Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:00 PM EDT

PDB ID	:	2OBE
Title	:	Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
Authors	:	Xue, F.; Rux, J.J.; Burnett, R.M.
Deposited on	:	2006-12-18
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

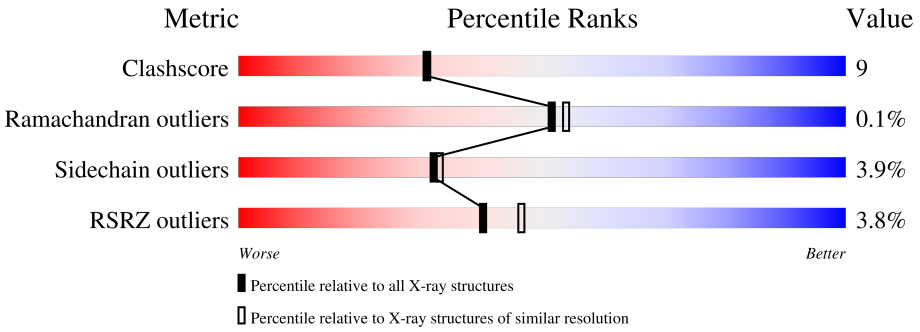
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	932	3% 83% 14% • •
1	B	932	3% 81% 14% • •
1	C	932	5% 78% 17% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2HP	A	1619	-	X	-	-
2	2HP	B	1605	-	X	-	-
2	2HP	B	1607	-	X	-	-
2	2HP	B	1609	-	X	-	-
2	2HP	B	1615	-	X	-	-
3	MPD	A	1704	X	-	X	-
3	MPD	A	1717	X	-	-	-
3	MPD	A	1720	X	-	X	-
3	MPD	B	1703	-	-	X	-
3	MPD	B	1709	-	-	X	-
3	MPD	B	1711	-	-	X	-
3	MPD	B	1718	X	-	-	-
3	MPD	B	1719	X	-	-	-
3	MPD	B	1721	X	-	-	-
3	MPD	B	1722	X	-	-	-
3	MPD	B	1724	X	-	-	-
3	MPD	C	1713	X	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23334 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.

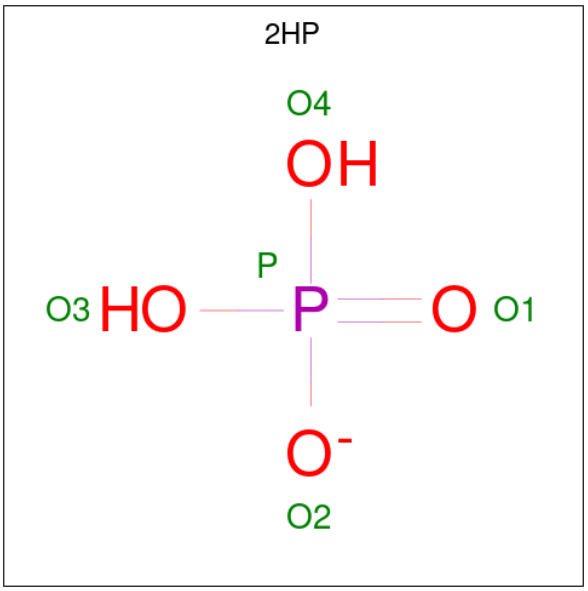
- Molecule 1 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	915	7208	4582	1217	1377	32	2	0	0
1	B	906	7169	4562	1206	1369	32	2	0	0
1	C	909	7134	4540	1201	1361	32	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	825	ASN	UNK	conflict	UNP Q8UY79
A	921	LEU	UNK	conflict	UNP Q8UY79
B	825	ASN	UNK	conflict	UNP Q8UY79
B	921	LEU	UNK	conflict	UNP Q8UY79
C	825	ASN	UNK	conflict	UNP Q8UY79
C	921	LEU	UNK	conflict	UNP Q8UY79

- Molecule 2 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H_2O_4P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	A	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0
			Total	O	P			
2	B	1	5	4	1		0	0

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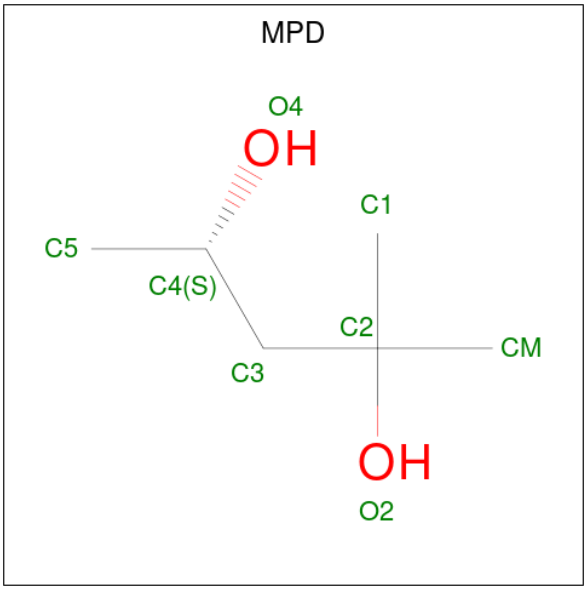
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	8	6	2		0	0
3	A	1	8	6	2		0	0
3	A	1	8	6	2		0	0
3	A	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	B	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0

- Molecule 4 is water.

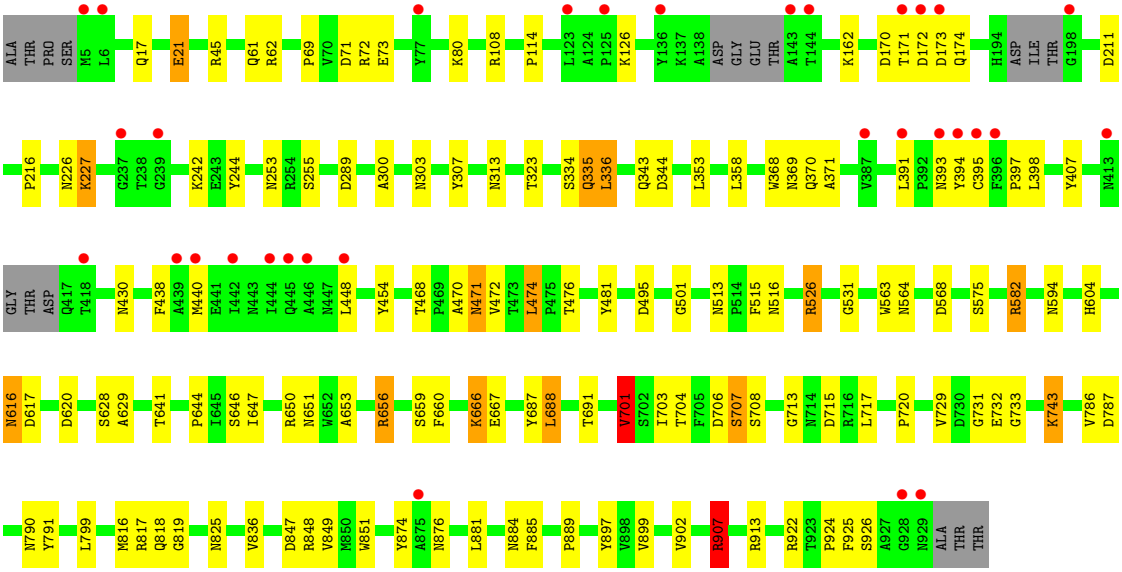
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	542	542	542	0	0
			Total	O		
4	B	563	563	563	0	0
			Total	O		
4	C	416	416	416	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

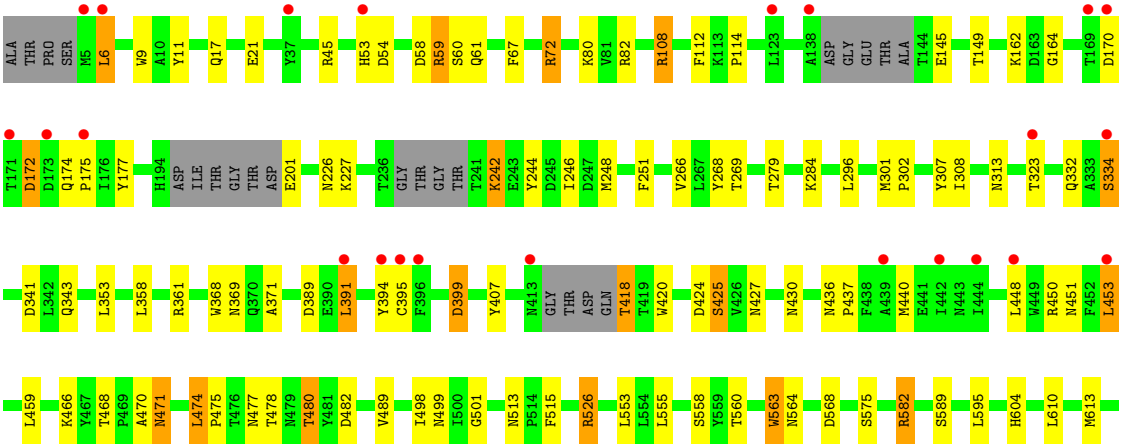
- Molecule 1: Hexon protein

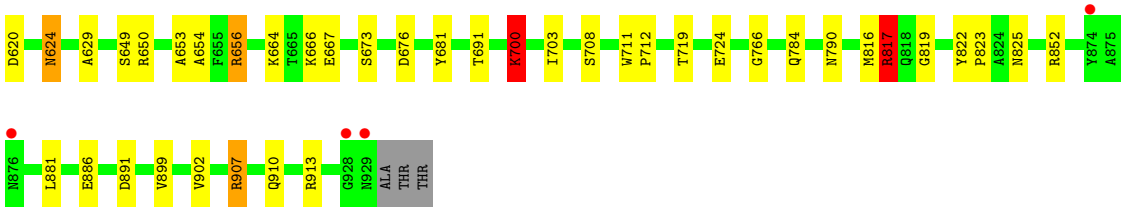
Chain A:



