



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 1HX6 / pdb_00001hx6
Title : P3, THE MAJOR COAT PROTEIN OF THE LIPID-CONTAINING BACTERIOPHAGE PRD1.
Authors : Benson, S.D.; Bamford, J.K.H.; Bamford, D.H.; Burnett, R.M.
Deposited on : 2001-01-11
Resolution : 1.65 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

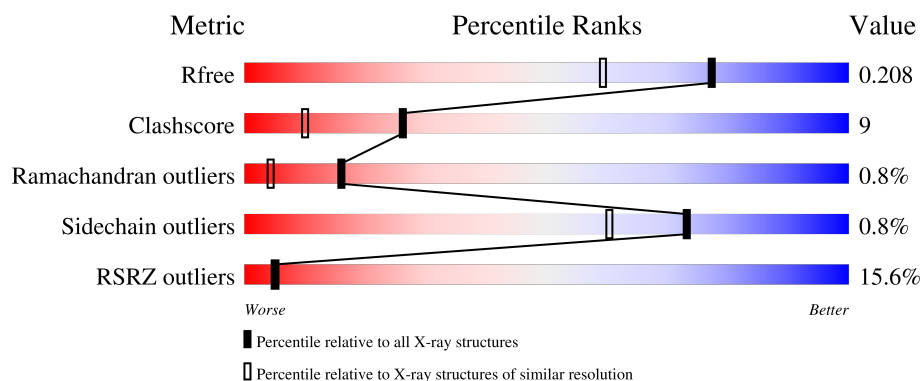
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	394	15% 75% 17% 6%
1	B	394	15% 78% 15% 5%
1	C	394	14% 78% 16% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10026 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 MAJOR CAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	24	0
			3047	1924	520	595	8			
1	B	374	Total	C	N	O	S	0	22	0
			3056	1932	518	598	8			
1	C	371	Total	C	N	O	S	0	15	0
			2988	1892	504	584	8			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	3	Total	Na	0	0
			3	3		
3	C	1	Total	Na	0	0
			1	1		

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



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

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

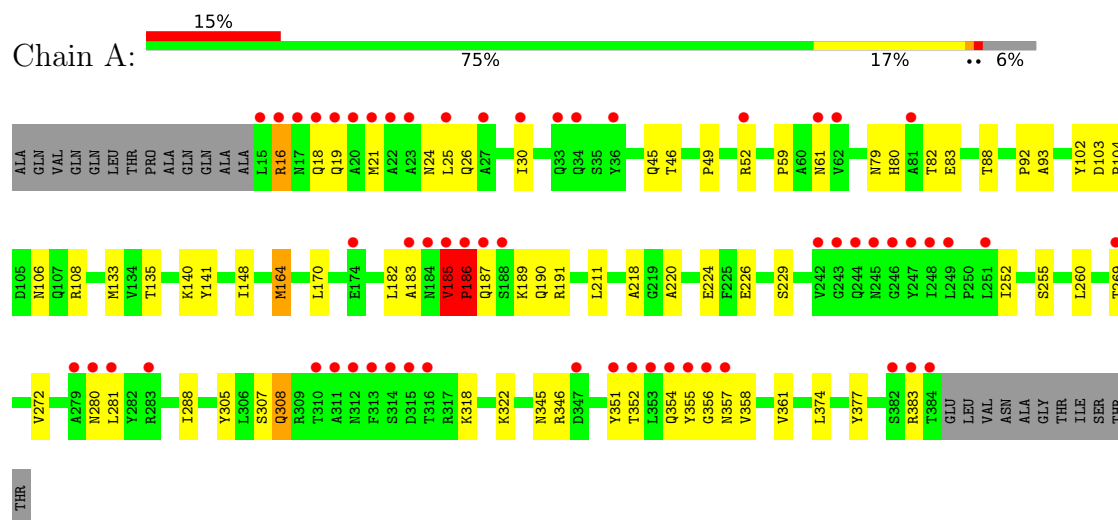
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total	O	0	0
			242	242		
5	B	289	Total	O	0	0
			289	289		
5	C	251	Total	O	0	0
			251	251		

