



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:20 AM UTC

PDB ID : 2OBE / pdb_00002obe
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 ⓘ 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

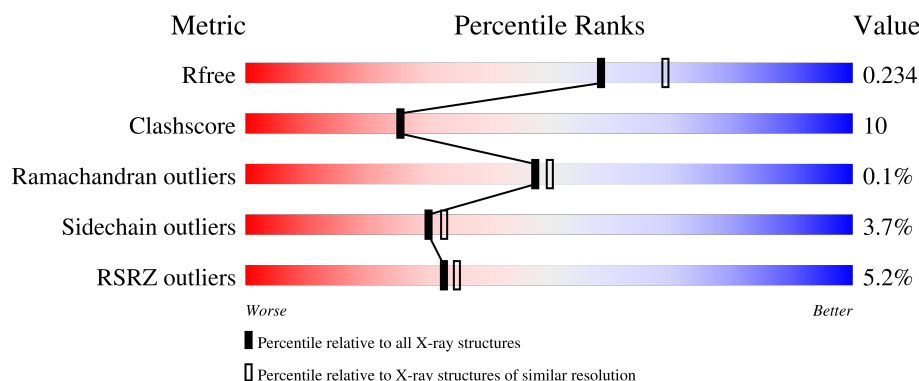
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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% 81% 14% . .
1	B	932	 3% 80% 14% . .
1	C	932	 9% 76% 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	1610	-	X	-	-
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	-	-
2	2HP	B	1622	-	X	-	-
2	2HP	C	1618	-	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

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.

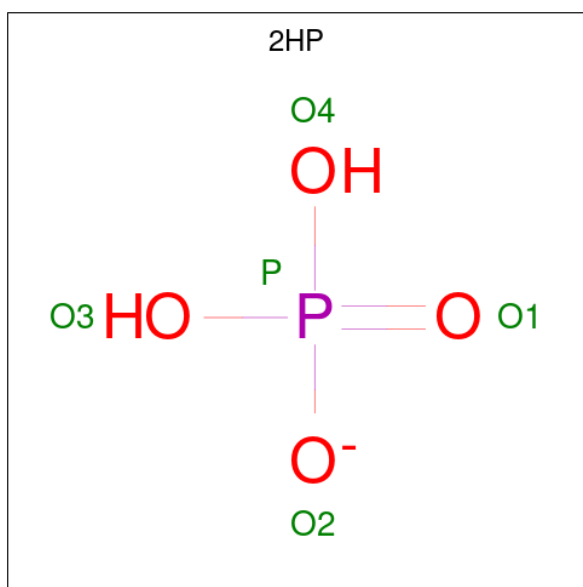
- Molecule 1 is a protein called Hexon protein.

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

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 (CCD ID: 2HP) (formula: $\text{H}_2\text{O}_4\text{P}$).



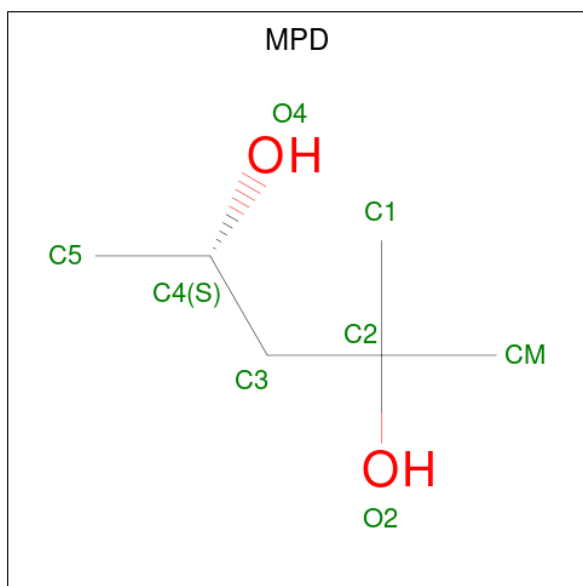
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total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

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

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

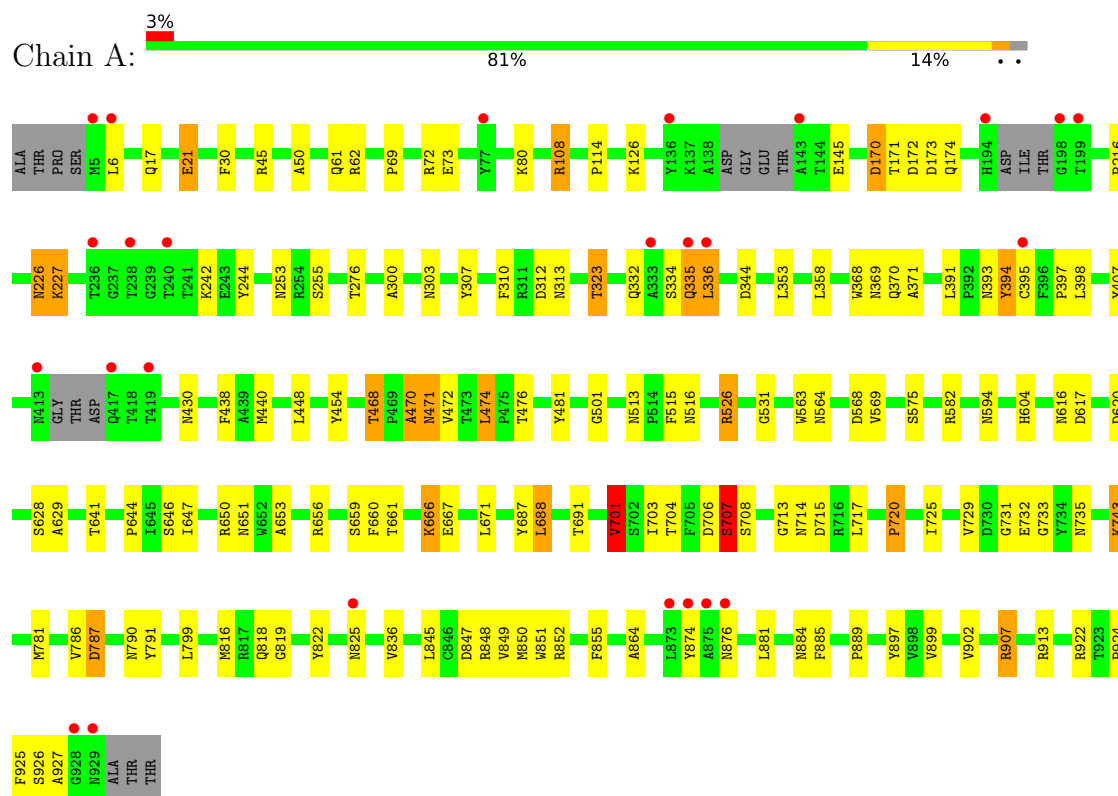
- Molecule 4 is water.