- Molecule 1: Hexon protein

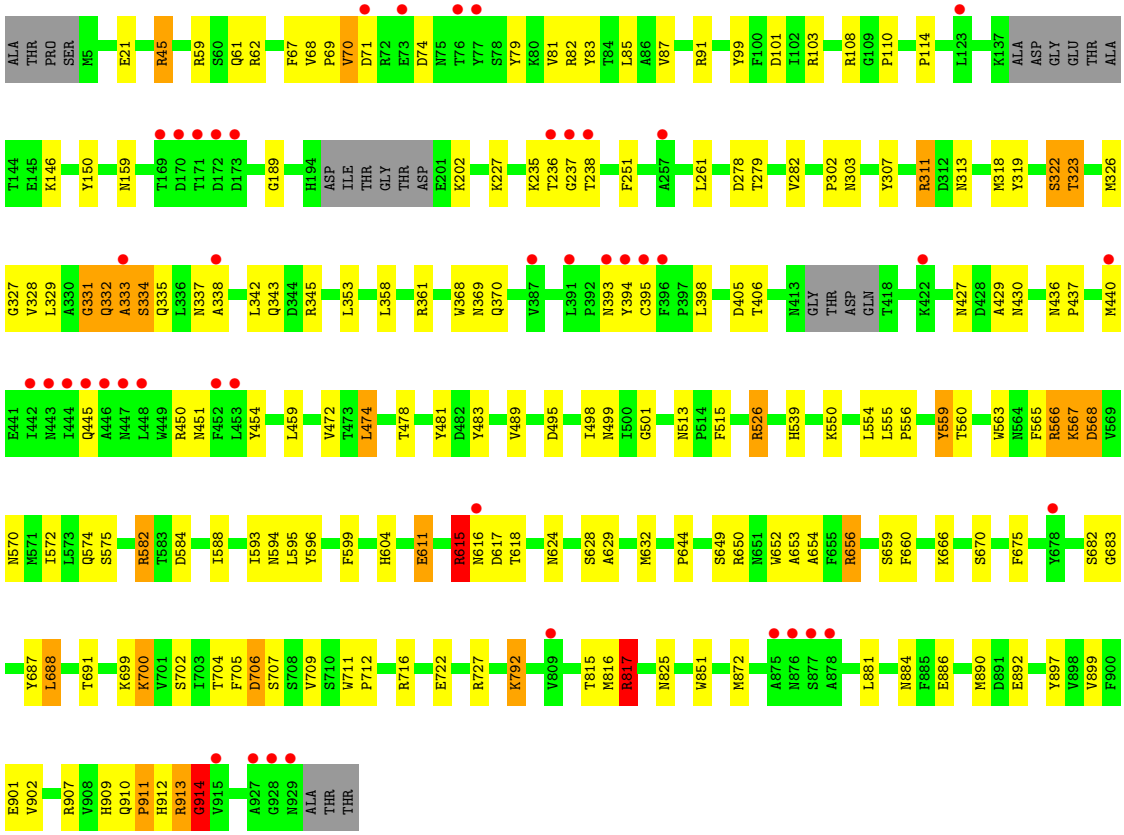
Chain B:





• Molecule 1: Hexon protein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	90.80Å 433.00Å 159.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.10 49.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.10) 93.7 (49.25-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.169 , 0.210 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23334	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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: MPD, 2HP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	9/7404 (0.1%)	0.95	21/10090 (0.2%)
1	B	1.00	10/7364 (0.1%)	1.04	24/10034 (0.2%)
1	C	1.22	42/7328 (0.6%)	1.02	32/9991 (0.3%)
All	All	1.07	61/22096 (0.3%)	1.00	77/30115 (0.3%)

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
1	B	0	1
1	C	0	5
All	All	0	7

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	825	ASN	CG-OD1	-30.50	0.56	1.24
1	B	825	ASN	CG-OD1	-24.34	0.70	1.24
1	C	615	ARG	NE-CZ	22.69	1.62	1.33
1	C	914	GLY	C-O	19.38	1.54	1.23
1	C	328	VAL	C-O	18.29	1.58	1.23
1	B	425	SER	CB-OG	17.80	1.65	1.42
1	C	912	HIS	C-O	12.83	1.47	1.23
1	C	825	ASN	CG-ND2	12.31	1.63	1.32
1	A	733	GLY	CA-C	11.98	1.71	1.51
1	C	337	ASN	C-N	11.06	1.59	1.34
1	C	70	VAL	C-O	10.76	1.43	1.23
1	C	567	LYS	CE-NZ	10.35	1.75	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	825	ASN	CG-OD1	-9.96	1.02	1.24
1	C	707	SER	C-O	9.73	1.41	1.23
1	C	913	ARG	CA-C	8.96	1.76	1.52
1	B	825	ASN	CG-ND2	8.34	1.53	1.32
1	A	731	GLY	C-N	8.25	1.53	1.34
1	C	566	ARG	CZ-NH1	8.16	1.43	1.33
1	A	707	SER	CB-OG	7.99	1.52	1.42
1	C	68	VAL	C-O	7.93	1.38	1.23
1	C	615	ARG	CZ-NH1	7.88	1.43	1.33
1	A	704	THR	C-N	7.82	1.52	1.34
1	C	912	HIS	CA-CB	7.68	1.70	1.53
1	C	914	GLY	N-CA	-7.64	1.34	1.46
1	C	278	ASP	CB-CG	-7.49	1.36	1.51
1	C	332	GLN	CB-CG	7.37	1.72	1.52
1	C	335	GLN	C-O	7.28	1.37	1.23
1	C	582	ARG	CZ-NH1	7.27	1.42	1.33
1	C	395	CYS	CB-SG	7.15	1.94	1.82
1	C	559	TYR	CG-CD2	7.12	1.48	1.39
1	C	912	HIS	C-N	7.00	1.50	1.34
1	C	327	GLY	CA-C	7.00	1.63	1.51
1	C	323	THR	C-N	6.94	1.45	1.33
1	B	11	TYR	CE2-CZ	6.85	1.47	1.38
1	C	594	ASN	CG-OD1	6.66	1.38	1.24
1	C	706	ASP	C-O	6.60	1.35	1.23
1	A	743	LYS	CE-NZ	6.23	1.64	1.49
1	A	732	GLU	CD-OE2	6.11	1.32	1.25
1	C	611	GLU	CD-OE2	6.07	1.32	1.25
1	C	323	THR	C-O	6.06	1.34	1.23
1	C	566	ARG	CG-CD	6.01	1.67	1.51
1	B	108	ARG	CD-NE	-5.99	1.36	1.46
1	C	567	LYS	CD-CE	5.96	1.66	1.51
1	B	11	TYR	CG-CD1	5.92	1.46	1.39
1	C	611	GLU	CB-CG	5.88	1.63	1.52
1	B	11	TYR	CG-CD2	5.84	1.46	1.39
1	C	395	CYS	CA-CB	5.82	1.66	1.53
1	B	395	CYS	CA-CB	5.72	1.66	1.53
1	C	333	ALA	C-N	5.70	1.47	1.34
1	A	526	ARG	CG-CD	5.64	1.66	1.51
1	A	526	ARG	CD-NE	-5.59	1.36	1.46
1	C	322	SER	CB-OG	5.57	1.49	1.42
1	C	21	GLU	CG-CD	5.46	1.60	1.51
1	C	554	LEU	CG-CD2	5.43	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	ARG	CD-NE	-5.42	1.37	1.46
1	C	87	VAL	CB-CG2	5.31	1.64	1.52
1	B	11	TYR	CE1-CZ	5.27	1.45	1.38
1	C	342	LEU	CA-CB	5.26	1.65	1.53
1	C	914	GLY	CA-C	5.24	1.60	1.51
1	C	911	PRO	C-O	5.22	1.33	1.23
1	C	582	ARG	CZ-NH2	5.12	1.39	1.33

