:ARG:NH1	1:E:100:ASP:O	1.88	1.07
1:A:98:THR:HB	1:A:100:ASP:OD1	1.56	1.05
1:B:26:ALA:O	2:N:411:LYS:NZ	1.91	1.03
1:E:165:GLN:H	1:E:165:GLN:NE2	1.56	1.03
1:E:98:THR:HB	1:E:100:ASP:OD1	1.61	1.01
1:F:98:THR:HB	1:F:100:ASP:OD1	1.62	1.00
1:F:26:ALA:O	2:R:411:LYS:NZ	1.93	1.00
1:B:98:THR:HB	1:B:100:ASP:OD1	1.62	0.99
1:E:165:GLN:HE21	1:E:165:GLN:N	1.62	0.96
1:B:165:GLN:H	1:B:165:GLN:NE2	1.63	0.95
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.31	0.94
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.82	0.93
2:M:497:ASN:HD22	2:M:499:GLU:H	1.15	0.93
2:N:390:LYS:HD3	6:N:747:HOH:O	1.71	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ALA:O	2:P:411:LYS:HE3	1.68	0.91
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.32	0.91
1:D:98:THR:OG1	1:D:102:GLY:N	2.05	0.90
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.87	0.90
1:D:165:GLN:NE2	1:D:165:GLN:H	1.70	0.89
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.88	0.89
1:D:26:ALA:O	2:P:411:LYS:CE	2.21	0.88
1:D:165:GLN:H	1:D:165:GLN:HE21	1.20	0.87
1:A:98:THR:OG1	1:A:102:GLY:N	2.08	0.87
2:Q:411:LYS:H	2:Q:411:LYS:CE	1.88	0.86
1:B:64:ARG:NH1	1:B:100:ASP:O	2.09	0.85
2:R:361:HIS:H	2:R:361:HIS:CD2	1.93	0.85
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.91	0.85
2:P:411:LYS:O	2:P:414:ARG:NH1	2.10	0.84
1:B:26:ALA:O	2:N:411:LYS:CE	2.26	0.84
2:R:411:LYS:H	2:R:411:LYS:CE	1.89	0.84
2:Q:361:HIS:CD2	2:Q:361:HIS:H	1.95	0.83
2:R:390:LYS:HE2	6:R:873:HOH:O	1.78	0.82
1:D:64:ARG:NH1	1:D:100:ASP:O	2.13	0.82
2:N:497:ASN:HD22	2:N:499:GLU:H	1.27	0.82
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.45	0.81
2:O:411:LYS:H	2:O:411:LYS:CE	1.93	0.80
1:C:54:GLN:HG3	1:C:184:ARG:NH2	1.96	0.80
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.64	0.79
1:C:100:ASP:CG	1:C:101:ALA:H	1.90	0.79
1:F:174:ARG:HE	1:F:181:THR:HG21	1.46	0.79
2:Q:390:LYS:HD2	6:Q:663:HOH:O	1.82	0.79
1:F:174:ARG:HE	1:F:181:THR:CG2	1.96	0.79
1:C:26:ALA:O	2:O:411:LYS:CE	2.30	0.78
1:F:78:GLU:HG2	2:R:301:PRO:HG2	1.63	0.78
1:D:98:THR:HB	1:D:100:ASP:OD1	1.84	0.78
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.30	0.76
2:M:497:ASN:ND2	2:M:499:GLU:H	1.84	0.76
2:O:411:LYS:H	2:O:411:LYS:HE2	1.50	0.76
2:Q:411:LYS:H	2:Q:411:LYS:HE2	1.50	0.75
1:F:177:VAL:O	1:F:180:LYS:HB3	1.85	0.75
1:F:100:ASP:CG	1:F:101:ALA:H	1.95	0.74
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.69	0.74
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.86	0.74
2:P:313:ARG:O	2:P:318:LYS:HE3	1.88	0.74
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:GLU:O	1:F:27:GLY:N	2.21	0.73
2:M:361:HIS:H	2:M:361:HIS:CD2	2.04	0.73
1:E:98:THR:OG1	1:E:102:GLY:N	2.21	0.73
1:D:24:GLU:O	1:D:27:GLY:N	2.21	0.73
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.71	0.73
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.53	0.73
1:B:176:GLU:HG3	1:B:180:LYS:O	1.88	0.73
2:R:361:HIS:H	2:R:361:HIS:HD2	1.34	0.73
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.72	0.72
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.13	0.72
2:N:361:HIS:CD2	2:N:361:HIS:H	2.08	0.72
2:O:413:ASP:C	2:O:414:ARG:HD2	2.14	0.72
1:A:163:GLN:HB2	6:A:819:HOH:O	1.89	0.72
1:D:64:ARG:NH1	1:D:64:ARG:HG2	2.01	0.71
1:A:165:GLN:CD	1:A:165:GLN:H	1.98	0.71
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.56	0.71
1:F:165:GLN:NE2	1:F:165:GLN:H	1.89	0.71
1:A:176:GLU:HG2	1:A:179:GLY:HA2	1.72	0.71
1:F:163:GLN:CB	1:F:165:GLN:HE22	2.04	0.70
1:F:165:GLN:H	1:F:165:GLN:CD	1.98	0.70
2:O:361:HIS:H	2:O:361:HIS:CD2	2.09	0.70
1:E:176:GLU:HG3	1:E:180:LYS:O	1.91	0.70
2:R:497:ASN:ND2	2:R:499:GLU:H	1.90	0.70
2:N:497:ASN:ND2	2:N:499:GLU:H	1.91	0.69
1:E:147:ASP:OD2	1:E:174:ARG:NH1	2.25	0.69
1:A:100:ASP:CG	1:A:101:ALA:H	2.01	0.69
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.57	0.69
1:F:64:ARG:HD3	1:F:99:PHE:O	1.93	0.69
2:R:497:ASN:HD22	2:R:499:GLU:H	1.39	0.69
1:E:165:GLN:H	1:E:165:GLN:HE21	0.76	0.68
2:P:411:LYS:HE2	2:P:411:LYS:H	0.64	0.68
2:O:390:LYS:HE2	6:O:798:HOH:O	1.94	0.68