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

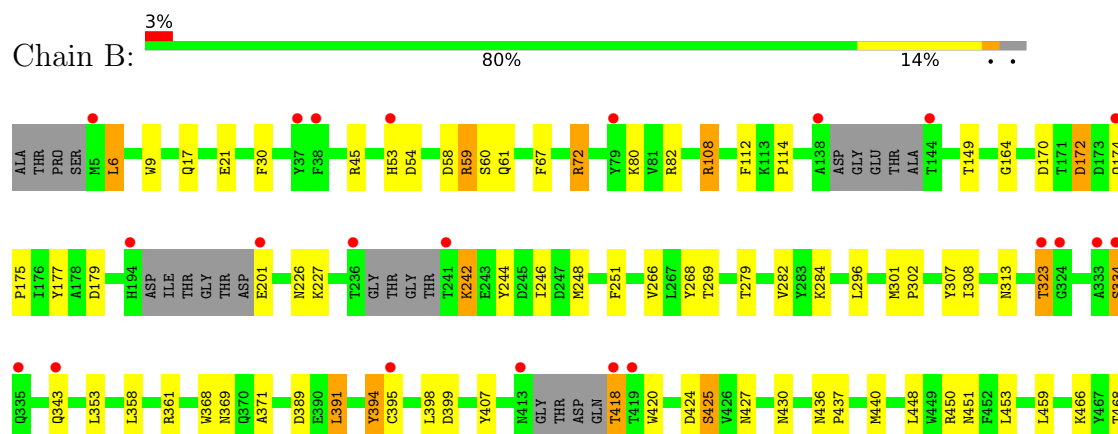
3 Residue-property plots [i](#)

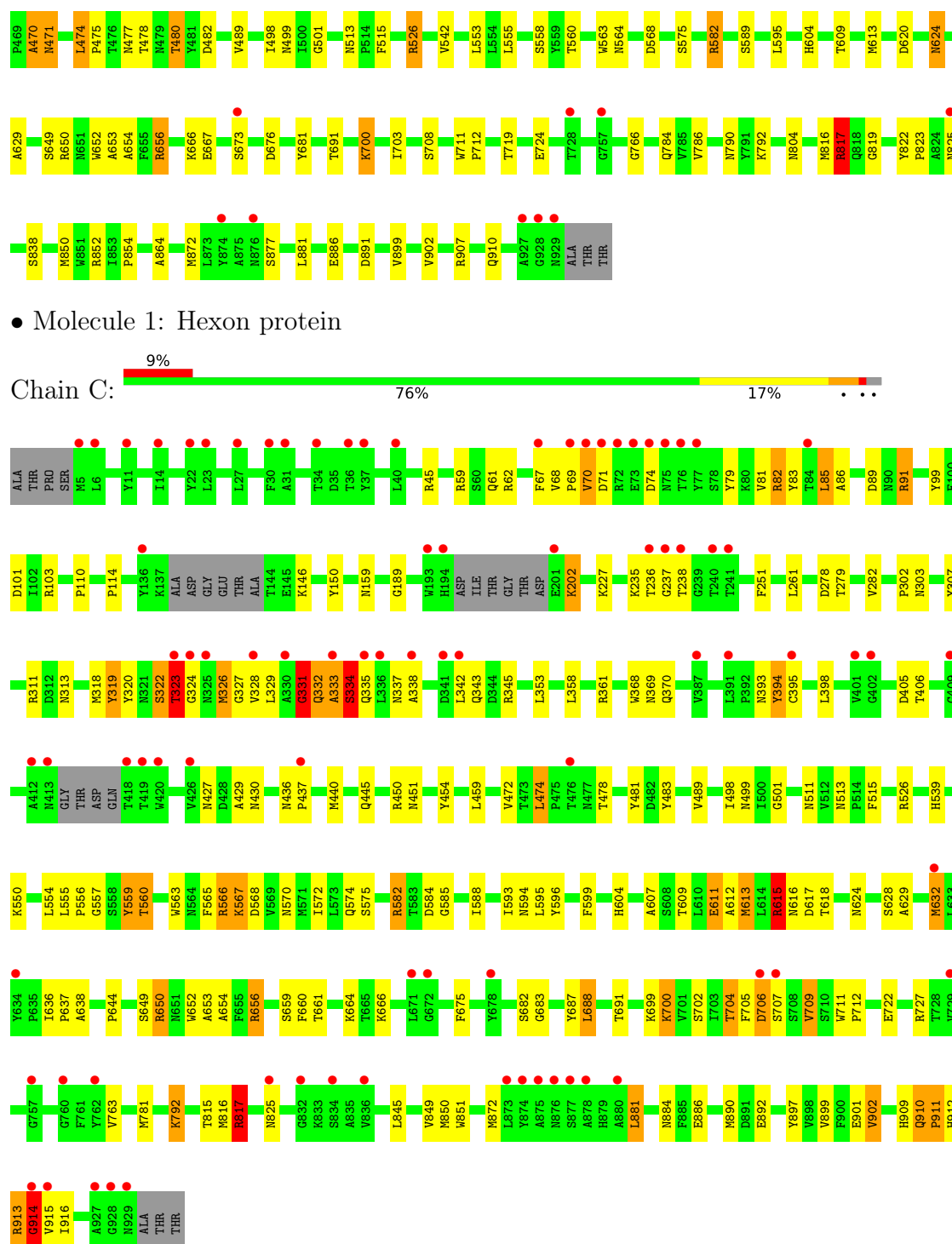
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Hexon protein





● Molecule 1: Hexon protein

4 Data and refinement statistics

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 49.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.10) 93.8 (49.27-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.169 , 0.210 0.168 , 0.234	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)	0.34 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2HP, MPD