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	526	ARG	NE-CZ-NH2	-24.16	108.22	120.30
1	B	817	ARG	NE-CZ-NH2	-23.25	108.68	120.30
1	A	526	ARG	NE-CZ-NH2	-22.85	108.87	120.30
1	B	817	ARG	NE-CZ-NH1	20.77	130.69	120.30
1	B	656	ARG	NE-CZ-NH2	-19.11	110.74	120.30
1	C	278	ASP	CB-CG-OD1	-16.92	103.07	118.30
1	B	526	ARG	NE-CZ-NH1	16.81	128.70	120.30
1	A	526	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	C	817	ARG	NE-CZ-NH2	-16.27	112.17	120.30
1	C	825	ASN	CB-CG-ND2	-16.01	78.28	116.70
1	B	656	ARG	NE-CZ-NH1	15.84	128.22	120.30
1	C	825	ASN	OD1-CG-ND2	15.34	157.17	121.90
1	B	825	ASN	CB-CG-ND2	-13.28	84.83	116.70
1	C	817	ARG	NE-CZ-NH1	13.15	126.88	120.30
1	B	582	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	C	656	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	108	ARG	NE-CZ-NH2	-12.19	114.20	120.30
1	B	108	ARG	NE-CZ-NH2	-11.89	114.36	120.30
1	C	656	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	B	825	ASN	OD1-CG-ND2	11.71	148.82	121.90
1	B	907	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	B	582	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	825	ASN	OD1-CG-ND2	10.77	146.67	121.90
1	A	907	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	C	615	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	A	108	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	C	278	ASP	CB-CG-OD2	10.05	127.35	118.30
1	B	817	ARG	CD-NE-CZ	10.01	137.61	123.60
1	C	526	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	C	311	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	907	ARG	NE-CZ-NH2	-9.28	115.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	582	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	289	ASP	CB-CG-OD1	-9.18	110.03	118.30
1	C	615	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	A	656	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	45	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	A	907	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	582	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	582	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	817	ARG	CG-CD-NE	-7.70	95.63	111.80
1	C	45	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	825	ASN	CB-CG-ND2	-7.51	98.68	116.70
1	B	108	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	656	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	526	ARG	CD-NE-CZ	7.17	133.64	123.60
1	C	817	ARG	CG-CD-NE	-6.94	97.23	111.80
1	B	526	ARG	CD-NE-CZ	6.76	133.07	123.60
1	C	311	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	108	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	701	VAL	CB-CA-C	-6.25	99.52	111.40
1	C	526	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	345	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	713	GLY	N-CA-C	-6.10	97.86	113.10
1	C	907	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	278	ASP	CB-CA-C	-5.97	98.46	110.40
1	B	656	ARG	CD-NE-CZ	5.93	131.91	123.60
1	B	700	LYS	CD-CE-NZ	5.93	125.35	111.70
1	C	568	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	211	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	62	ARG	CG-CD-NE	-5.81	99.59	111.80
1	C	554	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	B	453	LEU	CB-CG-CD1	5.66	120.62	111.00
1	C	912	HIS	O-C-N	5.62	131.70	122.70
1	C	328	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	B	913	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	907	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	341	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	399	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	817	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	526	ARG	CG-CD-NE	-5.21	100.86	111.80
1	C	615	ARG	CD-NE-CZ	-5.15	116.39	123.60
1	C	716	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	395	CYS	CA-CB-SG	-5.10	104.82	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	656	ARG	CD-NE-CZ	5.03	130.63	123.60
1	A	395	CYS	CA-CB-SG	-5.02	104.97	114.00
1	C	45	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	VAL	Peptide
1	B	817	ARG	Sidechain
1	C	236	THR	Peptide
1	C	323	THR	Peptide
1	C	331	GLY	Mainchain
1	C	615	ARG	Sidechain
1	C	914	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7208	0	6804	109	0
1	B	7169	0	6783	144	0
1	C	7134	0	6705	137	0
2	A	25	0	0	1	0
2	B	60	0	0	2	0
2	C	25	0	0	0	0
3	A	56	0	98	33	0
3	B	96	0	168	53	0
3	C	40	0	70	9	0
4	A	542	0	0	2	0
4	B	563	0	0	10	0
4	C	416	0	0	6	0
All	All	23334	0	20628	385	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 9.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:913:ARG:C	1:C:913:ARG:CA	1.76	1.49
1:C:567:LYS:NZ	1:C:567:LYS:CE	1.74	1.48
1:B:425:SER:CB	1:B:425:SER:OG	1.65	1.41
1:B:227:LYS:H	3:B:1703:MPD:C1	1.53	1.19
3:B:1711:MPD:H11	3:B:1711:MPD:C5	1.72	1.17
3:B:1711:MPD:C1	3:B:1711:MPD:H52	1.76	1.16
1:B:72:ARG:HG3	1:B:72:ARG:HH11	1.01	1.14
3:B:1707:MPD:C5	3:B:1707:MPD:H11	1.77	1.11
3:B:1707:MPD:C1	3:B:1707:MPD:H52	1.78	1.11
3:A:1716:MPD:H31	1:B:766:GLY:H	1.02	1.11
1:A:666:LYS:HB2	1:A:666:LYS:HZ3	1.19	1.04
3:B:1707:MPD:H11	3:B:1707:MPD:H52	1.07	1.04
1:A:227:LYS:H	1:A:227:LYS:HE2	0.94	1.04
1:B:852:ARG:HD3	4:B:2225:HOH:O	1.57	1.03
3:A:1717:MPD:H12	3:A:1717:MPD:C5	1.88	1.03
1:A:336:LEU:HD21	4:A:2233:HOH:O	1.57	1.03
3:A:1717:MPD:H12	3:A:1717:MPD:H53	1.02	1.01
1:B:226:ASN:HB2	3:B:1703:MPD:H13	1.43	1.01
3:C:1713:MPD:H11	4:C:2068:HOH:O	1.59	1.00
1:B:170:ASP:HB2	1:B:174:GLN:H	1.26	1.00
1:B:227:LYS:H	3:B:1703:MPD:H11	1.20	1.00
3:B:1711:MPD:H11	3:B:1711:MPD:H52	1.01	0.98
3:A:1717:MPD:H53	3:A:1717:MPD:C1	1.94	0.98
1:A:227:LYS:HE2	1:A:227:LYS:N	1.79	0.97
1:C:74:ASP:OD1	1:C:567:LYS:HE2	1.68	0.94
3:A:1720:MPD:H11	1:C:405:ASP:HB3	1.49	0.94
1:A:666:LYS:HB2	1:A:666:LYS:NZ	1.84	0.93
1:C:61:GLN:HE22	1:C:604:HIS:HE1	0.97	0.93
1:B:227:LYS:N	3:B:1703:MPD:C1	2.32	0.92
1:A:253:ASN:OD1	3:A:1720:MPD:H12	1.69	0.92
1:B:61:GLN:HE22	1:B:604:HIS:HE1	1.17	0.92
3:A:1717:MPD:HM1	1:C:227:LYS:H	1.36	0.91
3:A:1716:MPD:H31	1:B:766:GLY:N	1.85	0.90
1:C:319:TYR:CZ	1:C:566:ARG:HG2	2.06	0.90
1:B:719:THR:HG21	1:B:724:GLU:OE2	1.72	0.89
1:B:72:ARG:HH11	1:B:72:ARG:CG	1.79	0.89
3:B:1718:MPD:HO2	3:B:1718:MPD:HO4	1.07	0.89
1:B:72:ARG:HG3	1:B:72:ARG:NH1	1.83	0.89
1:A:743:LYS:HE2	1:C:596:TYR:CZ	2.09	0.88
1:A:170:ASP:HB3	1:A:172:ASP:H	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLN:HE22	1:C:604:HIS:CE1	1.88	0.88
1:B:227:LYS:H	3:B:1703:MPD:H13	1.40	0.87
1:C:61:GLN:NE2	1:C:604:HIS:HE1	1.73	0.86
3:A:1720:MPD:HM3	1:C:406:THR:H	1.39	0.85
1:B:418:THR:HA	3:B:1722:MPD:H4	1.56	0.84
1:A:791:TYR:CE1	1:A:836:VAL:HG23	2.12	0.84
1:A:651:ASN:HD21	1:A:653:ALA:HB3	1.45	0.82
1:C:616:ASN:HD22	1:C:618:THR:HG22	1.45	0.80
1:B:227:LYS:N	3:B:1703:MPD:H11	1.95	0.80
1:C:555:LEU:H	1:C:910:GLN:HE22	1.30	0.79
1:A:650:ARG:NH1	1:A:925:PHE:CE1	2.51	0.79
3:A:1720:MPD:CM	1:C:406:THR:H	1.95	0.78
1:B:226:ASN:CB	3:B:1703:MPD:H13	2.13	0.78
1:C:792:LYS:H	1:C:792:LYS:HD3	1.47	0.77
1:B:482:ASP:OD1	3:B:1718:MPD:H32	1.85	0.77
3:A:1716:MPD:H11	1:B:766:GLY:HA3	1.66	0.76
1:C:567:LYS:NZ	1:C:567:LYS:CG	2.48	0.76
1:A:393:ASN:HD21	1:C:451:ASN:HD21	1.33	0.76
1:B:513:ASN:H	3:B:1709:MPD:H51	1.51	0.76
1:A:227:LYS:H	1:A:227:LYS:CE	1.87	0.75
3:B:1719:MPD:CM	3:B:1719:MPD:O4	2.35	0.75