2:P:361:HIS:H	2:P:361:HIS:CD2	2.12	0.68
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.58	0.68
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.09	0.68
1:F:110:LYS:NZ	1:F:148:GLU:OE2	2.17	0.68
1:C:165:GLN:NE2	1:C:165:GLN:H	1.91	0.67
2:P:376:GLU:OE1	6:P:675:HOH:O	2.11	0.67
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.77	0.67
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.10	0.67
1:E:26:ALA:O	2:Q:411:LYS:CE	2.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLU:O	1:E:27:GLY:N	2.27	0.66
2:R:411:LYS:H	2:R:411:LYS:HE2	1.60	0.66
1:E:65:ASP:OD2	1:E:133:ARG:HD3	1.96	0.66
1:F:50:LEU:HD12	1:F:51:LEU:N	2.11	0.66
1:C:54:GLN:HG3	1:C:184:ARG:HH21	1.62	0.66
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.31	0.65
1:B:176:GLU:OE2	1:B:179:GLY:C	2.39	0.65
1:F:98:THR:OG1	1:F:102:GLY:N	2.28	0.65
2:Q:410:HIS:HA	2:Q:411:LYS:HZ1	1.61	0.65
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.43	0.65
2:N:361:HIS:H	2:N:361:HIS:HD2	1.44	0.65
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.79	0.65
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.31	0.65
2:R:505:ILE:HG22	2:R:507:LYS:HE2	1.79	0.64
1:A:143:LEU:C	1:A:143:LEU:HD23	2.22	0.64
1:D:100:ASP:CG	1:D:101:ALA:H	2.04	0.64
1:A:64:ARG:NH1	1:A:100:ASP:O	2.31	0.64
1:A:176:GLU:HG3	1:A:180:LYS:O	1.98	0.64
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.80	0.64
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.79	0.64
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.45	0.64
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.62	0.64
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.32	0.64
1:C:98:THR:OG1	1:C:102:GLY:N	2.30	0.63
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.29	0.63
1:D:165:GLN:HE21	1:D:165:GLN:N	1.94	0.63
1:B:26:ALA:O	2:N:411:LYS:HE3	1.98	0.63
2:Q:505:ILE:O	2:Q:507:LYS:HE3	1.99	0.63
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.34	0.62
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.14	0.62
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.63	0.62
2:Q:411:LYS:NZ	2:Q:411:LYS:H	1.98	0.62
2:R:522:ARG:NH1	6:R:814:HOH:O	2.29	0.62
1:C:24:GLU:O	1:C:27:GLY:N	2.28	0.62
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.82	0.62
2:M:361:HIS:H	2:M:361:HIS:HD2	1.47	0.61
1:B:165:GLN:NE2	1:B:165:GLN:N	2.42	0.61
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.00	0.61
2:N:390:LYS:HE2	6:N:828:HOH:O	1.99	0.61
1:B:134:GLY:HA3	2:N:326:THR:HG22	1.81	0.61
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.83	0.61
1:D:3:GLU:HA	1:D:3:GLU:OE1	2.01	0.60
1:F:143:LEU:C	1:F:143:LEU:HD23	2.26	0.60
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.83	0.60
2:R:410:HIS:HA	2:R:411:LYS:NZ	2.15	0.60
2:Q:411:LYS:HE2	2:Q:411:LYS:N	2.17	0.60
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.02	0.60
1:D:19:ILE:O	2:P:426:VAL:HG21	2.01	0.60
1:C:98:THR:HB	1:C:100:ASP:OD1	2.01	0.60
2:M:448:PRO:HB2	2:P:516:MET:HA	1.82	0.59
1:F:26:ALA:O	2:R:411:LYS:CE	2.50	0.59
2:O:473:LYS:HD2	2:O:474:LEU:N	2.17	0.59
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.68	0.59
2:N:447:TYR:OH	5:N:550:PHB:H5	2.03	0.59
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.18	0.59
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.27	0.59
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.98	0.59
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.68	0.59
2:R:497:ASN:HD22	2:R:497:ASN:C	2.11	0.59
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.03	0.58
1:D:114:VAL:HG23	1:D:122:MET:HE3	1.84	0.58
2:P:361:HIS:H	2:P:361:HIS:HD2	1.51	0.58
1:C:100:ASP:CG	1:C:101:ALA:N	2.60	0.58
2:N:416:LEU:HD23	2:N:416:LEU:C	2.28	0.58
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.01	0.58
1:F:78:GLU:CG	2:R:301:PRO:HG2	2.32	0.58
2:R:413:ASP:C	2:R:414:ARG:HD2	2.29	0.58
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.67	0.58
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.38	0.58
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.86	0.58