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	1.14	20/7404 (0.3%)	1.11	29/10090 (0.3%)
1	B	1.15	9/7364 (0.1%)	1.12	26/10034 (0.3%)
1	C	1.53	61/7328 (0.8%)	1.22	39/9991 (0.4%)
All	All	1.29	90/22096 (0.4%)	1.15	94/30115 (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 (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	825	ASN	CG-OD1	-35.11	0.56	1.23
1	C	328	VAL	C-O	30.06	1.58	1.24
1	B	825	ASN	CG-OD1	-27.97	0.70	1.23
1	C	615	ARG	NE-CZ	26.81	1.62	1.33
1	C	914	GLY	C-O	21.56	1.54	1.23
1	C	912	HIS	C-O	19.28	1.47	1.23
1	C	913	ARG	CA-C	19.09	1.76	1.52
1	C	337	ASN	C-N	18.92	1.59	1.33
1	C	70	VAL	C-O	15.21	1.43	1.24
1	C	825	ASN	CG-ND2	14.46	1.63	1.33
1	C	707	SER	C-O	14.17	1.41	1.24
1	A	731	GLY	C-N	14.13	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	THR	C-N	14.07	1.52	1.33
1	A	733	GLY	CA-C	13.47	1.71	1.51
1	C	912	HIS	C-N	12.26	1.50	1.33
1	B	425	SER	CB-OG	11.62	1.65	1.42
1	A	825	ASN	CG-OD1	-11.33	1.02	1.23
1	C	68	VAL	C-O	11.11	1.38	1.24
1	C	335	GLN	C-O	10.48	1.37	1.24
1	C	912	HIS	CA-CB	10.29	1.70	1.53
1	B	825	ASN	CG-ND2	9.74	1.53	1.33
1	C	333	ALA	C-N	9.63	1.47	1.33
1	C	706	ASP	C-O	9.45	1.35	1.24
1	C	395	CYS	CA-CB	9.00	1.66	1.53
1	C	323	THR	C-O	8.69	1.34	1.23
1	C	567	LYS	CE-NZ	8.53	1.75	1.49
1	B	395	CYS	CA-CB	8.43	1.66	1.53
1	C	650	ARG	C-N	8.32	1.45	1.33
1	C	323	THR	C-N	8.25	1.45	1.33
1	C	85	LEU	CA-C	8.05	1.63	1.52
1	C	594	ASN	CG-OD1	7.92	1.38	1.23
1	C	566	ARG	CZ-NH1	7.80	1.43	1.32
1	C	911	PRO	C-O	7.66	1.33	1.24
1	C	914	GLY	N-CA	-7.55	1.34	1.45
1	C	615	ARG	CZ-NH1	7.53	1.43	1.32
1	B	108	ARG	CD-NE	-7.13	1.36	1.46
1	C	582	ARG	CZ-NH1	6.96	1.42	1.32
1	A	395	CYS	CA-CB	6.89	1.63	1.53
1	C	881	LEU	C-O	6.88	1.31	1.23
1	C	332	GLN	CB-CG	6.66	1.72	1.52
1	A	526	ARG	CD-NE	-6.65	1.36	1.46
1	C	612	ALA	C-N	6.60	1.42	1.34
1	C	327	GLY	CA-C	6.53	1.63	1.52
1	A	787	ASP	C-O	6.48	1.31	1.24
1	C	86	ALA	CA-CB	6.44	1.62	1.53
1	B	526	ARG	CD-NE	-6.44	1.37	1.46
1	C	278	ASP	CB-CG	-6.41	1.36	1.52
1	A	276	THR	CA-CB	6.40	1.60	1.53
1	C	320	TYR	C-N	6.30	1.42	1.33
1	C	324	GLY	C-N	6.26	1.42	1.33
1	C	342	LEU	CA-CB	6.26	1.65	1.54
1	C	85	LEU	C-O	6.20	1.31	1.24
1	C	334	SER	C-O	6.19	1.31	1.24
1	A	50	ALA	CA-CB	6.15	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	735	ASN	C-O	6.14	1.32	1.23
1	C	704	THR	C-N	6.09	1.41	1.33
1	C	914	GLY	CA-C	6.02	1.60	1.51
1	C	91	ARG	N-CA	5.96	1.53	1.45
1	C	707	SER	C-N	5.95	1.41	1.33
1	C	916	ILE	C-O	5.91	1.30	1.24
1	C	319	TYR	C-O	5.89	1.31	1.24
1	C	707	SER	CA-C	5.89	1.60	1.52
1	C	585	GLY	C-N	5.89	1.41	1.33
1	C	554	LEU	CG-CD2	5.88	1.72	1.52
1	A	733	GLY	C-O	-5.86	1.16	1.24
1	C	902	VAL	CA-CB	5.82	1.62	1.54
1	C	910	GLN	CD-OE1	5.81	1.34	1.23
1	C	326	MET	SD-CE	5.80	1.94	1.79
1	C	607	ALA	CA-C	5.78	1.60	1.52
1	C	331	GLY	C-N	5.71	1.41	1.33
1	C	345	ARG	N-CA	5.67	1.52	1.45
1	C	612	ALA	CA-CB	5.65	1.62	1.53
1	C	557	GLY	N-CA	5.64	1.50	1.45
1	A	720	PRO	C-O	5.60	1.30	1.24
1	A	468	THR	C-O	-5.59	1.20	1.25
1	B	542	VAL	CA-CB	5.56	1.58	1.54
1	A	310	PHE	C-O	5.43	1.31	1.23
1	B	864	ALA	CA-CB	5.43	1.61	1.53
1	B	786	VAL	CA-CB	5.41	1.59	1.54
1	C	706	ASP	CA-C	5.36	1.59	1.52
1	C	613	MET	N-CA	5.26	1.52	1.46
1	A	707	SER	CB-OG	5.24	1.52	1.42
1	A	704	THR	C-O	5.22	1.30	1.23
1	A	312	ASP	CA-C	5.21	1.59	1.52
1	C	582	ARG	CD-NE	5.19	1.53	1.46
1	A	735	ASN	N-CA	-5.18	1.38	1.45
1	C	89	ASP	C-O	5.17	1.31	1.23
1	C	704	THR	CA-C	5.14	1.58	1.52
1	A	743	LYS	CE-NZ	5.09	1.64	1.49
1	A	864	ALA	CA-CB	5.05	1.61	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	825	ASN	OD1-CG-ND2	34.57	157.17	122.60
1	B	825	ASN	OD1-CG-ND2	26.22	148.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	825	ASN	CB-CG-ND2	-25.41	78.28	116.40
1	A	825	ASN	OD1-CG-ND2	24.07	146.67	122.60
1	B	825	ASN	CB-CG-ND2	-21.05	84.83	116.40
1	B	526	ARG	NE-CZ-NH2	-12.20	108.22	119.20