1:A:371:ALA:HB3	1:A:526:ARG:CD	2.17	0.73
1:A:371:ALA:HB3	1:A:526:ARG:HD3	1.70	0.73
1:B:61:GLN:NE2	1:B:604:HIS:HE1	1.84	0.73
3:A:1705:MPD:O4	3:A:1705:MPD:HM1	1.89	0.72
1:B:248:MET:CE	1:B:266:VAL:HG21	2.18	0.72
1:B:666:LYS:HD3	3:B:1709:MPD:HM2	1.70	0.72
1:A:647:ILE:HD13	1:A:881:LEU:HD23	1.70	0.72
1:A:650:ARG:NH1	1:A:925:PHE:CD1	2.58	0.72
1:B:164:GLY:CA	1:B:248:MET:HE1	2.19	0.72
1:B:164:GLY:HA3	1:B:248:MET:HE1	1.73	0.71
1:A:666:LYS:HD3	3:A:1704:MPD:H12	1.72	0.71
1:C:629:ALA:HB1	1:C:899:VAL:HG13	1.71	0.71
1:C:792:LYS:HD3	1:C:792:LYS:N	2.03	0.71
1:C:615:ARG:HH22	1:C:913:ARG:HA	1.54	0.70
3:A:1720:MPD:H13	1:C:406:THR:O	1.91	0.70
1:B:891:ASP:HB3	4:B:2254:HOH:O	1.91	0.70
1:B:164:GLY:HA2	1:B:248:MET:CE	2.22	0.69
1:C:666:LYS:NZ	3:C:1713:MPD:H13	2.07	0.69
1:A:743:LYS:HE2	1:C:596:TYR:CE1	2.28	0.68
1:C:235:LYS:C	1:C:237:GLY:HA3	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ALA:CB	1:C:899:VAL:HG13	2.24	0.68
1:B:334:SER:O	1:B:334:SER:OG	2.11	0.67
1:A:334:SER:O	1:A:335:GLN:CB	2.42	0.67
1:A:651:ASN:HD21	1:A:653:ALA:CB	2.08	0.67
1:A:687:TYR:HD1	1:A:688:LEU:HD13	1.57	0.67
1:A:791:TYR:CD1	1:A:836:VAL:HG23	2.30	0.67
1:B:470:ALA:O	1:B:471:ASN:OD1	2.11	0.67
1:B:629:ALA:CB	1:B:899:VAL:HG13	2.24	0.67
1:B:450:ARG:HD3	4:B:1903:HOH:O	1.94	0.67
1:C:74:ASP:OD1	1:C:567:LYS:CE	2.42	0.67
1:C:331:GLY:HA3	1:C:914:GLY:O	1.93	0.67
1:C:567:LYS:NZ	1:C:567:LYS:HG2	2.09	0.66
1:B:451:ASN:HD21	1:C:393:ASN:HD21	1.42	0.66
1:C:913:ARG:CA	1:C:914:GLY:N	2.56	0.66
1:B:555:LEU:H	1:B:910:GLN:HE22	1.42	0.66
1:C:472:VAL:HG12	1:C:474:LEU:HD13	1.77	0.66
1:B:80:LYS:HD3	3:B:1723:MPD:H11	1.76	0.66
1:A:666:LYS:CE	3:A:1704:MPD:H12	2.27	0.65
1:A:787:ASP:OD2	1:A:790:ASN:HB2	1.97	0.65
1:B:170:ASP:HB3	1:B:172:ASP:H	1.61	0.64
1:B:371:ALA:HB3	1:B:526:ARG:CD	2.27	0.64
1:B:624:ASN:ND2	3:B:1711:MPD:C1	2.61	0.64
1:B:72:ARG:CG	1:B:72:ARG:NH1	2.47	0.63
1:B:248:MET:HE2	1:B:266:VAL:HG21	1.79	0.63
1:A:743:LYS:HE3	1:C:99:TYR:OH	1.97	0.63
1:B:59:ARG:NH2	4:B:2122:HOH:O	2.32	0.63
1:A:170:ASP:HB2	1:A:174:GLN:H	1.65	0.62
1:A:743:LYS:HE2	1:C:596:TYR:CE2	2.33	0.62
1:C:319:TYR:CE2	1:C:566:ARG:HG2	2.33	0.62
1:B:170:ASP:HB3	1:B:172:ASP:N	2.15	0.62
1:C:282:VAL:HG13	1:C:815:THR:HG22	1.81	0.62
1:C:526:ARG:NH2	1:C:574:GLN:OE1	2.30	0.62
1:A:786:VAL:HG23	1:A:836:VAL:HG21	1.82	0.61
1:C:61:GLN:NE2	1:C:604:HIS:CE1	2.57	0.61
1:C:913:ARG:C	1:C:913:ARG:CB	2.67	0.61
1:B:371:ALA:HB3	1:B:526:ARG:HD3	1.83	0.61
1:B:399:ASP:OD1	1:C:150:TYR:OH	2.17	0.61
1:B:568:ASP:OD1	1:B:582:ARG:HD3	2.01	0.61
1:B:563:TRP:C	1:B:564:ASN:HD22	2.04	0.61
1:A:170:ASP:HB3	1:A:172:ASP:N	2.12	0.60
1:A:253:ASN:OD1	3:A:1720:MPD:C1	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:SER:CB	1:B:425:SER:HG	2.09	0.60
1:A:629:ALA:CB	1:A:899:VAL:HG13	2.31	0.60
1:A:666:LYS:CD	3:A:1704:MPD:H12	2.31	0.60
1:A:472:VAL:HG12	1:A:474:LEU:HD13	1.84	0.60
1:C:792:LYS:H	1:C:792:LYS:CD	2.14	0.60
1:B:513:ASN:H	3:B:1709:MPD:C5	2.14	0.59
1:A:666:LYS:HE3	3:A:1704:MPD:H12	1.85	0.59
1:C:550:LYS:HD2	4:C:2042:HOH:O	2.01	0.59
1:B:164:GLY:CA	1:B:248:MET:CE	2.79	0.59
1:C:699:LYS:HB2	1:C:886:GLU:HG2	1.85	0.59
1:A:470:ALA:O	1:A:471:ASN:OD1	2.19	0.59
1:B:424:ASP:O	1:C:146:LYS:HE2	2.03	0.59
1:B:667:GLU:OE2	3:B:1709:MPD:HM1	2.02	0.59
1:A:45:ARG:HD3	1:B:624:ASN:HB2	1.85	0.58
1:C:666:LYS:HD3	3:C:1713:MPD:HM3	1.84	0.58
1:B:468:THR:HG23	1:B:474:LEU:HD22	1.86	0.58
1:B:666:LYS:HD3	3:B:1709:MPD:H12	1.84	0.58
1:C:687:TYR:HD1	1:C:688:LEU:HD13	1.69	0.58
1:A:666:LYS:HZ3	1:A:666:LYS:CB	2.06	0.58
1:A:687:TYR:CD1	1:A:688:LEU:HD13	2.39	0.58
1:B:564:ASN:HD22	1:B:564:ASN:N	2.02	0.58
1:A:468:THR:HG23	1:A:474:LEU:HD22	1.86	0.57
1:B:164:GLY:HA2	1:B:248:MET:HE2	1.86	0.57
1:C:83:TYR:O	1:C:560:THR:HA	2.05	0.57
1:A:568:ASP:OD1	1:A:582:ARG:HD3	2.05	0.56
1:B:629:ALA:HB1	1:B:899:VAL:HG13	1.86	0.56
1:B:666:LYS:HD3	3:B:1709:MPD:CM	2.34	0.56
1:B:226:ASN:CA	3:B:1703:MPD:H13	2.35	0.56
1:C:445:GLN:HG2	4:C:1732:HOH:O	2.06	0.56
1:A:666:LYS:HD3	3:A:1704:MPD:C1	2.36	0.56
1:B:477:ASN:O	1:B:480:THR:HB	2.06	0.56
1:B:226:ASN:HA	3:B:1703:MPD:H12	1.87	0.55
3:B:1719:MPD:O4	3:B:1719:MPD:HM2	2.06	0.55
1:A:454:TYR:CD2	1:B:391:LEU:HD13	2.41	0.55
1:A:791:TYR:CZ	1:A:836:VAL:HG23	2.42	0.55
1:C:515:PHE:CD1	1:C:691:THR:HB	2.42	0.55
1:A:703:ILE:HG23	1:A:881:LEU:HD11	1.88	0.55
1:B:819:GLY:H	1:C:436:ASN:ND2	2.03	0.55
1:C:69:PRO:HB3	1:C:81:VAL:HG22	1.89	0.55
1:A:620:ASP:OD2	1:A:907:ARG:HD3	2.07	0.54
1:B:61:GLN:HE22	1:B:604:HIS:CE1	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG23	1:C:71:ASP:OD2	2.08	0.54
1:A:818:GLN:HE21	1:C:189:GLY:H	1.56	0.54
1:A:61:GLN:OE1	1:A:604:HIS:HE1	1.90	0.54
1:A:515:PHE:CD1	1:A:691:THR:HB	2.43	0.54
1:B:227:LYS:CB	3:B:1703:MPD:H11	2.38	0.54
1:A:656:ARG:HD3	1:A:902:VAL:O	2.08	0.54
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.72	0.54
1:C:67:PHE:HB2	1:C:595:LEU:HB3	1.90	0.54
1:C:615:ARG:NH2	1:C:913:ARG:HA	2.21	0.54
1:A:513:ASN:HB3	3:A:1704:MPD:H51	1.90	0.53
3:B:1719:MPD:O4	3:B:1719:MPD:HM1	2.08	0.53
1:B:227:LYS:N	3:B:1703:MPD:H13	2.11	0.53
1:A:666:LYS:NZ	1:A:666:LYS:CB	2.55	0.53
1:B:284:LYS:HE2	4:B:2044:HOH:O	2.07	0.53
1:C:570:ASN:ND2	1:C:582:ARG:HG3	2.24	0.53
3:B:1722:MPD:O4	3:B:1722:MPD:H11	2.08	0.53
1:A:303:ASN:HB3	1:A:481:TYR:OH	2.09	0.53
1:B:82:ARG:HE	1:B:560:THR:HG23	1.74	0.53
1:B:451:ASN:ND2	1:C:393:ASN:HD21	2.06	0.53
1:A:874:TYR:C	1:A:876:ASN:N	2.63	0.52
1:C:318:MET:HG2	1:C:565:PHE:CE1	2.44	0.52
1:A:73:GLU:OE1	1:A:80:LYS:HD2	2.08	0.52
1:B:515:PHE:CD1	1:B:691:THR:HB	2.45	0.52
1:B:676:ASP:OD1	2:B:1616:2HP:O1	2.27	0.52
1:C:333:ALA:O	1:C:334:SER:CB	2.56	0.52
1:A:216:PRO:HG2	1:A:300:ALA:HB2	1.91	0.52
1:A:667:GLU:OE2	3:A:1704:MPD:HM1	2.09	0.52
1:C:816:MET:SD	1:C:817:ARG:NH2	2.83	0.52
1:C:909:HIS:CD2	1:C:911:PRO:HD3	2.45	0.52
1:A:430:ASN:HD22	1:B:149:THR:H	1.58	0.52
1:C:450:ARG:HD3	4:C:1815:HOH:O	2.09	0.52
1:C:303:ASN:HB3	1:C:481:TYR:OH	2.10	0.52
1:C:666:LYS:CD	3:C:1713:MPD:HM3	2.39	0.52
1:B:226:ASN:HA	3:B:1703:MPD:C1	2.39	0.52
1:A:393:ASN:HD21	1:C:451:ASN:ND2	2.05	0.52
3:A:1720:MPD:C1	1:C:405:ASP:HB3	2.32	0.52
1:C:567:LYS:CG	1:C:567:LYS:HZ3	2.20	0.51
1:B:164:GLY:HA2	1:B:248:MET:HE1	1.88	0.51
1:A:516:ASN:HD22	3:A:1704:MPD:C5	2.24	0.51
1:A:242:LYS:HE2	1:A:244:TYR:OH	2.10	0.51
3:A:1720:MPD:HM3	1:C:406:THR:N	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:TYR:CD2	1:B:823:PRO:HD2	2.45	0.51
1:C:567:LYS:NZ	1:C:567:LYS:CD	2.68	0.51
1:B:58:ASP:OD1	1:B:58:ASP:N	2.39	0.50
1:B:301:MET:CG	1:B:302:PRO:HD2	2.42	0.50
1:C:567:LYS:HG2	1:C:567:LYS:HZ2	1.74	0.50
1:B:226:ASN:CA	3:B:1703:MPD:C1	2.88	0.50
1:A:659:SER:HA	1:A:851:TRP:O	2.12	0.50
1:C:687:TYR:CD1	1:C:688:LEU:HD13	2.46	0.50
1:B:114:PRO:HG2	1:C:501:GLY:HA3	1.94	0.50
1:B:482:ASP:CG	3:B:1718:MPD:H4	2.32	0.50
1:B:620:ASP:OD2	1:B:907:ARG:HD3	2.12	0.49
1:C:568:ASP:HB2	1:C:675:PHE:HE1	1.77	0.49
1:A:791:TYR:CD1	1:A:836:VAL:CG2	2.96	0.49
3:B:1723:MPD:O2	3:B:1723:MPD:H53	2.12	0.49
1:B:201:GLU:N	4:B:2154:HOH:O	2.46	0.49
1:C:568:ASP:OD1	1:C:582:ARG:HD3	2.13	0.49
1:C:711:TRP:CG	1:C:712:PRO:HA	2.48	0.49
1:C:313:ASN:HD21	1:C:370:GLN:HG3	1.78	0.49
1:A:847:ASP:O	1:A:848:ARG:HB2	2.11	0.49
1:B:427:ASN:HB3	1:B:430:ASN:HD21	1.77	0.49
1:B:61:GLN:NE2	1:B:604:HIS:CE1	2.72	0.48
1:C:478:THR:HG23	1:C:483:TYR:CE1	2.48	0.48