2:R:411:LYS:NZ	2:R:411:LYS:H	2.01	0.58
1:C:176:GLU:HG3	1:C:180:LYS:O	2.04	0.57
1:B:52:LEU:C	1:B:52:LEU:HD22	2.29	0.57
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.19	0.57
2:R:416:LEU:C	2:R:416:LEU:HD23	2.30	0.57
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.34	0.57
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.92	0.57
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.87	0.57
1:C:165:GLN:H	1:C:165:GLN:CD	2.11	0.56
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.87	0.56
1:A:165:GLN:NE2	1:A:165:GLN:H	2.02	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.87	0.56
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.88	0.56
2:R:356:PHE:CD2	2:R:428:ARG:HD3	2.40	0.56
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.86	0.56
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.21	0.56
2:Q:522:ARG:NH1	6:Q:686:HOH:O	2.38	0.56
1:B:165:GLN:H	1:B:165:GLN:CD	2.11	0.56
2:O:361:HIS:CD2	6:O:766:HOH:O	2.59	0.56
1:A:24:GLU:O	1:A:27:GLY:N	2.34	0.55
2:R:361:HIS:CD2	2:R:361:HIS:N	2.67	0.55
2:R:376:GLU:OE1	6:R:782:HOH:O	2.17	0.55
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.89	0.55
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.37	0.55
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.41	0.55
1:F:50:LEU:HD12	1:F:50:LEU:C	2.31	0.55
1:D:64:ARG:HH11	1:D:64:ARG:CG	2.12	0.55
1:F:100:ASP:OD1	1:F:100:ASP:N	2.36	0.55
1:F:122:MET:HE3	1:F:125:HIS:HE1	1.72	0.55
2:M:390:LYS:HD2	6:M:644:HOH:O	2.06	0.55
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.24	0.55
2:M:448:PRO:CB	2:P:516:MET:HA	2.37	0.55
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.06	0.55
2:M:488:MET:HE1	2:P:508:LEU:HD23	1.89	0.54
1:D:176:GLU:HA	1:D:180:LYS:O	2.07	0.54
2:Q:410:HIS:HA	2:Q:411:LYS:NZ	2.22	0.54
1:C:177:VAL:O	1:C:180:LYS:HB3	2.07	0.54
1:D:26:ALA:O	2:P:411:LYS:NZ	2.39	0.54
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.70	0.54
2:P:478:LEU:C	2:P:478:LEU:HD23	2.33	0.54
2:N:448:PRO:HD3	2:N:456:TRP:CZ3	2.43	0.54
1:A:52:LEU:C	1:A:52:LEU:HD22	2.33	0.54
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.36	0.54
2:M:497:ASN:HD22	2:M:499:GLU:N	1.95	0.54
2:M:416:LEU:C	2:M:416:LEU:HD23	2.33	0.53
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.23	0.53
1:B:165:GLN:H	1:B:165:GLN:HE21	1.48	0.53
1:C:64:ARG:HG2	1:C:64:ARG:HH11	1.70	0.53
2:P:497:ASN:HD22	2:P:499:GLU:H	1.54	0.53
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.90	0.53
1:E:39:LEU:CD1	1:E:106:LEU:HD11	2.38	0.53
1:E:84:ASN:OD1	1:E:86:GLU:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.91	0.53
2:O:416:LEU:C	2:O:416:LEU:HD23	2.33	0.53
1:E:39:LEU:HD11	1:E:106:LEU:HD11	1.91	0.53
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.24	0.52
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.24	0.52
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.44	0.52
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.91	0.52
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.42	0.52
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.09	0.52
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.75	0.52
1:A:176:GLU:HA	1:A:180:LYS:O	2.08	0.52
2:R:534:HIS:HB2	2:R:535:PHE:CD1	2.45	0.52
2:M:390:LYS:HD3	6:M:720:HOH:O	2.09	0.52
2:N:478:LEU:C	2:N:478:LEU:HD23	2.34	0.52
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.40	0.52
2:M:364:LEU:HB2	2:M:440:ARG:HD3	1.91	0.52
2:O:376:GLU:O	2:O:442:ILE:HA	2.10	0.52
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.66	0.52
1:C:114:VAL:HG23	1:C:122:MET:CE	2.40	0.52
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.10	0.51
2:N:522:ARG:NH1	6:N:770:HOH:O	2.24	0.51
1:F:174:ARG:HD2	1:F:183:TYR:OH	2.09	0.51
2:M:376:GLU:HG2	2:P:446:PRO:HD2	1.91	0.51
2:R:410:HIS:HA	2:R:411:LYS:HZ3	1.73	0.51
2:N:376:GLU:O	2:N:442:ILE:HA	2.10	0.51
2:O:361:HIS:HD2	6:O:766:HOH:O	1.93	0.51
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.93	0.51
1:F:100:ASP:CG	1:F:101:ALA:N	2.64	0.51
2:R:399:MET:HA	2:R:462:HIS:O	2.10	0.51