1	A	825	ASN	CB-CG-ND2	-11.82	98.68	116.40
1	B	817	ARG	NE-CZ-NH2	-11.69	108.68	119.20
1	A	526	ARG	NE-CZ-NH2	-11.47	108.87	119.20
1	B	817	ARG	CD-NE-CZ	9.44	137.61	124.40
1	B	656	ARG	NE-CZ-NH2	-9.40	110.74	119.20
1	B	817	ARG	NE-CZ-NH1	9.19	130.69	121.50
1	A	713	GLY	N-CA-C	-7.84	97.86	111.50
1	C	817	ARG	NE-CZ-NH2	-7.82	112.17	119.20
1	A	470	ALA	N-CA-C	-7.75	99.58	110.50
1	B	817	ARG	CG-CD-NE	-7.44	95.63	112.00
1	C	912	HIS	O-C-N	7.34	131.70	123.48
1	B	526	ARG	NE-CZ-NH1	7.20	128.70	121.50
1	A	701	VAL	CB-CA-C	-7.13	99.52	110.50
1	C	560	THR	CB-CA-C	7.11	122.02	109.72
1	A	733	GLY	O-C-N	7.09	130.34	122.47
1	C	560	THR	N-CA-C	-7.01	97.78	109.07
1	A	526	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	B	656	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	C	817	ARG	CG-CD-NE	-6.71	97.23	112.00
1	A	822	TYR	CA-C-N	-6.68	113.08	119.90
1	A	822	TYR	C-N-CA	-6.68	113.08	119.90
1	C	278	ASP	CB-CG-OD1	-6.67	103.07	118.40
1	A	526	ARG	CD-NE-CZ	6.60	133.64	124.40
1	A	323	THR	N-CA-C	6.59	119.02	111.11
1	C	709	VAL	N-CA-C	6.54	116.88	108.12
1	B	470	ALA	N-CA-C	-6.49	101.36	110.50
1	C	615	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	C	915	VAL	N-CA-CB	6.37	119.91	111.25
1	C	912	HIS	CA-C-N	-6.36	111.94	120.90
1	C	912	HIS	C-N-CA	-6.36	111.94	120.90
1	C	278	ASP	CB-CA-C	-6.29	98.46	109.02
1	C	394	TYR	CA-C-N	6.20	131.27	122.09
1	C	394	TYR	C-N-CA	6.20	131.27	122.09
1	B	526	ARG	CD-NE-CZ	6.19	133.07	124.40
1	A	170	ASP	N-CA-C	6.19	118.31	110.33
1	A	394	TYR	CA-C-N	6.16	130.88	122.19
1	A	394	TYR	C-N-CA	6.16	130.88	122.19
1	A	725	ILE	N-CA-C	-6.14	105.08	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	612	ALA	CA-C-N	-6.07	111.51	120.38
1	C	612	ALA	C-N-CA	-6.07	111.51	120.38
1	B	394	TYR	CA-C-N	6.03	131.64	122.65
1	B	394	TYR	C-N-CA	6.03	131.64	122.65
1	B	323	THR	N-CA-C	5.99	117.80	111.28
1	C	395	CYS	N-CA-C	-5.73	100.33	109.96
1	C	615	ARG	CD-NE-CZ	-5.72	116.39	124.40
1	B	395	CYS	N-CA-C	-5.71	100.40	109.76
1	C	913	ARG	CA-C-N	5.71	131.84	120.77
1	C	913	ARG	C-N-CA	5.71	131.84	120.77
1	B	877	SER	N-CA-C	5.65	117.56	109.14
1	A	62	ARG	CG-CD-NE	-5.64	99.59	112.00
1	C	656	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	732	GLU	CA-C-N	-5.59	114.77	122.26
1	A	732	GLU	C-N-CA	-5.59	114.77	122.26
1	B	825	ASN	N-CA-C	-5.57	105.84	113.30
1	C	82	ARG	CA-C-O	-5.56	113.93	120.60
1	A	108	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	A	732	GLU	N-CA-C	5.53	119.13	112.38
1	B	282	VAL	N-CA-C	-5.50	108.14	113.53
1	C	636	ILE	CB-CA-C	-5.50	105.86	111.08
1	A	671	LEU	N-CA-C	-5.49	106.46	112.72
1	C	332	GLN	N-CA-C	-5.48	104.70	111.33
1	C	849	VAL	CB-CA-C	-5.47	105.58	111.59
1	B	838	SER	N-CA-C	5.45	117.70	109.41
1	A	731	GLY	CA-C-N	-5.41	111.94	120.60
1	A	731	GLY	C-N-CA	-5.41	111.94	120.60
1	B	108	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	731	GLY	N-CA-C	5.38	119.00	112.49
1	C	817	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	B	656	ARG	CD-NE-CZ	5.36	131.91	124.40
1	B	582	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	C	763	VAL	CA-C-N	-5.32	114.77	120.03
1	C	763	VAL	C-N-CA	-5.32	114.77	120.03
1	C	323	THR	O-C-N	5.24	130.25	123.07
1	B	792	LYS	N-CA-C	5.24	117.73	111.71
1	A	927	ALA	N-CA-C	5.19	117.75	110.23
1	C	611	GLU	CB-CG-CD	-5.15	103.85	112.60
1	C	849	VAL	N-CA-C	5.14	115.65	110.05
1	C	559	TYR	CA-C-N	-5.12	115.93	123.00
1	C	559	TYR	C-N-CA	-5.12	115.93	123.00
1	C	332	GLN	CA-C-N	5.12	129.61	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	GLN	C-N-CA	5.12	129.61	121.99
1	A	569	VAL	N-CA-C	5.10	117.43	111.05
1	B	854	PRO	CB-CA-C	-5.06	104.47	111.21
1	A	526	ARG	CG-CD-NE	-5.06	100.86	112.00
1	B	804	ASN	N-CA-C	-5.06	100.02	108.32
1	A	855	PHE	N-CA-C	-5.05	103.65	110.68
1	C	85	LEU	CB-CA-C	-5.03	103.03	110.67
1	C	335	GLN	CA-C-O	-5.02	113.33	120.51