1:B:653:ALA:O	1:B:654:ALA:HB3	2.14	0.48
3:A:1716:MPD:H32	4:B:1988:HOH:O	2.14	0.48
1:A:172:ASP:O	1:A:173:ASP:HB2	2.14	0.48
1:A:651:ASN:ND2	1:A:653:ALA:H	2.11	0.48
1:C:454:TYR:CE1	1:C:489:VAL:HG13	2.48	0.48
1:C:513:ASN:HB3	3:C:1713:MPD:H51	1.94	0.48
1:A:307:TYR:O	1:A:575:SER:HA	2.14	0.48
1:B:307:TYR:O	1:B:575:SER:HA	2.13	0.48
1:B:610:LEU:HA	1:B:613:MET:HE2	1.96	0.48
1:A:701:VAL:HG13	1:A:885:PHE:CD2	2.49	0.47
1:C:110:PRO:HD2	1:C:584:ASP:O	2.14	0.47
1:A:126:LYS:HE2	1:B:389:ASP:O	2.15	0.47
1:B:248:MET:HE3	1:B:266:VAL:HG21	1.93	0.47
1:A:501:GLY:HA3	1:C:114:PRO:HG2	1.96	0.47
1:C:103:ARG:HG3	1:C:539:HIS:CD2	2.49	0.47
1:C:700:LYS:HD3	1:C:722:GLU:OE2	2.15	0.47
1:C:572:ILE:HD11	1:C:588:ILE:HG21	1.95	0.47
1:B:816:MET:HA	1:C:394:TYR:OH	2.15	0.47
1:A:472:VAL:CG1	1:A:474:LEU:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:GLY:H	1:B:436:ASN:ND2	2.13	0.47
1:B:475:PRO:HG2	1:B:480:THR:HG21	1.96	0.47
1:C:666:LYS:CE	3:C:1713:MPD:H13	2.45	0.47
3:B:1711:MPD:C5	3:B:1711:MPD:C1	2.44	0.47
1:A:786:VAL:HG23	1:A:836:VAL:CG2	2.45	0.46
3:A:1702:MPD:HM1	4:A:1815:HOH:O	2.14	0.46
1:B:666:LYS:CD	3:B:1709:MPD:H12	2.45	0.46
3:A:1716:MPD:HM2	4:B:2251:HOH:O	2.15	0.46
1:B:667:GLU:HG2	1:B:681:TYR:CZ	2.50	0.46
3:C:1714:MPD:H11	3:C:1714:MPD:O4	2.16	0.46
1:A:440:MET:HE1	1:B:440:MET:HG2	1.97	0.46
1:B:700:LYS:HB3	1:B:700:LYS:HE3	1.73	0.46
1:C:550:LYS:NZ	4:C:2076:HOH:O	2.35	0.46
1:B:175:PRO:HB2	1:B:177:TYR:CE1	2.51	0.46
1:C:459:LEU:HD23	1:C:489:VAL:CG1	2.45	0.46
1:C:816:MET:HE3	1:C:817:ARG:HH21	1.81	0.46
1:C:568:ASP:HB2	1:C:675:PHE:CE1	2.51	0.46
1:C:555:LEU:HB3	1:C:556:PRO:HD2	1.98	0.46
1:C:652:TRP:HB2	1:C:872:MET:HG2	1.97	0.46
1:C:659:SER:HA	1:C:851:TRP:O	2.15	0.46
3:A:1704:MPD:HM1	3:A:1704:MPD:H4	1.54	0.45
1:C:307:TYR:O	1:C:575:SER:HA	2.16	0.45
1:A:717:LEU:HB2	1:A:720:PRO:HA	1.97	0.45
1:C:599:PHE:CD1	1:C:599:PHE:N	2.84	0.45
1:B:513:ASN:HB2	3:B:1709:MPD:H51	1.98	0.45
1:B:555:LEU:H	1:B:910:GLN:NE2	2.10	0.45
1:B:624:ASN:ND2	3:B:1711:MPD:H12	2.29	0.45
1:B:819:GLY:H	1:C:436:ASN:HD22	1.63	0.45
1:C:279:THR:HG22	1:C:302:PRO:HA	1.98	0.45
1:C:656:ARG:NH1	1:C:901:GLU:HB3	2.31	0.45
1:A:922:ARG:O	1:A:926:SER:HA	2.16	0.45
1:B:819:GLY:O	1:C:437:PRO:HD3	2.17	0.45
1:C:498:ILE:O	1:C:499:ASN:C	2.55	0.45
1:B:513:ASN:CB	3:B:1709:MPD:H51	2.47	0.45
1:C:704:THR:O	1:C:881:LEU:HD12	2.16	0.45
3:B:1709:MPD:HM1	3:B:1709:MPD:H4	1.67	0.45
3:B:1723:MPD:O4	3:B:1723:MPD:HM1	2.16	0.45
1:C:574:GLN:HA	1:C:682:SER:O	2.16	0.45
1:A:616:ASN:HD22	1:A:617:ASP:N	2.15	0.45
1:A:641:THR:HG22	1:A:889:PRO:HD3	1.99	0.45
1:C:644:PRO:HA	1:C:884:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HA	1:A:80:LYS:O	2.17	0.45
1:B:80:LYS:HB3	3:B:1723:MPD:HM3	1.99	0.45
1:C:85:LEU:N	1:C:559:TYR:O	2.49	0.45
1:A:394:TYR:OH	1:C:816:MET:HA	2.18	0.44
1:B:498:ILE:O	1:B:499:ASN:C	2.54	0.44
1:B:700:LYS:HG2	1:B:886:GLU:HB3	1.98	0.44
3:A:1720:MPD:HM3	1:C:406:THR:HB	2.00	0.44
1:A:667:GLU:OE2	3:A:1704:MPD:CM	2.66	0.44
1:A:650:ARG:HE	1:A:650:ARG:HB3	1.66	0.44
1:B:242:LYS:HE2	1:B:244:TYR:OH	2.18	0.44
1:B:420:TRP:HB2	1:C:261:LEU:O	2.16	0.44
1:A:69:PRO:HD3	1:A:594:ASN:HD22	1.83	0.44
1:C:617:ASP:OD1	1:C:909:HIS:CE1	2.71	0.44
1:B:313:ASN:HA	1:B:368:TRP:O	2.18	0.44
1:B:656:ARG:HD3	1:B:902:VAL:O	2.18	0.44
2:A:1610:2HP:O2	1:C:539:HIS:ND1	2.41	0.44
1:B:6:LEU:HD23	1:B:9:TRP:CE3	2.53	0.44
1:B:17:GLN:HB3	1:B:21:GLU:HB2	2.00	0.44
1:A:255:SER:OG	3:A:1720:MPD:H4	2.18	0.43
1:B:564:ASN:N	1:B:564:ASN:ND2	2.66	0.43
1:A:430:ASN:ND2	1:B:149:THR:H	2.15	0.43
1:B:279:THR:HG22	1:B:302:PRO:HA	2.00	0.43
1:B:418:THR:CA	3:B:1722:MPD:H4	2.40	0.43
1:B:666:LYS:HD3	3:B:1709:MPD:C1	2.48	0.43
1:B:470:ALA:O	1:B:471:ASN:CB	2.63	0.43
1:A:17:GLN:HB3	1:A:21:GLU:HB2	2.01	0.43
1:A:816:MET:HA	1:B:394:TYR:OH	2.17	0.43
1:A:874:TYR:C	1:A:876:ASN:H	2.21	0.43
1:B:112:PHE:HB2	1:B:308:ILE:HD12	2.00	0.43
1:B:301:MET:HG2	1:B:302:PRO:HD2	1.98	0.43
1:C:319:TYR:CZ	1:C:566:ARG:CG	2.92	0.43
1:B:67:PHE:HB2	1:B:595:LEU:HB3	2.00	0.43
1:C:644:PRO:CA	1:C:884:ASN:HD22	2.31	0.43
1:C:653:ALA:O	1:C:654:ALA:HB3	2.17	0.43
1:A:344:ASP:HB3	1:A:922:ARG:HH12	1.84	0.43
3:B:1723:MPD:O2	3:B:1723:MPD:C5	2.66	0.43
1:C:70:VAL:N	1:C:82:ARG:O	2.50	0.43
1:C:555:LEU:HD12	1:C:910:GLN:HB2	2.00	0.43
1:A:564:ASN:N	1:A:564:ASN:HD22	2.17	0.43
1:A:313:ASN:HD21	1:A:370:GLN:HG3	1.84	0.43
1:C:319:TYR:CE2	1:C:566:ARG:CG	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:ARG:HD3	1:C:902:VAL:O	2.18	0.43
1:C:329:LEU:O	1:C:338:ALA:N	2.50	0.42
1:A:407:TYR:HB3	1:B:251:PHE:HB3	2.01	0.42
3:C:1713:MPD:C1	4:C:2068:HOH:O	2.37	0.42
1:C:101:ASP:OD1	1:C:539:HIS:NE2	2.52	0.42
1:A:114:PRO:O	1:B:501:GLY:HA2	2.19	0.42
1:A:715:ASP:O	1:C:62:ARG:HA	2.20	0.42
1:A:660:PHE:HA	1:A:897:TYR:O	2.19	0.42
1:A:743:LYS:CE	1:C:596:TYR:CE1	3.00	0.42
1:C:70:VAL:HG22	1:C:82:ARG:O	2.20	0.42
1:C:660:PHE:HA	1:C:897:TYR:O	2.20	0.42
3:B:1707:MPD:H51	4:B:2256:HOH:O	2.19	0.42
1:B:468:THR:CG2	1:B:474:LEU:HD22	2.49	0.42
1:C:427:ASN:HB3	1:C:430:ASN:HD21	1.85	0.42
1:B:248:MET:HE1	1:B:268:TYR:OH	2.19	0.41
1:B:650:ARG:HE	1:B:650:ARG:HB3	1.69	0.41
1:A:644:PRO:HB3	1:A:884:ASN:HD22	1.85	0.41
1:A:706:ASP:O	1:A:708:SER:N	2.53	0.41
1:B:58:ASP:OD1	2:B:1606:2HP:O3	2.38	0.41
1:A:313:ASN:HA	1:A:368:TRP:O	2.20	0.41
1:C:629:ALA:CB	1:C:899:VAL:CG1	2.98	0.41
1:C:311:ARG:NH2	1:C:683:GLY:O	2.34	0.41
1:C:650:ARG:HE	1:C:650:ARG:HB3	1.52	0.41
1:C:705:PHE:O	1:C:706:ASP:C	2.58	0.41
1:B:466:LYS:HG2	1:B:489:VAL:HG22	2.03	0.41
1:A:563:TRP:C	1:A:564:ASN:HD22	2.24	0.41
1:A:799:LEU:HD23	3:A:1705:MPD:H31	2.03	0.41
1:A:924:PRO:O	1:A:925:PHE:HB2	2.20	0.41
1:B:407:TYR:HB3	1:C:251:PHE:HB3	2.03	0.41
1:C:565:PHE:CD2	1:C:565:PHE:N	2.89	0.41
1:A:242:LYS:HE2	1:A:244:TYR:CZ	2.56	0.41
1:B:246:ILE:HA	1:B:269:THR:O	2.21	0.41
1:B:323:THR:N	1:B:343:GLN:OE1	2.42	0.41
1:B:790:ASN:ND2	4:B:2247:HOH:O	2.38	0.41
3:B:1721:MPD:H11	3:B:1721:MPD:H4	1.77	0.41
1:C:611:GLU:O	1:C:615:ARG:HG3	2.21	0.41
1:C:666:LYS:HZ3	3:C:1713:MPD:H13	1.86	0.41
1:A:819:GLY:O	1:B:437:PRO:HD3	2.21	0.41
3:A:1720:MPD:HM3	1:C:406:THR:CB	2.51	0.41
1:B:711:TRP:CG	1:B:712:PRO:HA	2.56	0.41
1:C:704:THR:HA	1:C:709:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLY:HA3	1:B:784:GLN:OE1	2.20	0.40
1:A:470:ALA:O	1:A:471:ASN:CB	2.68	0.40
1:B:53:HIS:O	1:B:54:ASP:HB2	2.20	0.40
1:B:667:GLU:OE2	3:B:1709:MPD:CM	2.68	0.40
1:B:703:ILE:HG23	1:B:881:LEU:HD11	2.02	0.40
1:C:313:ASN:HA	1:C:368:TRP:O	2.22	0.40
1:C:890:MET:C	1:C:892:GLU:H	2.25	0.40
1:B:482:ASP:OD1	3:B:1718:MPD:H4	2.22	0.40
1:B:624:ASN:CG	3:B:1711:MPD:C1	2.90	0.40
1:C:79:TYR:CE2	1:C:593:ILE:HD12	2.57	0.40
1:C:406:THR:HG22	1:C:429:ALA:HA	2.03	0.40
1:A:170:ASP:HB2	1:A:174:GLN:N	2.32	0.40
1:A:397:PRO:HD3	1:A:438:PHE:O	2.20	0.40
1:A:629:ALA:HB1	1:A:899:VAL:HG13	2.03	0.40
1:B:553:LEU:HD12	1:B:553:LEU:HA	1.93	0.40
1:B:664:LYS:HZ2	3:B:1709:MPD:H52	1.86	0.40
1:C:159:ASN:OD1	1:C:202:LYS:HE2	2.22	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	907/932 (97%)	873 (96%)	32 (4%)	2 (0%)	47 49
1	B	896/932 (96%)	858 (96%)	38 (4%)	0	100 100
1	C	901/932 (97%)	858 (95%)	41 (5%)	2 (0%)	47 49
All	All	2704/2796 (97%)	2589 (96%)	111 (4%)	4 (0%)	51 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	SER
1	A	335	GLN
1	C	334	SER
1	C	238	THR