1:B:123:ALA:HB3	1:B:144:TYR:CE1	2.46	0.51
2:Q:390:LYS:HD3	6:Q:743:HOH:O	2.10	0.51
1:F:78:GLU:HB3	1:F:80:GLN:NE2	2.26	0.51
1:F:36:TRP:CG	1:F:37:ASN:H	2.29	0.51
1:A:18:HIS:CE1	1:A:99:PHE:CE1	2.99	0.51
1:C:98:THR:OG1	1:C:101:ALA:HB3	2.11	0.51
1:B:165:GLN:N	1:B:165:GLN:HE21	2.06	0.51
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.92	0.51
1:B:98:THR:O	1:B:102:GLY:HA2	2.11	0.50
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.76	0.50
1:C:98:THR:HG1	1:C:101:ALA:HB3	1.76	0.50
1:E:100:ASP:CG	1:E:101:ALA:H	2.18	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.11	0.50
2:N:362:ASP:OD1	2:N:440:ARG:HD3	2.11	0.50
2:N:414:ARG:NE	2:N:414:ARG:HA	2.25	0.50
1:A:180:LYS:HG2	1:A:181:THR:N	2.26	0.50
1:B:176:GLU:HG3	1:B:180:LYS:C	2.36	0.50
1:F:56:TYR:CE1	1:F:62:LEU:HD23	2.46	0.50
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.47	0.50
2:Q:443:LYS:HE2	6:Q:714:HOH:O	2.11	0.50
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.20	0.50
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.47	0.50
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.93	0.50
2:R:306:SER:CB	2:R:530:GLN:HE21	2.24	0.50
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.93	0.49
1:F:18:HIS:HD1	1:F:99:PHE:HZ	1.59	0.49
1:D:18:HIS:HD1	1:D:99:PHE:HZ	1.59	0.49
2:P:390:LYS:HD2	6:P:681:HOH:O	2.13	0.49
2:P:416:LEU:C	2:P:416:LEU:HD23	2.38	0.49
1:F:51:LEU:HD12	1:F:106:LEU:HD23	1.95	0.49
1:F:174:ARG:HD2	1:F:183:TYR:CZ	2.47	0.49
1:F:50:LEU:HB2	1:F:180:LYS:HE2	1.94	0.49
1:F:80:GLN:O	1:F:91:SER:HB2	2.13	0.49
2:N:447:TYR:CE1	2:N:460:HIS:HE1	2.31	0.48
2:N:413:ASP:C	2:N:414:ARG:HD2	2.38	0.48
1:E:176:GLU:HG3	1:E:180:LYS:C	2.37	0.48
1:F:147:ASP:OD2	1:F:174:ARG:NH1	2.46	0.48
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.81	0.48
1:D:24:GLU:O	1:D:27:GLY:CA	2.62	0.48
2:N:497:ASN:HD22	2:N:499:GLU:N	2.04	0.48
2:R:405:GLY:HA3	6:R:792:HOH:O	2.13	0.48
2:R:505:ILE:HG22	2:R:507:LYS:CE	2.43	0.48
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.96	0.48
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.77	0.48
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.95	0.48
1:E:41:LYS:HD2	1:E:87:ASN:O	2.13	0.48
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.49	0.48
2:N:414:ARG:HD2	2:N:414:ARG:N	2.29	0.47
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.43	0.47
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.11	0.47
2:M:362:ASP:CG	2:M:440:ARG:HD2	2.39	0.47
2:P:356:PHE:HD1	2:P:428:ARG:HD3	1.79	0.47
1:E:18:HIS:CE1	6:E:843:HOH:O	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.47	0.47
1:F:147:ASP:OD2	1:F:183:TYR:OH	2.32	0.47
2:O:356:PHE:HD2	2:O:428:ARG:HD2	1.79	0.47
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.44	0.47
2:O:411:LYS:HE2	2:O:411:LYS:N	2.23	0.47
1:F:18:HIS:HE1	1:F:99:PHE:HE1	1.62	0.47
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.25	0.47
2:O:361:HIS:H	2:O:361:HIS:HD2	1.59	0.47
1:E:176:GLU:HA	1:E:180:LYS:O	2.13	0.47
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.96	0.47
1:D:25:ALA:C	1:D:27:GLY:N	2.71	0.47
1:E:36:TRP:CG	1:E:37:ASN:H	2.33	0.47
2:Q:392:VAL:HG12	2:Q:395:THR:HB	1.96	0.47
1:A:133:ARG:HG3	2:M:326:THR:HG21	1.96	0.47
2:M:447:TYR:HB2	2:M:448:PRO:HD2	1.95	0.47
1:C:50:LEU:O	1:C:182:ALA:HA	2.15	0.47
2:O:356:PHE:CD2	2:O:428:ARG:HD3	2.50	0.47
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.30	0.47
1:F:25:ALA:C	1:F:27:GLY:H	2.23	0.47
1:F:147:ASP:OD2	1:F:174:ARG:CD	2.63	0.47
2:R:408:TYR:HE1	2:R:447:TYR:CZ	2.33	0.47
2:O:497:ASN:C	2:O:497:ASN:HD22	2.22	0.47
1:D:100:ASP:CG	1:D:101:ALA:N	2.72	0.47
1:D:165:GLN:H	1:D:165:GLN:CD	2.20	0.47
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.96	0.47
2:Q:416:LEU:C	2:Q:416:LEU:CD2	2.86	0.47
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.30	0.47
1:B:100:ASP:CG	1:B:101:ALA:H	2.23	0.47
1:D:39:LEU:HD13	1:D:106:LEU:HD21	1.97	0.47
1:E:98:THR:HG1	1:E:103:GLU:H	1.62	0.47
2:R:505:ILE:O	2:R:507:LYS:HE3	2.15	0.47
2:P:410:HIS:HA	2:P:411:LYS:NZ	2.30	0.47