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

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	118	0
1	B	7169	0	6783	150	0
1	C	7134	0	6705	144	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	54	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	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23334	0	20628	405	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 10.

All (405) 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	1.52
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:B:164:GLY:HA2	1:B:248:MET:HE1	1.29	1.10
1:B:164:GLY:CA	1:B:248:MET:HE1	1.84	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:61:GLN:HE22	1:C:604:HIS:CE1	1.88	0.88
1:B:248:MET:HE2	1:B:266:VAL:HG21	1.55	0.87
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:C:567:LYS:HZ2	1:C:567:LYS:HG2	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:C:235:LYS:C	1:C:237:GLY:HA3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLY:HA3	1:B:248:MET:HE1	1.69	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:248:MET:HE3	1:B:268:TYR:CZ	2.26	0.70
1:B:891:ASP:HB3	4:B:2254:HOH:O	1.91	0.70
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: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:913:ARG:C	1:C:913:ARG:CB	2.67	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:440:MET:HE2	1:B:440:MET:CG	2.25	0.66
1:B:563:TRP:C	1:B:564:ASN:HD22	2.04	0.65
1:A:666:LYS:CE	3:A:1704:MPD:H12	2.27	0.65
1:A:781:MET:HE1	1:A:845:LEU:HG	1.77	0.65
1:C:567:LYS:NZ	1:C:567:LYS:HG2	2.09	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:C:661:THR:HG22	1:C:850:MET:HE3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:440:MET:HE2	1:B:440:MET:HG3	1.81	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: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: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
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: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:C:666:LYS:HZ1	3:C:1713:MPD:H13	1.68	0.58
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:B:425:SER:CB	1:B:425:SER:HG	2.09	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:A:661:THR:HG22	1:A:850:MET:HE3	1.84	0.58
1:A:468:THR:HG23	1:A:474:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:482:ASP:CG	3:B:1718:MPD:H4	2.32	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
1:A:874:TYR:C	1:A:876:ASN:N	2.63	0.54
1:A:440:MET:HE2	1:B:440:MET:HG2	1.89	0.54
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:B:564:ASN:HD22	1:B:564:ASN:N	2.02	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:248:MET:HE2	1:B:266:VAL:CG2	2.34	0.53
1:B:451:ASN:ND2	1:C:393:ASN:HD21	2.06	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:652:TRP:HB2	1:B:872:MET:HE2	1.92	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
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: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:816:MET:HE3	1:C:817:ARG:HH21	1.75	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:C:498:ILE:O	1:C:499:ASN:C	2.55	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:B:498:ILE:O	1:B:499:ASN:C	2.54	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:C:781:MET:HE1	1:C:845:LEU:HG	1.94	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:874:TYR:C	1:A:876:ASN:H	2.21	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:A:701:VAL:HG13	1:A:885:PHE:CD2	2.49	0.47
1:B:850:MET:HE1	1:B:899:VAL:HG23	1.97	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: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:C:913:ARG:C	1:C:913:ARG:N	2.64	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
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
1:A:30:PHE:CG	1:B:613:MET:HE1	2.51	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:B:700:LYS:HB3	1:B:700:LYS:HE3	1.73	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:568:ASP:HB2	1:C:675:PHE:CE1	2.51	0.46
1:C:705:PHE:O	1:C:706:ASP:C	2.58	0.46
1:A:563:TRP:C	1:A:564:ASN:HD22	2.24	0.46
3:B:1719:MPD:HM2	3:B:1719:MPD:HO4	1.80	0.46
1:C:511:ASN:O	1:C:664:LYS:NZ	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:624:ASN:CG	3:B:1711:MPD:C1	2.90	0.45
1:B:819:GLY:O	1:C:437:PRO:HD3	2.17	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
1:C:890:MET:C	1:C:892:GLU:H	2.25	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
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:30:PHE:CD1	1:B:30:PHE:C	2.95	0.44
1:B:700:LYS:HG2	1:B:886:GLU:HB3	1.98	0.44
1:C:609:THR:HG22	1:C:613:MET:HE2	1.99	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:714:ASN:O	1:A:715:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:637:PRO:O	1:C:638:ALA:C	2.61	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: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:B:470:ALA:O	1:B:471:ASN:CG	2.61	0.43
1:C:322:SER:O	1:C:323:THR:C	2.60	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
1:B:179:ASP:C	1:B:179:ASP:OD1	2.62	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:470:ALA:O	1:A:471:ASN:CG	2.62	0.43
1:A:564:ASN:HD22	1:A:564:ASN:N	2.17	0.43
1:A:313:ASN:HD21	1:A:370:GLN:HG3	1.84	0.43
1:B:624:ASN:CG	3:B:1711:MPD:H13	2.44	0.43
1:C:319:TYR:CE2	1:C:566:ARG:CG	3.01	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ASN:HB3	1:C:430:ASN:HD21	1.85	0.42
1:B:650:ARG:HE	1:B:650:ARG:HB3	1.69	0.41
1:C:568:ASP:CG	1:C:582:ARG:HH11	2.28	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:B:609:THR:HG22	1:B:613:MET:HE2	2.02	0.41
1:C:629:ALA:CB	1:C:899:VAL:CG1	2.98	0.41
1:C:632:MET:HE2	1:C:632:MET:HB3	1.98	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:B:466:LYS:HG2	1:B:489:VAL:HG22	2.03	0.41
1:A:706:ASP:O	1:A:707:SER:C	2.64	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:226:ASN:C	1:A:226:ASN:HD22	2.29	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: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:B:816:MET:HE2	1:B:816:MET:HB3	1.96	0.41
1:C:704:THR:HA	1:C:709:VAL:O	2.21	0.41
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:B:482:ASP:OD1	3:B:1718:MPD:H4	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	43	44
1	B	896/932 (96%)	858 (96%)	38 (4%)	0	100	100
1	C	901/932 (97%)	858 (95%)	41 (5%)	2 (0%)	43	44
All	All	2704/2796 (97%)	2589 (96%)	111 (4%)	4 (0%)	48	50

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%)	30	33
1	B	764/799 (96%)	733 (96%)	31 (4%)	27	29
1	C	750/799 (94%)	724 (96%)	26 (4%)	32	35
All	All	2278/2397 (95%)	2193 (96%)	85 (4%)	30	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	21	GLU
1	A	108	ARG
1	A	145	GLU
1	A	171	THR
1	A	226	ASN
1	A	227	LYS
1	A	323	THR
1	A	332	GLN
1	A	336	LEU
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	628	SER
1	A	646	SER
1	A	666	LYS
1	A	688	LEU
1	A	701	VAL
1	A	729	VAL
1	A	852	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	172	ASP

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Mol	Chain	Res	Type
1	B	242	LYS
1	B	296	LEU
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	398	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	589	SER
1	B	624	ASN
1	B	649	SER
1	B	673	SER
1	B	700	LYS
1	B	708	SER
1	B	817	ARG
1	C	45	ARG
1	C	59	ARG
1	C	91	ARG
1	C	202	LYS
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	563	TRP
1	C	624	ASN

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Mol	Chain	Res	Type
1	C	628	SER
1	C	632	MET
1	C	649	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 (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	53	HIS
1	A	75	ASN
1	A	90	ASN
1	A	133	GLN
1	A	226	ASN
1	A	231	GLN
1	A	313	ASN
1	A	325	ASN
1	A	393	ASN
1	A	430	ASN
1	A	564	ASN
1	A	594	ASN
1	A	604	HIS
1	A	616	ASN
1	A	651	ASN
1	A	777	ASN
1	A	818	GLN
1	A	871	ASN
1	A	884	ASN
1	B	8	GLN
1	B	61	GLN
1	B	133	GLN
1	B	233	ASN
1	B	253	ASN
1	B	313	ASN
1	B	325	ASN
1	B	369	ASN
1	B	393	ASN

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Mol	Chain	Res	Type
1	B	430	ASN
1	B	436	ASN
1	B	447	ASN
1	B	451	ASN
1	B	471	ASN
1	B	564	ASN
1	B	604	HIS
1	B	624	ASN
1	B	642	ASN
1	B	777	ASN
1	B	803	HIS
1	B	910	GLN
1	C	29	GLN
1	C	61	GLN
1	C	133	GLN
1	C	231	GLN
1	C	253	ASN
1	C	313	ASN
1	C	332	GLN
1	C	393	ASN
1	C	430	ASN
1	C	436	ASN
1	C	447	ASN
1	C	451	ASN
1	C	604	HIS
1	C	616	ASN
1	C	651	ASN
1	C	738	GLN
1	C	753	HIS
1	C	871	ASN
1	C	884	ASN
1	C	910	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 [i](#)