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	764/799 (96%)	736 (96%)	28 (4%)	34	35
1	B	764/799 (96%)	730 (96%)	34 (4%)	27	27
1	C	750/799 (94%)	723 (96%)	27 (4%)	35	36
All	All	2278/2397 (95%)	2189 (96%)	89 (4%)	32	33

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	162	LYS
1	A	171	THR
1	A	226	ASN
1	A	227	LYS
1	A	323	THR
1	A	336	LEU
1	A	343	GLN
1	A	353	LEU
1	A	358	LEU
1	A	369	ASN
1	A	391	LEU
1	A	398	LEU
1	A	448	LEU
1	A	471	ASN
1	A	474	LEU
1	A	476	THR
1	A	495	ASP
1	A	616	ASN

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Mol	Chain	Res	Type
1	A	628	SER
1	A	646	SER
1	A	666	LYS
1	A	688	LEU
1	A	701	VAL
1	A	729	VAL
1	A	817	ARG
1	A	907	ARG
1	A	913	ARG
1	B	6	LEU
1	B	59	ARG
1	B	60	SER
1	B	72	ARG
1	B	108	ARG
1	B	145	GLU
1	B	162	LYS
1	B	172	ASP
1	B	242	LYS
1	B	296	LEU
1	B	332	GLN
1	B	334	SER
1	B	353	LEU
1	B	358	LEU
1	B	361	ARG
1	B	369	ASN
1	B	391	LEU
1	B	418	THR
1	B	448	LEU
1	B	453	LEU
1	B	459	LEU
1	B	471	ASN
1	B	474	LEU
1	B	478	THR
1	B	480	THR
1	B	558	SER
1	B	563	TRP
1	B	589	SER
1	B	624	ASN
1	B	649	SER
1	B	673	SER
1	B	700	LYS
1	B	708	SER

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Mol	Chain	Res	Type
1	B	817	ARG
1	C	45	ARG
1	C	59	ARG
1	C	91	ARG
1	C	322	SER
1	C	326	MET
1	C	332	GLN
1	C	343	GLN
1	C	353	LEU
1	C	358	LEU
1	C	361	ARG
1	C	369	ASN
1	C	398	LEU
1	C	440	MET
1	C	474	LEU
1	C	495	ASP
1	C	563	TRP
1	C	624	ASN
1	C	628	SER
1	C	632	MET
1	C	649	SER
1	C	670	SER
1	C	688	LEU
1	C	700	LYS
1	C	702	SER
1	C	727	ARG
1	C	792	LYS
1	C	817	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	130	ASN
1	A	226	ASN
1	A	231	GLN
1	A	313	ASN
1	A	325	ASN
1	A	430	ASN
1	A	564	ASN
1	A	594	ASN
1	A	604	HIS