1:A:50:LEU:O	1:A:182:ALA:HA	2.15	0.46
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.97	0.46
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.74	0.46
1:D:25:ALA:C	1:D:27:GLY:H	2.22	0.46
1:C:36:TRP:CG	1:C:37:ASN:H	2.33	0.46
1:C:64:ARG:HH11	1:C:64:ARG:CG	2.27	0.46
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.83	0.46
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.98	0.46
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.45	0.46
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.15	0.46
2:O:497:ASN:HD22	2:O:499:GLU:H	1.64	0.46
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.72	0.46
1:C:176:GLU:HG3	1:C:180:LYS:C	2.41	0.46
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.98	0.46
1:D:188:ARG:HG3	1:D:188:ARG:HH11	1.81	0.46
2:P:359:HIS:O	2:P:366:ASN:HB3	2.16	0.46
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.51	0.46
2:R:411:LYS:HE2	2:R:411:LYS:HB2	1.62	0.46
2:R:447:TYR:OH	5:R:550:PHB:H5	2.16	0.46
1:A:165:GLN:CD	1:A:165:GLN:N	2.72	0.46
2:N:359:HIS:O	2:N:366:ASN:HB3	2.16	0.46
1:D:36:TRP:CG	1:D:37:ASN:H	2.34	0.46
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.97	0.46
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.98	0.45
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.45	0.45
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.98	0.45
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.97	0.45
2:O:356:PHE:HD2	2:O:428:ARG:CD	2.28	0.45
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.31	0.45
1:B:177:VAL:O	1:B:180:LYS:HB3	2.16	0.45
1:C:18:HIS:CE1	6:C:843:HOH:O	2.69	0.45
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.15	0.45
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.31	0.45
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.16	0.45
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.98	0.45
2:N:486:ILE:HB	2:N:487:PRO:HD3	1.97	0.45
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.32	0.45
2:R:400:TRP:HA	2:R:425:GLY:O	2.16	0.45
1:B:114:VAL:HG23	1:B:122:MET:CE	2.43	0.45
2:O:399:MET:HA	2:O:462:HIS:O	2.16	0.45
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.47	0.45
2:R:516:MET:HB3	2:R:516:MET:HE3	1.79	0.45
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.80	0.45
1:A:100:ASP:CG	1:A:101:ALA:N	2.73	0.45
1:E:143:LEU:HD23	1:E:143:LEU:C	2.42	0.45
2:R:362:ASP:OD1	2:R:440:ARG:HD2	2.17	0.45
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.99	0.45
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.99	0.44
1:F:24:GLU:O	1:F:27:GLY:CA	2.65	0.44

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	2.62	0.44
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.85	0.44
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.17	0.44
2:P:410:HIS:HA	2:P:411:LYS:CE	2.47	0.44
2:P:416:LEU:C	2:P:416:LEU:CD2	2.91	0.44
1:E:163:GLN:HB3	1:E:165:GLN:HE22	1.80	0.44
2:Q:411:LYS:HE2	2:Q:411:LYS:HB2	1.69	0.44
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.52	0.44
2:N:497:ASN:HD22	2:N:497:ASN:C	2.25	0.44
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.52	0.44
2:O:414:ARG:HD2	2:O:414:ARG:N	2.31	0.44
2:O:497:ASN:ND2	2:O:499:GLU:H	2.15	0.44
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.80	0.44
2:M:400:TRP:HA	2:M:425:GLY:O	2.17	0.44
1:B:176:GLU:HG3	1:B:180:LYS:N	2.33	0.44
1:D:24:GLU:O	1:D:27:GLY:HA2	2.18	0.44
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.18	0.44
1:B:64:ARG:HD3	1:B:99:PHE:O	2.17	0.44
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.89	0.44
1:F:176:GLU:HA	1:F:180:LYS:O	2.18	0.44
2:M:413:ASP:O	2:M:414:ARG:NH1	2.51	0.43
2:P:313:ARG:O	2:P:318:LYS:CE	2.61	0.43
2:P:318:LYS:HA	2:P:318:LYS:HD3	1.57	0.43
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.82	0.43
2:R:473:LYS:HD2	2:R:474:LEU:N	2.33	0.43
1:B:147:ASP:OD2	1:B:183:TYR:OH	2.29	0.43
1:A:18:HIS:CE1	1:A:99:PHE:HE1	2.36	0.43
1:B:180:LYS:HD2	1:B:181:THR:N	2.33	0.43
1:D:64:ARG:NH1	1:D:64:ARG:CG	2.64	0.43
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.99	0.43