There are no oligosaccharides 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
3	MPD	A	1706	-	7,7,7	0.34	0	9,10,10	0.95	0
3	MPD	A	1705	-	7,7,7	0.36	0	9,10,10	0.73	0
3	MPD	C	1701	-	7,7,7	0.37	0	9,10,10	0.80	0
3	MPD	C	1715	-	7,7,7	0.33	0	9,10,10	0.33	0
2	2HP	A	1610	-	4,4,4	5.50	2 (50%)	6,6,6	1.89	2 (33%)
2	2HP	B	1622	-	4,4,4	5.27	3 (75%)	6,6,6	1.77	1 (16%)
2	2HP	B	1614	-	4,4,4	5.91	2 (50%)	6,6,6	1.30	1 (16%)
3	MPD	B	1724	-	7,7,7	0.33	0	9,10,10	0.65	0
2	2HP	A	1602	-	4,4,4	5.91	2 (50%)	6,6,6	1.40	1 (16%)
2	2HP	C	1611	-	4,4,4	6.12	2 (50%)	6,6,6	1.01	0
3	MPD	B	1722	-	7,7,7	0.57	0	9,10,10	0.49	0
3	MPD	B	1723	-	7,7,7	0.44	0	9,10,10	0.66	0
3	MPD	C	1713	-	7,7,7	0.57	0	9,10,10	1.31	1 (11%)
3	MPD	A	1716	-	7,7,7	1.05	0	9,10,10	1.13	0
3	MPD	A	1704	-	7,7,7	0.75	0	9,10,10	0.76	1 (11%)
3	MPD	B	1707	-	7,7,7	0.41	0	9,10,10	0.43	0
3	MPD	A	1720	-	7,7,7	0.36	0	9,10,10	0.85	0
3	MPD	A	1702	-	7,7,7	0.48	0	9,10,10	1.90	4 (44%)
2	2HP	B	1608	-	4,4,4	6.15	2 (50%)	6,6,6	1.14	1 (16%)
3	MPD	B	1709	-	7,7,7	1.16	1 (14%)	9,10,10	1.13	1 (11%)
2	2HP	C	1617	-	4,4,4	6.43	2 (50%)	6,6,6	1.51	1 (16%)
2	2HP	B	1605	-	4,4,4	6.02	2 (50%)	6,6,6	1.64	2 (33%)
2	2HP	A	1620	-	4,4,4	6.05	2 (50%)	6,6,6	0.94	0
2	2HP	C	1604	-	4,4,4	5.32	2 (50%)	6,6,6	1.47	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2HP	C	1613	-	4,4,4	6.02	2 (50%)	6,6,6	1.47	1 (16%)
2	2HP	C	1618	-	4,4,4	5.79	2 (50%)	6,6,6	1.53	2 (33%)
2	2HP	B	1615	-	4,4,4	6.55	2 (50%)	6,6,6	1.73	3 (50%)
3	MPD	A	1717	-	7,7,7	0.58	0	9,10,10	0.86	0
2	2HP	B	1616	-	4,4,4	6.43	2 (50%)	6,6,6	0.82	0
3	MPD	C	1712	-	7,7,7	0.62	0	9,10,10	0.96	0
3	MPD	B	1703	-	7,7,7	0.72	0	9,10,10	0.79	0
2	2HP	A	1619	-	4,4,4	6.52	2 (50%)	6,6,6	1.55	2 (33%)
2	2HP	A	1603	-	4,4,4	5.57	2 (50%)	6,6,6	1.16	0
3	MPD	B	1718	-	7,7,7	0.89	0	9,10,10	1.50	2 (22%)
2	2HP	B	1612	-	4,4,4	6.17	2 (50%)	6,6,6	1.14	0
3	MPD	B	1719	-	7,7,7	0.38	0	9,10,10	0.84	0
3	MPD	C	1714	-	7,7,7	0.43	0	9,10,10	0.30	0
3	MPD	B	1721	-	7,7,7	0.33	0	9,10,10	0.60	0
2	2HP	B	1609	-	4,4,4	4.64	2 (50%)	6,6,6	2.27	3 (50%)
3	MPD	B	1711	-	7,7,7	0.39	0	9,10,10	0.97	0
3	MPD	B	1708	-	7,7,7	0.37	0	9,10,10	0.44	0
2	2HP	B	1601	-	4,4,4	5.25	2 (50%)	6,6,6	1.41	1 (16%)
2	2HP	B	1621	-	4,4,4	6.20	2 (50%)	6,6,6	0.99	0
2	2HP	B	1606	-	4,4,4	5.56	2 (50%)	6,6,6	0.91	0
3	MPD	B	1710	-	7,7,7	0.59	0	9,10,10	0.61	0
2	2HP	B	1607	-	4,4,4	5.71	2 (50%)	6,6,6	1.87	2 (33%)

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	1706	-	-	0/5/5/5	-
3	MPD	A	1705	-	-	2/5/5/5	-
3	MPD	C	1701	-	-	3/5/5/5	-
3	MPD	C	1715	-	-	0/5/5/5	-
3	MPD	B	1724	-	1/1/2/2	2/5/5/5	-
3	MPD	B	1722	-	1/1/2/2	3/5/5/5	-
3	MPD	B	1723	-	-	0/5/5/5	-
3	MPD	C	1713	-	1/1/2/2	4/5/5/5	-
3	MPD	A	1704	-	1/1/2/2	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	1707	-	-	5/5/5/5	-
3	MPD	A	1720	-	1/1/2/2	5/5/5/5	-
3	MPD	A	1702	-	-	0/5/5/5	-
3	MPD	B	1709	-	-	2/5/5/5	-
3	MPD	A	1717	-	1/1/2/2	3/5/5/5	-
3	MPD	C	1712	-	-	4/5/5/5	-
3	MPD	B	1703	-	-	0/5/5/5	-
3	MPD	B	1718	-	1/1/2/2	3/5/5/5	-
3	MPD	B	1719	-	1/1/2/2	2/5/5/5	-
3	MPD	C	1714	-	-	1/5/5/5	-
3	MPD	B	1721	-	1/1/2/2	1/5/5/5	-
3	MPD	B	1711	-	-	4/5/5/5	-
3	MPD	B	1708	-	-	0/5/5/5	-
3	MPD	A	1716	-	-	4/5/5/5	-