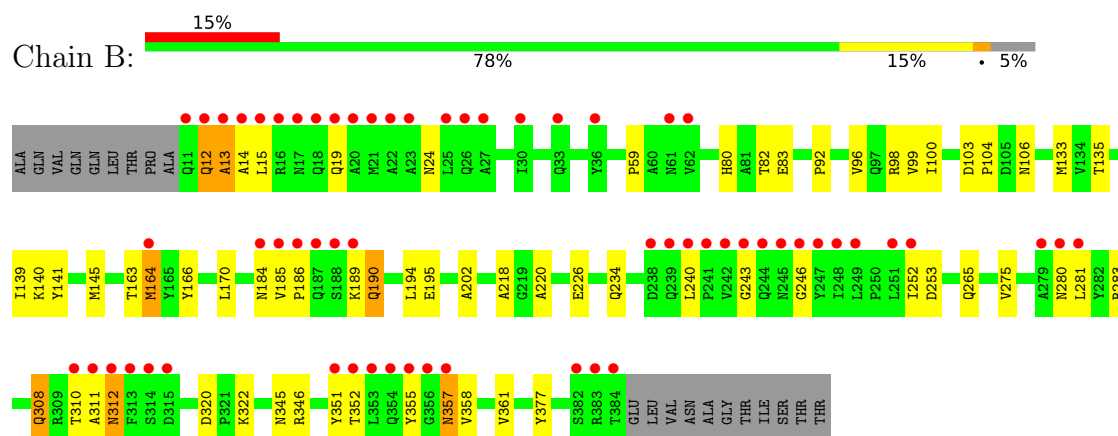
3 Residue-property plots [i](#)

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.