1:E:68:LEU:HD12	1:E:68:LEU:N	2.34	0.43
2:Q:414:ARG:HD2	2:Q:414:ARG:N	2.32	0.43
2:R:411:LYS:H	2:R:411:LYS:CD	2.30	0.43
1:B:20:GLY:C	1:B:21:LEU:HD23	2.43	0.43
1:D:18:HIS:CE1	1:D:99:PHE:CE1	3.06	0.43
1:B:155:CYS:O	1:B:159:ASN:ND2	2.49	0.43
2:R:314:ASN:OD1	2:R:318:LYS:HE2	2.19	0.43
1:A:100:ASP:OD1	1:A:100:ASP:N	2.41	0.43
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.49	0.43
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.80	0.43
2:O:356:PHE:CE2	2:O:428:ARG:HD3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:393:PRO:O	2:O:393:PRO:HG2	2.18	0.43
2:P:400:TRP:HA	2:P:425:GLY:O	2.18	0.43
1:B:50:LEU:HD11	1:B:105:THR:HB	2.01	0.43
1:B:144:TYR:CE2	1:B:158:LEU:HD13	2.53	0.43
2:N:373:PRO:HB3	2:N:423:PHE:HB2	2.01	0.43
2:O:478:LEU:HD12	2:O:523:PHE:CD2	2.54	0.43
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.34	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.01	0.43
2:N:416:LEU:HD23	2:N:417:ALA:N	2.33	0.43
1:D:164:PRO:O	1:D:167:ARG:HB2	2.19	0.43
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.84	0.43
1:C:26:ALA:O	2:O:411:LYS:HE3	2.15	0.42
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.01	0.42
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.54	0.42
1:F:174:ARG:NE	1:F:181:THR:HG21	2.25	0.42
2:R:356:PHE:HD2	2:R:428:ARG:HD3	1.81	0.42
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.55	0.42
1:C:19:ILE:HD13	1:C:19:ILE:HG21	1.81	0.42
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.84	0.42
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.79	0.42
2:R:416:LEU:HD23	2:R:417:ALA:N	2.34	0.42
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.35	0.42
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.35	0.42
1:F:74:ASP:HB2	6:F:690:HOH:O	2.19	0.42
2:R:437:TYR:CD1	2:R:437:TYR:C	2.97	0.42
1:A:155:CYS:HB3	1:A:158:LEU:HB2	2.02	0.42
2:M:517:ASP:C	2:M:517:ASP:OD1	2.63	0.42
1:C:84:ASN:OD1	1:C:86:GLU:HB2	2.20	0.42
2:O:437:TYR:CD1	2:O:437:TYR:C	2.97	0.42
1:D:51:LEU:O	1:D:105:THR:HA	2.20	0.42
1:E:92:PHE:CD1	2:Q:349:PRO:HG3	2.54	0.42
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.55	0.42
1:A:44:ALA:O	1:A:48:HIS:NE2	2.42	0.42
2:N:516:MET:HE3	2:N:516:MET:HB3	1.94	0.42
1:C:143:LEU:HD23	1:C:143:LEU:C	2.45	0.42
1:D:143:LEU:C	1:D:143:LEU:HD23	2.45	0.42
1:D:191:GLY:O	1:D:194:GLU:HB2	2.19	0.42
2:Q:307:ARG:HD3	2:Q:307:ARG:HA	1.86	0.42
2:Q:488:MET:CE	1:F:1:PRO:HG2	2.49	0.42
1:F:176:GLU:HG3	1:F:180:LYS:N	2.34	0.42
2:R:497:ASN:HD22	2:R:498:PRO:N	2.16	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:328:ILE:HD12	2:N:335:ALA:HB2	2.01	0.42
2:M:383:ARG:HH11	2:M:383:ARG:HD3	1.57	0.42
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.54	0.42
1:D:50:LEU:O	1:D:182:ALA:HA	2.20	0.42
2:P:360:ASP:HB3	2:P:428:ARG:CG	2.50	0.42
1:E:61:HIS:CE1	1:F:163:GLN:HG3	2.54	0.42
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.80	0.42
1:D:150:GLN:O	1:D:154:LYS:HG2	2.20	0.42
1:E:33:GLN:HG2	1:E:85:LEU:HD12	2.01	0.42
1:F:50:LEU:CB	1:F:180:LYS:HE2	2.50	0.42
1:A:176:GLU:OE2	1:A:179:GLY:C	2.63	0.41
2:M:534:HIS:HD1	2:M:534:HIS:C	2.28	0.41
1:F:131:PHE:O	1:F:132:ALA:HB2	2.20	0.41
1:B:176:GLU:OE2	1:B:179:GLY:O	2.38	0.41
1:E:100:ASP:OD1	1:E:100:ASP:N	2.45	0.41
2:R:363:LEU:HD23	2:R:425:GLY:HA2	2.01	0.41
2:R:411:LYS:HE2	2:R:411:LYS:N	2.31	0.41
1:B:4:LEU:HD22	2:P:511:ASN:CG	2.45	0.41
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.50	0.41
1:F:50:LEU:O	1:F:182:ALA:HA	2.20	0.41
2:R:360:ASP:HB3	2:R:428:ARG:HG3	2.02	0.41
1:C:100:ASP:OD1	1:C:100:ASP:N	2.32	0.41
2:Q:399:MET:HA	2:Q:462:HIS:O	2.19	0.41
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	3.08	0.41
1:B:115:ASN:HA	1:B:121:PRO:HA	2.03	0.41
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.55	0.41
2:P:437:TYR:CD1	2:P:437:TYR:C	2.99	0.41
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.64	0.41
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.55	0.41
2:M:360:ASP:HB3	2:M:428:ARG:HG3	2.03	0.41
1:C:131:PHE:O	1:C:132:ALA:HB2	2.21	0.41