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Mol	Chain	Res	Type
1	A	616	ASN
1	A	651	ASN
1	A	803	HIS
1	A	818	GLN
1	A	871	ASN
1	A	884	ASN
1	B	8	GLN
1	B	61	GLN
1	B	253	ASN
1	B	313	ASN
1	B	325	ASN
1	B	430	ASN
1	B	436	ASN
1	B	451	ASN
1	B	471	ASN
1	B	564	ASN
1	B	604	HIS
1	B	624	ASN
1	B	790	ASN
1	B	825	ASN
1	B	910	GLN
1	C	29	GLN
1	C	61	GLN
1	C	130	ASN
1	C	231	GLN
1	C	253	ASN
1	C	313	ASN
1	C	332	GLN
1	C	427	ASN
1	C	430	ASN
1	C	436	ASN
1	C	451	ASN
1	C	604	HIS
1	C	616	ASN
1	C	790	ASN
1	C	825	ASN
1	C	871	ASN
1	C	884	ASN
1	C	910	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)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2HP	C	1611	-	4,4,4	5.94	2 (50%)	6,6,6	0.98	0
2	2HP	A	1620	-	4,4,4	5.87	2 (50%)	6,6,6	0.91	0
3	MPD	A	1720	-	7,7,7	0.34	0	9,10,10	0.78	0
3	MPD	B	1718	-	7,7,7	0.87	0	9,10,10	1.50	2 (22%)
3	MPD	B	1703	-	7,7,7	0.72	0	9,10,10	0.75	0
3	MPD	B	1710	-	7,7,7	0.55	0	9,10,10	0.67	0
2	2HP	B	1616	-	4,4,4	6.24	2 (50%)	6,6,6	0.79	0
2	2HP	B	1601	-	4,4,4	5.09	2 (50%)	6,6,6	1.37	1 (16%)
2	2HP	C	1613	-	4,4,4	5.84	2 (50%)	6,6,6	1.42	1 (16%)
3	MPD	A	1704	-	7,7,7	0.70	0	9,10,10	0.77	1 (11%)
2	2HP	A	1602	-	4,4,4	5.73	2 (50%)	6,6,6	1.36	1 (16%)
2	2HP	C	1618	-	4,4,4	5.62	2 (50%)	6,6,6	1.48	1 (16%)
3	MPD	A	1705	-	7,7,7	0.33	0	9,10,10	0.76	1 (11%)
3	MPD	A	1702	-	7,7,7	0.45	0	9,10,10	1.84	4 (44%)
3	MPD	C	1701	-	7,7,7	0.35	0	9,10,10	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2HP	B	1614	-	4,4,4	5.74	2 (50%)	6,6,6	1.26	1 (16%)
3	MPD	C	1713	-	7,7,7	0.53	0	9,10,10	1.31	1 (11%)
3	MPD	B	1721	-	7,7,7	0.31	0	9,10,10	0.60	0
3	MPD	B	1711	-	7,7,7	0.36	0	9,10,10	0.99	0
2	2HP	C	1604	-	4,4,4	5.16	2 (50%)	6,6,6	1.43	1 (16%)
2	2HP	C	1617	-	4,4,4	6.23	2 (50%)	6,6,6	1.46	1 (16%)
3	MPD	B	1708	-	7,7,7	0.35	0	9,10,10	0.47	0
2	2HP	B	1621	-	4,4,4	6.01	2 (50%)	6,6,6	0.95	0
2	2HP	B	1609	-	4,4,4	4.51	2 (50%)	6,6,6	2.20	3 (50%)
3	MPD	A	1706	-	7,7,7	0.30	0	9,10,10	0.96	0
3	MPD	C	1712	-	7,7,7	0.63	0	9,10,10	0.96	1 (11%)
2	2HP	A	1610	-	4,4,4	5.33	2 (50%)	6,6,6	1.84	1 (16%)
2	2HP	A	1619	-	4,4,4	6.32	2 (50%)	6,6,6	1.50	2 (33%)
2	2HP	B	1608	-	4,4,4	5.96	2 (50%)	6,6,6	1.11	1 (16%)
2	2HP	B	1605	-	4,4,4	5.84	2 (50%)	6,6,6	1.58	2 (33%)
3	MPD	C	1714	-	7,7,7	0.41	0	9,10,10	0.33	0
2	2HP	B	1612	-	4,4,4	5.98	2 (50%)	6,6,6	1.11	0
3	MPD	A	1717	-	7,7,7	0.57	0	9,10,10	0.89	0
3	MPD	B	1723	-	7,7,7	0.41	0	9,10,10	0.69	0
2	2HP	B	1622	-	4,4,4	5.11	2 (50%)	6,6,6	1.70	1 (16%)
3	MPD	C	1715	-	7,7,7	0.29	0	9,10,10	0.33	0
3	MPD	B	1709	-	7,7,7	1.10	0	9,10,10	1.12	1 (11%)
2	2HP	A	1603	-	4,4,4	5.40	2 (50%)	6,6,6	1.12	0
2	2HP	B	1607	-	4,4,4	5.54	2 (50%)	6,6,6	1.82	2 (33%)
3	MPD	B	1719	-	7,7,7	0.37	0	9,10,10	0.85	0
3	MPD	B	1722	-	7,7,7	0.56	0	9,10,10	0.52	0
3	MPD	B	1724	-	7,7,7	0.32	0	9,10,10	0.67	0
2	2HP	B	1615	-	4,4,4	6.35	2 (50%)	6,6,6	1.68	3 (50%)
3	MPD	B	1707	-	7,7,7	0.40	0	9,10,10	0.44	0
3	MPD	A	1716	-	7,7,7	1.01	0	9,10,10	1.12	0
2	2HP	B	1606	-	4,4,4	5.39	2 (50%)	6,6,6	0.88	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
3	MPD	A	1720	-	1/1/2/2	4/5/5/5	-
3	MPD	B	1718	-	1/1/2/2	2/5/5/5	-
3	MPD	B	1703	-	-	0/5/5/5	-
3	MPD	B	1710	-	-	0/5/5/5	-
3	MPD	A	1704	-	1/1/2/2	5/5/5/5	-
3	MPD	A	1705	-	-	2/5/5/5	-
3	MPD	C	1713	-	1/1/2/2	5/5/5/5	-
3	MPD	A	1702	-	-	0/5/5/5	-
3	MPD	C	1701	-	-	3/5/5/5	-
3	MPD	B	1721	-	1/1/2/2	0/5/5/5	-
3	MPD	B	1711	-	-	4/5/5/5	-
3	MPD	B	1708	-	-	0/5/5/5	-
3	MPD	C	1712	-	-	3/5/5/5	-
3	MPD	A	1706	-	-	0/5/5/5	-
3	MPD	C	1714	-	-	0/5/5/5	-
3	MPD	A	1717	-	1/1/2/2	3/5/5/5	-
3	MPD	B	1723	-	-	1/5/5/5	-
3	MPD	C	1715	-	-	0/5/5/5	-
3	MPD	B	1709	-	-	2/5/5/5	-
3	MPD	B	1719	-	1/1/2/2	2/5/5/5	-
3	MPD	B	1722	-	1/1/2/2	2/5/5/5	-
3	MPD	B	1724	-	1/1/2/2	2/5/5/5	-
3	MPD	B	1707	-	-	5/5/5/5	-
3	MPD	A	1716	-	-	2/5/5/5	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1615	2HP	P-O4	9.88	1.84	1.54
2	C	1617	2HP	P-O3	9.31	1.82	1.54
2	B	1616	2HP	P-O3	9.14	1.82	1.54
2	A	1619	2HP	P-O4	8.94	1.81	1.54
2	A	1619	2HP	P-O3	8.93	1.81	1.54
2	C	1611	2HP	P-O4	8.89	1.81	1.54
2	B	1612	2HP	P-O3	8.72	1.80	1.54
2	B	1621	2HP	P-O4	8.54	1.80	1.54
2	B	1608	2HP	P-O3	8.42	1.79	1.54
2	B	1605	2HP	P-O3	8.40	1.79	1.54
2	C	1613	2HP	P-O4	8.38	1.79	1.54
2	B	1621	2HP	P-O3	8.37	1.79	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1616	2HP	P-O4	8.36	1.79	1.54
2	B	1608	2HP	P-O4	8.33	1.79	1.54
2	A	1620	2HP	P-O3	8.32	1.79	1.54
2	B	1614	2HP	P-O3	8.24	1.79	1.54
2	A	1620	2HP	P-O4	8.19	1.79	1.54
2	C	1618	2HP	P-O4	8.18	1.79	1.54
2	B	1607	2HP	P-O4	8.16	1.79	1.54
2	C	1617	2HP	P-O4	8.10	1.79	1.54
2	B	1612	2HP	P-O4	8.10	1.78	1.54
2	B	1605	2HP	P-O4	8.09	1.78	1.54
2	A	1602	2HP	P-O4	8.04	1.78	1.54
2	A	1602	2HP	P-O3	7.99	1.78	1.54
2	A	1603	2HP	P-O4	7.91	1.78	1.54
2	B	1614	2HP	P-O4	7.88	1.78	1.54
2	C	1613	2HP	P-O3	7.86	1.78	1.54
2	C	1611	2HP	P-O3	7.83	1.78	1.54
2	B	1606	2HP	P-O3	7.82	1.78	1.54
2	B	1615	2HP	P-O3	7.78	1.78	1.54
2	C	1618	2HP	P-O3	7.64	1.77	1.54
2	B	1622	2HP	P-O3	7.64	1.77	1.54
2	B	1601	2HP	P-O3	7.59	1.77	1.54
2	A	1610	2HP	P-O3	7.57	1.77	1.54
2	B	1607	2HP	P-O3	7.47	1.77	1.54
2	B	1606	2HP	P-O4	7.38	1.76	1.54
2	C	1604	2HP	P-O3	7.37	1.76	1.54
2	A	1610	2HP	P-O4	7.37	1.76	1.54
2	A	1603	2HP	P-O3	7.18	1.76	1.54
2	C	1604	2HP	P-O4	7.11	1.76	1.54
2	B	1622	2HP	P-O4	6.49	1.74	1.54
2	B	1609	2HP	P-O3	6.40	1.73	1.54
2	B	1601	2HP	P-O4	6.35	1.73	1.54
2	B	1609	2HP	P-O4	6.23	1.73	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1610	2HP	O2-P-O1	3.78	124.74	110.89
2	B	1609	2HP	O4-P-O2	-3.30	97.38	107.97
2	B	1622	2HP	O4-P-O3	3.14	118.06	107.97
3	B	1709	MPD	O4-C4-C5	3.05	122.59	109.38
2	B	1607	2HP	O2-P-O1	2.98	121.80	110.89
2	C	1617	2HP	O2-P-O1	2.85	121.33	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1702	MPD	O2-C2-C1	2.67	116.64	108.08
2	B	1609	2HP	O3-P-O1	-2.66	101.18	110.89
2	B	1607	2HP	O4-P-O3	-2.60	99.62	107.97
3	B	1718	MPD	O2-C2-C3	-2.59	100.08	109.80
3	A	1702	MPD	CM-C2-C3	2.56	121.87	109.96
3	A	1702	MPD	C1-C2-C3	-2.54	98.13	109.96
3	A	1702	MPD	CM-C2-C1	-2.51	105.34	110.57
2	A	1602	2HP	O4-P-O3	-2.51	99.93	107.97
2	A	1619	2HP	O2-P-O1	2.50	120.04	110.89
2	A	1619	2HP	O3-P-O1	-2.50	101.76	110.89
2	C	1604	2HP	O3-P-O2	-2.49	99.97	107.97
2	B	1615	2HP	O2-P-O1	2.48	119.97	110.89
2	B	1614	2HP	O2-P-O1	2.41	119.73	110.89
2	B	1609	2HP	O2-P-O1	2.37	119.56	110.89
2	B	1608	2HP	O2-P-O1	2.28	119.24	110.89
3	C	1713	MPD	O4-C4-C5	2.26	119.15	109.38
2	B	1605	2HP	O2-P-O1	2.21	119.00	110.89
3	A	1704	MPD	O4-C4-C5	2.18	118.83	109.38
2	B	1605	2HP	O3-P-O1	-2.18	102.93	110.89
3	C	1712	MPD	CM-C2-C1	-2.08	106.24	110.57
2	B	1615	2HP	O3-P-O2	-2.06	101.34	107.97
3	A	1705	MPD	CM-C2-C1	2.05	114.85	110.57
2	B	1601	2HP	O2-P-O1	2.05	118.39	110.89
2	B	1615	2HP	O4-P-O1	-2.03	103.47	110.89
2	C	1613	2HP	O3-P-O2	2.03	114.47	107.97
3	B	1718	MPD	O4-C4-C3	2.02	119.51	111.36
2	C	1618	2HP	O3-P-O2	-2.01	101.52	107.97

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1704	MPD	C4
3	A	1717	MPD	C4
3	A	1720	MPD	C4
3	B	1718	MPD	C4
3	B	1719	MPD	C4
3	B	1721	MPD	C4
3	B	1722	MPD	C4
3	B	1724	MPD	C4
3	C	1713	MPD	C4