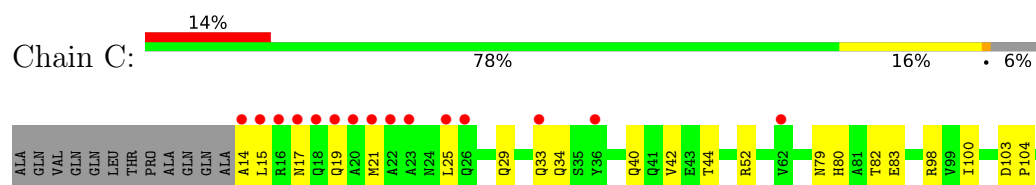
• Molecule 1: MAJOR CAPSID PROTEIN

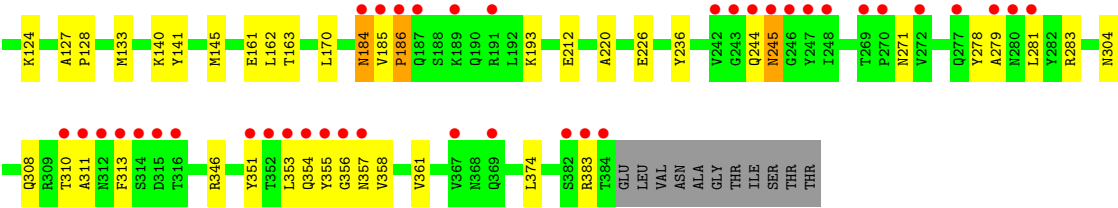


• Molecule 1: MAJOR CAPSID PROTEIN



• Molecule 1: MAJOR CAPSID PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.96Å 121.30Å 126.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.45 – 1.65 53.45 – 1.65	Depositor EDS
% Data completeness (in resolution range)	82.6 (53.45-1.65) 80.8 (53.45-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	4.70	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.52Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.208 0.205 , 0.208	Depositor DCC
R_{free} test set	1617 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10026	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: NA, CL, 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	0.48	1/3113 (0.0%)	0.96	10/4255 (0.2%)
1	B	0.51	1/3121 (0.0%)	0.98	14/4265 (0.3%)
1	C	0.48	0/3053	1.00	14/4173 (0.3%)
All	All	0.49	2/9287 (0.0%)	0.98	38/12693 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	MET	SD-CE	-8.12	1.59	1.79
1	B	164	MET	CB-CG	7.64	1.75	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	MET	CB-CG-SD	-11.70	77.61	112.70
1	A	170	LEU	N-CA-C	-10.73	97.74	112.12
1	C	170	LEU	N-CA-C	-10.31	98.31	112.12
1	B	170	LEU	N-CA-C	-9.35	99.33	112.13
1	B	190	GLN	N-CA-C	-8.35	99.76	110.53
1	C	226	GLU	N-CA-C	-8.09	103.00	113.12
1	A	226	GLU	N-CA-C	-8.07	101.77	111.69
1	C	141	TYR	N-CA-C	-7.92	100.31	110.53
1	A	141	TYR	N-CA-C	-7.18	101.57	110.41
1	B	226	GLU	N-CA-C	-7.17	102.48	112.45
1	C	140	LYS	N-CA-C	7.14	121.77	110.70
1	B	141	TYR	N-CA-C	-7.10	101.37	110.53
1	A	361	VAL	N-CA-C	6.58	117.95	108.48
1	C	361	VAL	N-CA-C	6.48	117.82	108.48
1	C	278	TYR	N-CA-C	-6.45	96.25	108.17
1	C	220	ALA	N-CA-C	6.28	118.65	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	GLN	N-CA-C	6.26	119.39	111.69
1	C	185	VAL	CA-C-N	6.23	127.62	119.84
1	C	185	VAL	C-N-CA	6.23	127.62	119.84
1	B	220	ALA	N-CA-C	6.16	118.79	111.33
1	B	361	VAL	N-CA-C	6.09	117.24	108.48
1	B	140	LYS	N-CA-C	5.87	123.30	110.80
1	C	346	ARG	N-CA-C	5.81	117.29	111.07
1	B	308	GLN	N-CA-C	-5.76	99.03	108.76
1	C	308	GLN	N-CA-C	-5.73	99.56	108.90
1	B	357	ASN	N-CA-C	-5.57	103.18	110.53
1	A	220	ALA	N-CA-C	5.52	118.01	111.33
1	C	42	VAL	CB-CA-C	-5.51	106.01	111.30
1	A	308	GLN	N-CA-C	-5.48	99.49	108.76
1	B	202	ALA	N-CA-C	5.47	119.67	112.89
1	B	275	VAL	N-CA-C	5.33	115.63	108.17
1	A	88	THR	N-CA-C	-5.28	103.06	110.35
1	C	279	ALA	N-CA-C	5.23	118.92	112.54
1	A	140	LYS	N-CA-C	5.21	121.89	110.80
1	A	189	LYS	N-CA-C	5.14	118.09	110.48
1	B	346	ARG	N-CA-C	5.05	116.78	111.28
1	A	148	ILE	N-CA-C	-5.04	100.39	107.75
1	B	320	ASP	N-CA-C	-5.02	102.97	110.20

There are no chirality outliers.

There are no planarity outliers.