1:E:165:GLN:NE2	1:E:165:GLN:N	2.41	0.41
2:M:362:ASP:OD1	2:M:440:ARG:CD	2.68	0.41
2:N:400:TRP:HA	2:N:425:GLY:O	2.21	0.41
1:D:35:ILE:HG21	1:D:92:PHE:CE2	2.55	0.41
1:E:5:LEU:HA	1:E:6:PRO:HD3	1.86	0.41
1:E:188:ARG:HH11	1:E:188:ARG:HG3	1.84	0.41
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.68	0.41
1:E:188:ARG:HG3	1:E:188:ARG:NH1	2.36	0.41
1:A:25:ALA:C	1:A:27:GLY:H	2.29	0.41
1:A:78:GLU:HG2	2:M:301:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:478:LEU:HD23	2:O:478:LEU:C	2.46	0.41
1:D:52:LEU:C	1:D:52:LEU:HD22	2.46	0.41
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.74	0.41
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.03	0.41
1:E:51:LEU:HD11	1:E:126:ILE:HD12	2.03	0.41
1:F:98:THR:O	1:F:102:GLY:HA2	2.21	0.41
1:F:158:LEU:HD12	1:F:161:ILE:HD12	2.02	0.41
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.51	0.41
2:R:383:ARG:HA	2:R:435:GLY:O	2.21	0.41
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.50	0.40
2:N:383:ARG:HG3	2:N:436:TYR:CZ	2.56	0.40
2:O:381:ALA:O	2:O:522:ARG:HA	2.21	0.40
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.79	0.40
1:E:74:ASP:N	1:E:78:GLU:O	2.50	0.40
1:E:114:VAL:HG23	1:E:122:MET:CE	2.51	0.40
2:Q:396:LEU:HA	2:Q:396:LEU:HD12	1.90	0.40
1:C:52:LEU:CD2	1:C:184:ARG:HH12	2.35	0.40
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.35	0.40
1:B:74:ASP:HB2	6:B:690:HOH:O	2.19	0.40
1:D:18:HIS:CE1	6:D:843:HOH:O	2.75	0.40
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.57	0.40
2:P:487:PRO:O	2:P:493:LYS:HD3	2.21	0.40
1:E:52:LEU:HA	1:E:104:TRP:O	2.21	0.40
1:F:53:GLY:HA3	1:F:185:PHE:O	2.20	0.40
1:F:113:VAL:HG13	1:F:122:MET:O	2.22	0.40
1:A:36:TRP:CG	1:A:37:ASN:H	2.39	0.40
1:B:143:LEU:HD23	1:B:143:LEU:C	2.46	0.40
1:E:122:MET:HE3	1:E:122:MET:HB2	1.95	0.40
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.75	0.40
1:D:77:GLY:O	1:D:114:VAL:HG12	2.22	0.40
1:D:177:VAL:O	1:D:180:LYS:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	13/200 (6%)	12 (92%)	1 (8%)	0	100	100
1	D	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	224 (98%)	5 (2%)	0	100	100
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
All	All	1523/1752 (87%)	1469 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/163 (63%)	96 (93%)	7 (7%)	14	5
1	B	162/163 (99%)	152 (94%)	10 (6%)	16	7
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	14
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	10
1	E	162/163 (99%)	155 (96%)	7 (4%)	26	14
1	F	162/163 (99%)	154 (95%)	8 (5%)	22	10
2	M	196/202 (97%)	185 (94%)	11 (6%)	19	8
2	N	196/202 (97%)	184 (94%)	12 (6%)	17	7
2	O	196/202 (97%)	188 (96%)	8 (4%)	27	16
2	P	196/202 (97%)	185 (94%)	11 (6%)	19	8
2	Q	196/202 (97%)	187 (95%)	9 (5%)	24	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	196/202 (97%)	187 (95%)	9 (5%)	24	12
All	All	2089/2190 (95%)	1982 (95%)	107 (5%)	21	10

All (107) 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	78	GLU
1	A	106	LEU
1	A	143	LEU
1	A	165	GLN
2	M	372	LEU
2	M	395	THR
2	M	411	LYS
2	M	416	LEU
2	M	434	ASP
2	M	440	ARG
2	M	442	ILE
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	52	LEU
1	B	106	LEU
1	B	141	THR
1	B	150	GLN
1	B	165	GLN
1	B	176	GLU
1	B	184	ARG
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	433	SER
2	N	440	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	442	ILE
2	N	497	ASN
2	N	499	GLU
2	N	507	LYS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	78	GLU
1	C	106	LEU
1	C	165	GLN
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	434	ASP
2	O	442	ILE
2	O	465	ILE
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	42	PRO
1	D	52	LEU
1	D	106	LEU
1	D	133	ARG
1	D	165	GLN
2	P	395	THR
2	P	411	LYS
2	P	414	ARG
2	P	416	LEU
2	P	434	ASP
2	P	440	ARG
2	P	478	LEU
2	P	488	MET
2	P	503	GLN
2	P	507	LYS
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	68	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	372	LEU
2	Q	395	THR
2	Q	411	LYS
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	440	ARG
2	Q	499	GLU