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1704	MPD	CM-C2-C3-C4
3	A	1705	MPD	C2-C3-C4-O4
3	A	1716	MPD	C2-C3-C4-O4
3	A	1717	MPD	C2-C3-C4-O4
3	A	1717	MPD	C2-C3-C4-C5
3	B	1707	MPD	C1-C2-C3-C4
3	B	1707	MPD	O2-C2-C3-C4
3	B	1707	MPD	C2-C3-C4-O4
3	B	1707	MPD	C2-C3-C4-C5
3	B	1711	MPD	C2-C3-C4-C5
3	B	1724	MPD	C2-C3-C4-C5
3	C	1713	MPD	CM-C2-C3-C4
3	A	1704	MPD	O2-C2-C3-C4
3	C	1701	MPD	O2-C2-C3-C4
3	C	1713	MPD	O2-C2-C3-C4
3	A	1704	MPD	C2-C3-C4-C5
3	A	1705	MPD	C2-C3-C4-C5
3	A	1720	MPD	C2-C3-C4-C5
3	B	1709	MPD	C2-C3-C4-C5
3	B	1722	MPD	C2-C3-C4-C5
3	C	1712	MPD	C2-C3-C4-C5
3	C	1713	MPD	C2-C3-C4-C5
3	A	1720	MPD	C2-C3-C4-O4
3	B	1718	MPD	C2-C3-C4-O4
3	B	1722	MPD	C2-C3-C4-O4
3	C	1712	MPD	C2-C3-C4-O4
3	A	1704	MPD	C1-C2-C3-C4
3	A	1717	MPD	C1-C2-C3-C4
3	A	1720	MPD	CM-C2-C3-C4
3	B	1707	MPD	CM-C2-C3-C4
3	B	1709	MPD	CM-C2-C3-C4
3	B	1711	MPD	C1-C2-C3-C4
3	B	1719	MPD	CM-C2-C3-C4
3	C	1701	MPD	C1-C2-C3-C4
3	C	1701	MPD	CM-C2-C3-C4
3	C	1712	MPD	C1-C2-C3-C4
3	C	1713	MPD	C1-C2-C3-C4
3	A	1716	MPD	O2-C2-C3-C4
3	A	1720	MPD	O2-C2-C3-C4
3	B	1711	MPD	O2-C2-C3-C4
3	B	1719	MPD	O2-C2-C3-C4
3	B	1718	MPD	C2-C3-C4-C5
3	B	1723	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1704	MPD	C2-C3-C4-O4
3	B	1711	MPD	C2-C3-C4-O4
3	B	1724	MPD	C2-C3-C4-O4
3	C	1713	MPD	C2-C3-C4-O4

There are no ring outliers.

20 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1720	MPD	11	0
3	B	1718	MPD	4	0
3	B	1703	MPD	13	0
2	B	1616	2HP	1	0
3	A	1704	MPD	10	0
3	A	1705	MPD	2	0
3	A	1702	MPD	1	0
3	C	1713	MPD	8	0
3	B	1721	MPD	1	0
3	B	1711	MPD	7	0
2	A	1610	2HP	1	0
3	C	1714	MPD	1	0
3	A	1717	MPD	4	0
3	B	1723	MPD	5	0
3	B	1709	MPD	13	0
3	B	1719	MPD	3	0
3	B	1722	MPD	3	0
3	B	1707	MPD	4	0
3	A	1716	MPD	5	0
2	B	1606	2HP	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)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	915/932 (98%)	-0.03	32 (3%)	44	50	29, 36, 52, 73	1 (0%)
1	B	906/932 (97%)	0.02	27 (2%)	50	56	28, 36, 49, 73	1 (0%)
1	C	909/932 (97%)	0.18	44 (4%)	30	36	28, 36, 50, 73	1 (0%)
All	All	2730/2796 (97%)	0.06	103 (3%)	40	46	28, 36, 50, 73	3 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	928	GLY	8.8
1	C	876	ASN	8.3
1	A	5	MET	6.6
1	C	875	ALA	6.2
1	C	395	CYS	6.0
1	B	395	CYS	5.6
1	C	928	GLY	5.6
1	C	172	ASP	5.5
1	A	929	ASN	5.4
1	B	874	TYR	5.2
1	C	878	ALA	5.1
1	C	448	LEU	4.9
1	C	237	GLY	4.9
1	C	444	ILE	4.8
1	A	395	CYS	4.6
1	B	442	ILE	4.5
1	C	678	TYR	4.5
1	A	442	ILE	4.3
1	B	6	LEU	4.2
1	C	929	ASN	4.2
1	C	877	SER	4.2
1	A	237	GLY	4.0
1	A	171	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	173	ASP	4.0
1	B	448	LEU	4.0
1	A	6	LEU	4.0
1	A	239	GLY	3.9
1	B	444	ILE	3.9
1	C	442	ILE	3.9
1	C	927	ALA	3.7
1	C	236	THR	3.7
1	A	198	GLY	3.7
1	A	444	ILE	3.5
1	C	333	ALA	3.5
1	A	875	ALA	3.5
1	C	238	THR	3.5
1	B	175	PRO	3.4
1	A	143	ALA	3.4
1	C	171	THR	3.3
1	C	394	TYR	3.3
1	B	5	MET	3.2
1	A	448	LEU	3.2
1	B	123	LEU	3.2
1	B	171	THR	3.2
1	B	394	TYR	3.1
1	B	876	ASN	3.0
1	B	169	THR	3.0
1	B	173	ASP	3.0
1	C	446	ALA	3.0
1	A	136	TYR	2.9
1	A	144	THR	2.9
1	C	396	PHE	2.9
1	A	387	VAL	2.9
1	C	71	ASP	2.8
1	A	173	ASP	2.8
1	C	616	ASN	2.8
1	B	138	ALA	2.8
1	A	396	PHE	2.7
1	A	77	TYR	2.7
1	A	123	LEU	2.7
1	A	394	TYR	2.7
1	B	396	PHE	2.7
1	A	172	ASP	2.7
1	B	323	THR	2.7
1	B	929	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	439	ALA	2.7
1	B	334	SER	2.6
1	C	123	LEU	2.6
1	C	169	THR	2.6
1	C	257	ALA	2.6
1	A	391	LEU	2.6
1	B	453	LEU	2.5
1	A	125	PRO	2.5
1	A	445	GLN	2.5
1	A	418	THR	2.5
1	B	53	HIS	2.5
1	C	77	TYR	2.5
1	A	446	ALA	2.4
1	C	443	ASN	2.4
1	C	453	LEU	2.4
1	C	387	VAL	2.4
1	B	391	LEU	2.3
1	C	338	ALA	2.3
1	C	447	ASN	2.3
1	C	73	GLU	2.3
1	C	440	MET	2.3
1	B	170	ASP	2.2
1	C	445	GLN	2.2
1	C	809	VAL	2.2
1	A	413	ASN	2.2
1	B	928	GLY	2.2
1	A	440	MET	2.2
1	A	439	ALA	2.2
1	C	452	PHE	2.1
1	C	170	ASP	2.1
1	B	413	ASN	2.1
1	C	76	THR	2.1
1	B	37	TYR	2.1
1	C	391	LEU	2.1
1	C	393	ASN	2.1
1	C	915	VAL	2.1
1	C	422	LYS	2.1
1	A	393	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	A	1717	8/8	0.44	0.24	67,69,70,70	0
3	MPD	B	1722	8/8	0.59	0.17	95,95,95,95	0
3	MPD	B	1703	8/8	0.73	0.22	61,62,63,64	0
3	MPD	B	1718	8/8	0.81	0.25	34,37,44,44	0
3	MPD	A	1720	8/8	0.82	0.25	63,65,66,66	0
3	MPD	A	1716	8/8	0.82	0.21	33,36,41,44	0
3	MPD	B	1709	8/8	0.83	0.16	28,33,39,42	0
3	MPD	A	1704	8/8	0.84	0.22	35,39,41,46	0
2	2HP	B	1612	5/5	0.84	0.23	77,78,79,79	0
3	MPD	C	1701	8/8	0.84	0.22	55,55,57,57	0
3	MPD	B	1708	8/8	0.85	0.20	71,72,72,73	0
3	MPD	B	1723	8/8	0.86	0.20	70,74,75,76	0
2	2HP	B	1622	5/5	0.86	0.22	34,37,46,46	0
3	MPD	C	1712	8/8	0.87	0.23	42,45,46,49	0
2	2HP	B	1608	5/5	0.89	0.30	78,78,79,79	0
3	MPD	B	1721	8/8	0.89	0.24	61,62,63,64	0
3	MPD	A	1702	8/8	0.90	0.14	41,45,46,48	0
3	MPD	C	1713	8/8	0.90	0.19	39,42,44,44	0
3	MPD	B	1707	8/8	0.91	0.21	49,52,54,54	0
2	2HP	C	1617	5/5	0.91	0.28	46,50,52,53	0
3	MPD	C	1714	8/8	0.91	0.25	54,55,56,57	0
2	2HP	B	1605	5/5	0.92	0.18	53,55,56,56	0
2	2HP	A	1619	5/5	0.92	0.25	59,60,60,61	0
3	MPD	B	1719	8/8	0.93	0.11	44,47,49,49	0
2	2HP	B	1621	5/5	0.93	0.27	72,72,73,74	0
3	MPD	B	1711	8/8	0.93	0.20	55,55,56,57	0
3	MPD	A	1706	8/8	0.93	0.20	60,61,62,63	0
2	2HP	A	1620	5/5	0.94	0.36	69,71,71,71	0
3	MPD	A	1705	8/8	0.94	0.19	58,58,58,59	0
3	MPD	C	1715	8/8	0.94	0.24	64,66,67,67	0
2	2HP	C	1613	5/5	0.95	0.16	49,51,52,52	0
3	MPD	B	1710	8/8	0.95	0.21	44,45,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	B	1724	8/8	0.95	0.16	58,60,61,61	0
2	2HP	B	1606	5/5	0.95	0.16	52,52,55,56	0
2	2HP	C	1611	5/5	0.96	0.22	54,54,55,56	0
2	2HP	B	1607	5/5	0.96	0.11	45,45,48,48	0
2	2HP	B	1615	5/5	0.96	0.24	41,41,42,42	0
2	2HP	C	1618	5/5	0.96	0.11	56,57,58,59	0
2	2HP	B	1616	5/5	0.97	0.29	58,59,61,61	0
2	2HP	B	1614	5/5	0.97	0.16	60,60,61,62	0
2	2HP	A	1610	5/5	0.97	0.15	51,51,53,54	0
2	2HP	C	1604	5/5	0.97	0.14	51,52,53,53	0
2	2HP	B	1609	5/5	0.98	0.13	35,35,37,38	0
2	2HP	A	1603	5/5	0.98	0.22	42,43,44,45	0
2	2HP	B	1601	5/5	0.98	0.07	37,38,41,41	0
2	2HP	A	1602	5/5	0.99	0.17	36,39,43,45	0

6.5 Other polymers (i)

There are no such residues in this entry.