3	MPD	B	1710	-	-	1/5/5/5	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1615	2HP	P-O4	10.18	1.84	1.54
2	C	1617	2HP	P-O3	9.60	1.82	1.54
2	B	1616	2HP	P-O3	9.42	1.82	1.54
2	A	1619	2HP	P-O4	9.22	1.81	1.54
2	A	1619	2HP	P-O3	9.20	1.81	1.54
2	C	1611	2HP	P-O4	9.16	1.81	1.54
2	B	1612	2HP	P-O3	8.99	1.80	1.54
2	B	1621	2HP	P-O4	8.80	1.80	1.54
2	B	1608	2HP	P-O3	8.68	1.79	1.54
2	B	1605	2HP	P-O3	8.66	1.79	1.54
2	C	1613	2HP	P-O4	8.64	1.79	1.54
2	B	1621	2HP	P-O3	8.63	1.79	1.54
2	B	1616	2HP	P-O4	8.62	1.79	1.54
2	B	1608	2HP	P-O4	8.59	1.79	1.54
2	A	1620	2HP	P-O3	8.58	1.79	1.54
2	B	1614	2HP	P-O3	8.49	1.79	1.54
2	A	1620	2HP	P-O4	8.44	1.79	1.54
2	C	1618	2HP	P-O4	8.44	1.79	1.54
2	B	1607	2HP	P-O4	8.41	1.79	1.54
2	C	1617	2HP	P-O4	8.35	1.79	1.54
2	B	1612	2HP	P-O4	8.35	1.78	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1605	2HP	P-O4	8.34	1.78	1.54
2	A	1602	2HP	P-O4	8.29	1.78	1.54
2	A	1602	2HP	P-O3	8.24	1.78	1.54
2	A	1603	2HP	P-O4	8.16	1.78	1.54
2	B	1614	2HP	P-O4	8.12	1.78	1.54
2	C	1613	2HP	P-O3	8.10	1.78	1.54
2	C	1611	2HP	P-O3	8.07	1.78	1.54
2	B	1606	2HP	P-O3	8.06	1.78	1.54
2	B	1615	2HP	P-O3	8.02	1.78	1.54
2	C	1618	2HP	P-O3	7.88	1.77	1.54
2	B	1622	2HP	P-O3	7.87	1.77	1.54
2	B	1601	2HP	P-O3	7.82	1.77	1.54
2	A	1610	2HP	P-O3	7.80	1.77	1.54
2	B	1607	2HP	P-O3	7.70	1.77	1.54
2	B	1606	2HP	P-O4	7.60	1.76	1.54
2	C	1604	2HP	P-O3	7.60	1.76	1.54
2	A	1610	2HP	P-O4	7.60	1.76	1.54
2	A	1603	2HP	P-O3	7.40	1.76	1.54
2	C	1604	2HP	P-O4	7.32	1.76	1.54
2	B	1622	2HP	P-O4	6.69	1.74	1.54
2	B	1609	2HP	P-O3	6.59	1.73	1.54
2	B	1601	2HP	P-O4	6.55	1.73	1.54
2	B	1609	2HP	P-O4	6.42	1.73	1.54
2	B	1622	2HP	P-O1	2.11	1.55	1.50
3	B	1709	MPD	O4-C4	2.03	1.51	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1610	2HP	O2-P-O1	3.90	124.74	110.95
2	B	1609	2HP	O4-P-O2	-3.39	97.38	107.91
2	B	1622	2HP	O4-P-O3	3.26	118.06	107.91
2	B	1607	2HP	O2-P-O1	3.07	121.80	110.95
3	B	1709	MPD	O4-C4-C5	3.05	122.59	109.45
2	C	1617	2HP	O2-P-O1	2.93	121.33	110.95
3	A	1702	MPD	C1-C2-C3	-2.80	98.13	110.20
3	A	1702	MPD	O2-C2-C1	2.78	116.64	107.99
2	B	1609	2HP	O3-P-O1	-2.76	101.18	110.95
3	A	1702	MPD	CM-C2-C3	2.71	121.87	110.20
2	B	1607	2HP	O4-P-O3	-2.66	99.62	107.91
2	A	1619	2HP	O3-P-O1	-2.60	101.76	110.95
2	A	1619	2HP	O2-P-O1	2.57	120.04	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1602	2HP	O4-P-O3	-2.57	99.93	107.91
2	C	1604	2HP	O3-P-O2	-2.55	99.97	107.91
2	B	1615	2HP	O2-P-O1	2.55	119.97	110.95
2	B	1614	2HP	O2-P-O1	2.48	119.73	110.95
3	B	1718	MPD	O2-C2-C3	-2.46	100.08	109.27
2	B	1609	2HP	O2-P-O1	2.43	119.56	110.95
3	A	1702	MPD	CM-C2-C1	-2.36	105.34	110.63
2	B	1608	2HP	O2-P-O1	2.34	119.24	110.95
2	B	1605	2HP	O2-P-O1	2.28	119.00	110.95
2	B	1605	2HP	O3-P-O1	-2.27	102.93	110.95
3	C	1713	MPD	O4-C4-C5	2.25	119.15	109.45
3	A	1704	MPD	O4-C4-C5	2.18	118.83	109.45
2	B	1615	2HP	O4-P-O1	-2.12	103.47	110.95
2	B	1615	2HP	O3-P-O2	-2.11	101.34	107.91
2	C	1613	2HP	O3-P-O2	2.11	114.47	107.91
2	B	1601	2HP	O2-P-O1	2.10	118.39	110.95
2	C	1618	2HP	O3-P-O2	-2.06	101.52	107.91
3	B	1718	MPD	O4-C4-C3	2.05	119.51	111.35
2	A	1610	2HP	O4-P-O2	-2.02	101.63	107.91
2	C	1618	2HP	O4-P-O1	-2.02	103.81	110.95