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	50	LEU
1	F	52	LEU
1	F	114	VAL
1	F	165	GLN
1	F	178	ASP
1	F	180	LYS
2	R	372	LEU
2	R	395	THR
2	R	411	LYS
2	R	416	LEU
2	R	434	ASP
2	R	442	ILE
2	R	473	LYS
2	R	478	LEU
2	R	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	163	GLN
1	A	165	GLN
2	M	314	ASN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
2	M	514	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	140	HIS
1	B	163	GLN
1	B	165	GLN
2	N	361	HIS
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	28	ASN
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	59	ASN
1	D	163	GLN
1	D	165	GLN
2	P	305	ASN
2	P	359	HIS
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	514	ASN
2	P	530	GLN
1	E	54	GLN
1	E	59	ASN
1	E	140	HIS
1	E	163	GLN
1	E	165	GLN
2	Q	334	GLN
2	Q	361	HIS
2	Q	394	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	165	GLN
2	R	334	GLN
2	R	361	HIS
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 oligosaccharides 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	PHB	O	551	-	10,10,10	1.45	2 (20%)	13,13,13	0.85	0
4	BME	P	601	2	3,3,3	0.62	0	2,2,2	0.84	0
5	PHB	P	551	-	10,10,10	1.23	1 (10%)	13,13,13	1.00	0
5	PHB	N	550	3	10,10,10	0.99	1 (10%)	13,13,13	0.90	0
4	BME	M	601	2	3,3,3	0.37	0	2,2,2	0.56	0
5	PHB	O	550	3	10,10,10	1.37	2 (20%)	13,13,13	1.17	1 (7%)
5	PHB	Q	550	3	10,10,10	1.28	1 (10%)	13,13,13	1.08	1 (7%)
4	BME	O	601	2	3,3,3	0.65	0	2,2,2	0.75	0
5	PHB	Q	551	-	10,10,10	1.35	1 (10%)	13,13,13	0.95	1 (7%)
5	PHB	R	551	-	10,10,10	1.12	1 (10%)	13,13,13	1.05	1 (7%)
4	BME	Q	601	2	3,3,3	0.68	0	2,2,2	0.89	0
5	PHB	M	551	-	10,10,10	1.24	1 (10%)	13,13,13	1.23	2 (15%)
5	PHB	R	550	3	10,10,10	1.15	1 (10%)	13,13,13	0.90	1 (7%)
5	PHB	N	551	-	10,10,10	1.28	1 (10%)	13,13,13	0.99	1 (7%)
4	BME	R	601	2	3,3,3	0.31	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BME	N	601	2	3,3,3	0.20	0	2,2,2	0.13	0
5	PHB	M	550	3	10,10,10	1.38	3 (30%)	13,13,13	1.40	2 (15%)
5	PHB	P	550	3	10,10,10	1.14	1 (10%)	13,13,13	1.30	2 (15%)

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	PHB	O	551	-	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
5	PHB	P	551	-	-	0/4/4/4	0/1/1/1
5	PHB	N	550	3	-	0/4/4/4	0/1/1/1
4	BME	M	601	2	-	0/1/1/1	-
5	PHB	O	550	3	-	0/4/4/4	0/1/1/1
5	PHB	Q	550	3	-	0/4/4/4	0/1/1/1
4	BME	O	601	2	-	1/1/1/1	-
5	PHB	Q	551	-	-	0/4/4/4	0/1/1/1
5	PHB	R	551	-	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	-
5	PHB	M	551	-	-	0/4/4/4	0/1/1/1
5	PHB	R	550	3	-	0/4/4/4	0/1/1/1
5	PHB	N	551	-	-	0/4/4/4	0/1/1/1
4	BME	R	601	2	-	1/1/1/1	-
4	BME	N	601	2	-	1/1/1/1	-
5	PHB	M	550	3	-	0/4/4/4	0/1/1/1
5	PHB	P	550	3	-	0/4/4/4	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	551	PHB	C1-C1'	2.96	1.55	1.49
5	M	551	PHB	C1-C1'	2.83	1.55	1.49
5	Q	551	PHB	C1-C1'	2.56	1.54	1.49
5	O	551	PHB	C2-C1	2.55	1.43	1.39
5	P	551	PHB	C1-C1'	2.50	1.54	1.49
5	O	551	PHB	C1-C1'	2.50	1.54	1.49
5	R	551	PHB	C1-C1'	2.40	1.54	1.49
5	O	550	PHB	O2'-C1'	-2.38	1.23	1.30
5	M	550	PHB	O2'-C1'	-2.28	1.23	1.30
5	Q	550	PHB	C1-C1'	2.27	1.54	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	PHB	O2'-C1'	-2.26	1.23	1.30
5	R	550	PHB	C1-C1'	2.25	1.54	1.49
5	M	550	PHB	C3-C2	2.18	1.42	1.38
5	O	550	PHB	C1-C1'	2.15	1.54	1.49
5	N	550	PHB	C1-C1'	2.08	1.53	1.49
5	M	550	PHB	C1-C1'	2.04	1.53	1.49

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	550	PHB	O2'-C1'-O1'	-3.75	115.29	123.35
5	M	551	PHB	O2'-C1'-C1	3.04	122.64	114.84
5	P	550	PHB	O2'-C1'-O1'	-3.01	116.87	123.35
5	M	551	PHB	O2'-C1'-O1'	-2.96	117.00	123.35
5	N	551	PHB	O2'-C1'-C1	2.77	121.96	114.84
5	R	551	PHB	O2'-C1'-O1'	-2.46	118.06	123.35
5	Q	551	PHB	O2'-C1'-C1	2.33	120.83	114.84
5	P	550	PHB	O2'-C1'-C1	2.32	120.79	114.84
5	R	550	PHB	O2'-C1'-O1'	-2.25	118.52	123.35
5	O	550	PHB	O2'-C1'-O1'	-2.18	118.66	123.35
5	M	550	PHB	O2'-C1'-C1	2.03	120.06	114.84
5	Q	550	PHB	O2'-C1'-O1'	-2.00	119.05	123.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	550	PHB	1	0
5	R	550	PHB	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.