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 (54) 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	1716	MPD	C2-C3-C4-C5
3	A	1717	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	A	1717	MPD	C2-C3-C4-C5
3	B	1707	MPD	C1-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	B	1721	MPD	O2-C2-C3-C4
3	C	1714	MPD	O2-C2-C3-C4
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	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	O2-C2-C3-C4
3	B	1707	MPD	O2-C2-C3-C4
3	B	1722	MPD	O2-C2-C3-C4
3	C	1701	MPD	O2-C2-C3-C4
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
3	A	1716	MPD	C1-C2-C3-C4
3	A	1716	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	1720	MPD	C1-C2-C3-C4
3	B	1710	MPD	C1-C2-C3-C4
3	B	1711	MPD	CM-C2-C3-C4
3	B	1718	MPD	C1-C2-C3-C4
3	B	1718	MPD	CM-C2-C3-C4
3	B	1719	MPD	C1-C2-C3-C4
3	C	1712	MPD	CM-C2-C3-C4

There are no ring outliers.

20 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1705	MPD	2	0
2	A	1610	2HP	1	0
3	B	1722	MPD	3	0
3	B	1723	MPD	5	0
3	C	1713	MPD	8	0
3	A	1716	MPD	5	0
3	A	1704	MPD	10	0
3	B	1707	MPD	4	0
3	A	1720	MPD	11	0
3	A	1702	MPD	1	0
3	B	1709	MPD	12	0
3	A	1717	MPD	4	0
2	B	1616	2HP	1	0
3	B	1703	MPD	13	0
3	B	1718	MPD	4	0
3	B	1719	MPD	4	0
3	C	1714	MPD	1	0
3	B	1721	MPD	1	0
3	B	1711	MPD	8	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.28	25 (2%)	56	59	24, 36, 52, 73	1 (0%)
1	B	906/932 (97%)	0.34	31 (3%)	48	50	25, 36, 49, 73	1 (0%)
1	C	909/932 (97%)	0.86	85 (9%)	14	14	24, 36, 50, 73	1 (0%)
All	All	2730/2796 (97%)	0.49	141 (5%)	33	35	24, 36, 50, 73	3 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	928	GLY	9.5
1	C	418	THR	6.1
1	C	413	ASN	5.9
1	C	929	ASN	5.1
1	A	929	ASN	4.9
1	B	413	ASN	4.8
1	A	875	ALA	4.6
1	C	876	ASN	4.6
1	B	929	ASN	4.4
1	B	236	THR	4.3
1	C	395	CYS	4.2
1	C	419	THR	4.1
1	B	138	ALA	4.0
1	A	413	ASN	4.0
1	C	71	ASP	4.0
1	A	77	TYR	3.9
1	A	199	THR	3.9
1	C	874	TYR	3.8
1	B	144	THR	3.7
1	C	237	GLY	3.7
1	C	73	GLU	3.7
1	B	419	THR	3.7
1	A	419	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	241	THR	3.5
1	A	198	GLY	3.5
1	B	395	CYS	3.5
1	C	336	LEU	3.4
1	B	876	ASN	3.4
1	B	5	MET	3.4
1	C	30	PHE	3.3
1	B	323	THR	3.3
1	C	240	THR	3.3
1	B	874	TYR	3.3
1	A	5	MET	3.3
1	A	240	THR	3.2
1	C	201	GLU	3.2
1	B	241	THR	3.2
1	C	729	VAL	3.2
1	C	323	THR	3.2
1	A	395	CYS	3.2
1	B	194	HIS	3.1
1	B	201	GLU	3.1
1	C	825	ASN	3.1
1	C	333	ALA	3.1
1	C	412	ALA	3.1
1	C	11	TYR	3.0
1	C	760	GLY	3.0
1	A	874	TYR	3.0
1	B	927	ALA	2.9
1	C	5	MET	2.9
1	C	875	ALA	2.9
1	A	417	GLN	2.9
1	C	193	TRP	2.9
1	B	335	GLN	2.8
1	C	873	LEU	2.8
1	C	36	THR	2.8
1	C	328	VAL	2.8
1	A	333	ALA	2.7
1	C	678	TYR	2.7
1	C	672	GLY	2.7
1	C	338	ALA	2.7
1	A	825	ASN	2.7
1	A	143	ALA	2.6
1	A	873	LEU	2.6
1	B	37	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	426	VAL	2.6
1	C	31	ALA	2.6
1	C	6	LEU	2.6
1	C	236	THR	2.6
1	A	194	HIS	2.5
1	B	928	GLY	2.5
1	C	70	VAL	2.5
1	A	236	THR	2.5
1	C	878	ALA	2.5
1	C	832	GLY	2.5
1	C	34	THR	2.5
1	C	238	THR	2.5
1	C	69	PRO	2.5
1	A	876	ASN	2.5
1	B	79	TYR	2.4
1	C	335	GLN	2.4
1	A	336	LEU	2.4
1	B	728	THR	2.4
1	C	634	TYR	2.4
1	C	325	ASN	2.4
1	B	418	THR	2.4
1	A	136	TYR	2.3
1	C	880	ALA	2.3
1	C	927	ALA	2.3
1	A	6	LEU	2.3
1	C	928	GLY	2.3
1	C	836	VAL	2.3
1	C	632	MET	2.3
1	C	194	HIS	2.3
1	C	22	TYR	2.3
1	C	420	TRP	2.3
1	B	343	GLN	2.3
1	C	706	ASP	2.3
1	C	391	LEU	2.3
1	B	38	PHE	2.2
1	A	238	THR	2.2
1	C	915	VAL	2.2
1	C	74	ASP	2.2
1	C	402	GLY	2.2
1	C	40	LEU	2.2
1	C	76	THR	2.2
1	C	757	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	77	TYR	2.2
1	C	72	ARG	2.2
1	C	67	PHE	2.2
1	C	84	THR	2.2
1	C	341	ASP	2.2
1	C	387	VAL	2.2
1	C	330	ALA	2.2
1	B	53	HIS	2.2
1	C	37	TYR	2.2
1	B	333	ALA	2.1
1	C	75	ASN	2.1
1	C	136	TYR	2.1
1	C	762	TYR	2.1
1	C	437	PRO	2.1
1	B	334	SER	2.1
1	B	673	SER	2.1
1	C	23	LEU	2.1
1	C	671	LEU	2.1
1	C	707	SER	2.1
1	B	825	ASN	2.1
1	C	401	VAL	2.1
1	C	342	LEU	2.1
1	C	877	SER	2.1
1	A	335	GLN	2.1
1	C	914	GLY	2.1
1	C	834	SER	2.1
1	C	27	LEU	2.0
1	B	174	GLN	2.0
1	C	476	THR	2.0
1	C	409	GLY	2.0
1	C	14	ILE	2.0
1	B	324	GLY	2.0
1	B	757	GLY	2.0
1	C	324	GLY	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
3	MPD	B	1722	8/8	0.56	0.20	95,95,95,95	0
3	MPD	A	1717	8/8	0.57	0.24	67,69,70,70	0
3	MPD	B	1703	8/8	0.69	0.20	61,62,63,64	0
3	MPD	A	1720	8/8	0.70	0.17	63,65,66,66	0
2	2HP	B	1612	5/5	0.73	0.14	77,78,79,79	0
2	2HP	B	1621	5/5	0.79	0.12	72,72,73,74	0
3	MPD	B	1723	8/8	0.81	0.20	70,74,75,76	0
3	MPD	C	1701	8/8	0.81	0.18	55,55,57,57	0
3	MPD	A	1716	8/8	0.82	0.16	33,36,41,44	0
3	MPD	A	1704	8/8	0.82	0.15	35,39,41,46	0
3	MPD	B	1711	8/8	0.82	0.17	55,55,56,57	0
3	MPD	C	1712	8/8	0.82	0.15	42,45,46,49	0
3	MPD	C	1714	8/8	0.82	0.16	54,55,56,57	0
3	MPD	B	1721	8/8	0.83	0.18	61,62,63,64	0
2	2HP	A	1619	5/5	0.83	0.12	59,60,60,61	0
3	MPD	C	1713	8/8	0.83	0.16	39,42,44,44	0
3	MPD	B	1718	8/8	0.83	0.16	34,37,44,44	0
2	2HP	B	1608	5/5	0.84	0.14	78,78,79,79	0
3	MPD	B	1708	8/8	0.84	0.17	71,72,72,73	0
3	MPD	B	1709	8/8	0.84	0.15	28,33,39,42	0
3	MPD	A	1705	8/8	0.86	0.14	58,58,58,59	0
2	2HP	C	1611	5/5	0.86	0.21	54,54,55,56	0
2	2HP	C	1617	5/5	0.86	0.23	46,50,52,53	0
2	2HP	A	1620	5/5	0.86	0.12	69,71,71,71	0
3	MPD	A	1702	8/8	0.88	0.13	41,45,46,48	0
2	2HP	B	1605	5/5	0.88	0.15	53,55,56,56	0
3	MPD	A	1706	8/8	0.89	0.15	60,61,62,63	0
2	2HP	C	1618	5/5	0.89	0.12	56,57,58,59	0
2	2HP	C	1604	5/5	0.90	0.17	51,52,53,53	0
2	2HP	B	1616	5/5	0.90	0.11	58,59,61,61	0
3	MPD	B	1710	8/8	0.90	0.12	44,45,47,47	0
2	2HP	A	1610	5/5	0.90	0.13	51,51,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2HP	B	1622	5/5	0.90	0.22	34,37,46,46	0
3	MPD	B	1707	8/8	0.90	0.12	49,52,54,54	0
3	MPD	C	1715	8/8	0.90	0.16	64,66,67,67	0
3	MPD	B	1724	8/8	0.91	0.14	58,60,61,61	0
3	MPD	B	1719	8/8	0.91	0.12	44,47,49,49	0
2	2HP	C	1613	5/5	0.91	0.14	49,51,52,52	0
2	2HP	B	1614	5/5	0.93	0.08	60,60,61,62	0
2	2HP	B	1615	5/5	0.93	0.18	41,41,42,42	0
2	2HP	A	1603	5/5	0.94	0.20	42,43,44,45	0
2	2HP	B	1607	5/5	0.94	0.12	45,45,48,48	0
2	2HP	B	1606	5/5	0.95	0.11	52,52,55,56	0
2	2HP	B	1609	5/5	0.96	0.12	35,35,37,38	0
2	2HP	A	1602	5/5	0.96	0.12	36,39,43,45	0
2	2HP	B	1601	5/5	0.96	0.09	37,38,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.