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	3047	0	2910	70	0
1	B	3056	0	2923	59	0
1	C	2988	0	2863	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	40	0	70	1	0
4	B	56	0	98	1	0
4	C	48	0	84	1	0
5	A	242	0	0	5	0
5	B	289	0	0	2	0
5	C	251	0	0	8	0
All	All	10026	0	8948	172	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 (172) 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:B:164:MET:CB	1:B:164:MET:CG	1.75	1.58
1:B:164:MET:CB	1:B:164:MET:SD	2.22	1.26
1:B:164:MET:CE	1:B:164:MET:HB3	1.71	1.19
1:B:164:MET:HB3	1:B:164:MET:HE3	1.17	1.10
1:B:92:PRO:O	1:B:164:MET:HE2	1.61	1.00
1:B:164:MET:SD	1:B:164:MET:HB3	1.96	1.00
1:A:93:ALA:HA	1:A:164:MET:HE3	1.54	0.89
1:A:164:MET:HE1	1:B:139:ILE:HD11	1.55	0.87
1:B:164:MET:CB	1:B:164:MET:HE3	2.05	0.86
1:A:93:ALA:CA	1:A:164:MET:HE3	2.10	0.82
1:A:80:HIS:CD2	1:A:83:GLU:H	2.00	0.79
1:A:308:GLN:HE22	1:A:345:ASN:HD21	1.32	0.78
1:B:164:MET:CB	1:B:164:MET:CE	2.50	0.78
1:A:59:PRO:HG2	1:A:190:GLN:HB2	1.70	0.72
1:A:322[B]:LYS:HD3	1:B:163:THR:HG21	1.72	0.72
1:C:80:HIS:CD2	1:C:83:GLU:H	2.08	0.71
1:C:357:ASN:HD22	1:C:358:VAL:H	1.38	0.71
1:B:133[A]:MET:HE2	1:B:135:THR:HG22	1.72	0.71
1:A:322[B]:LYS:CD	1:B:163:THR:HG21	2.20	0.71
1:A:52[A]:ARG:HD2	5:A:1595:HOH:O	1.90	0.70
1:B:80:HIS:CD2	1:B:83:GLU:H	2.08	0.70
1:A:80:HIS:HD2	1:A:83:GLU:H	1.37	0.69
1:A:185:VAL:H	1:A:186:PRO:HD2	1.57	0.68
1:A:133[B]:MET:HE2	1:A:135:THR:HG22	1.75	0.68
1:C:98:ARG:NH2	1:C:111[A]:GLU:OE2	2.26	0.68
1:B:308:GLN:HE22	1:B:345:ASN:HD21	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269[A]:THR:HG23	1:A:272:VAL:HB	1.75	0.67
1:C:80:HIS:HD2	1:C:82:THR:H	1.42	0.67
1:A:80:HIS:HD2	1:A:82:THR:H	1.43	0.67
1:A:280:ASN:HD22	1:A:355[A]:TYR:N	1.93	0.66
1:C:14:ALA:HA	1:C:17:ASN:HD22	1.59	0.66
1:A:185:VAL:HG23	1:A:186:PRO:HD3	1.78	0.66
1:A:280:ASN:O	1:A:281:LEU:HB3	1.96	0.66
1:B:24:ASN:HD21	1:B:253:ASP:H	1.43	0.65
1:B:80:HIS:HD2	1:B:83:GLU:H	1.44	0.65
1:A:308:GLN:HE22	1:A:345:ASN:ND2	1.94	0.65
1:B:184:ASN:O	1:B:186:PRO:HD3	1.97	0.65
1:C:80:HIS:HD2	1:C:83:GLU:H	1.42	0.65
1:C:29:GLN:O	1:C:33:GLN:HG2	1.97	0.64
1:A:93:ALA:N	1:A:164:MET:HE3	2.13	0.63
1:B:80:HIS:HD2	1:B:82:THR:H	1.47	0.63
1:A:185:VAL:O	1:A:187:GLN:N	2.32	0.63
1:A:79[B]:ASN:ND2	1:A:224:GLU:OE2	2.32	0.62
1:B:59:PRO:HG2	1:B:190:GLN:HB2	1.81	0.62
1:A:280:ASN:HA	1:A:352[B]:THR:OG1	1.99	0.62
1:A:92:PRO:C	1:A:164:MET:HE2	2.25	0.62
1:B:98[B]:ARG:HD3	1:B:195:GLU:OE1	1.98	0.62
1:B:357:ASN:HD22	1:B:358:VAL:H	1.48	0.61
1:A:45:GLN:NE2	1:A:52[B]:ARG:HH12	1.99	0.61
1:C:52:ARG:NH2	5:C:1057:HOH:O	2.30	0.59
1:C:281:LEU:HD23	1:C:353:LEU:HD11	1.84	0.59
1:B:96:VAL:HG11	1:B:99[B]:VAL:HG13	1.83	0.59
1:A:92:PRO:C	1:A:164:MET:CE	2.76	0.59
1:C:100:ILE:HG13	1:C:111[A]:GLU:HG3	1.84	0.59
1:A:92:PRO:HB2	1:A:164:MET:HE2	1.85	0.58
1:A:92:PRO:CB	1:A:164:MET:HE2	2.34	0.58
1:C:357:ASN:HD22	1:C:358:VAL:N	2.00	0.57
1:A:80:HIS:CD2	1:A:82:THR:H	2.22	0.57
1:C:108:ARG:HG2	1:C:108:ARG:HH11	1.69	0.57
1:C:40:GLN:NE2	1:C:236:TYR:OH	2.38	0.56
1:C:80:HIS:CD2	1:C:82:THR:H	2.23	0.56
1:B:164:MET:HE1	1:B:166:TYR:CE1	2.41	0.56
1:C:103:ASP:HB2	1:C:104:PRO:CD	2.36	0.55
1:C:184:ASN:O	1:C:186:PRO:HD3	2.05	0.55
1:A:352[B]:THR:C	1:A:354[B]:GLN:H	2.14	0.55
1:A:255[B]:SER:HA	1:A:383:ARG:HD2	1.87	0.55
1:B:80:HIS:CD2	1:B:82:THR:H	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:NE2	1:A:345:ASN:HD21	2.04	0.55
1:B:308:GLN:HE22	1:B:345:ASN:ND2	2.05	0.54
1:C:44[A]:THR:HG22	5:C:1052:HOH:O	2.08	0.54
1:A:93:ALA:N	1:A:164:MET:CE	2.70	0.54
1:B:12:GLN:C	1:B:14:ALA:H	2.14	0.54
1:A:182:LEU:O	1:A:186:PRO:HG2	2.07	0.54
1:C:351:TYR:HD2	1:C:354:GLN:HG3	1.73	0.53
1:A:61:ASN:HB3	1:A:183:ALA:O	2.09	0.53
1:B:357:ASN:ND2	1:B:358:VAL:H	2.07	0.52
1:B:15:LEU:O	1:B:19:GLN:HG3	2.11	0.51
1:B:322[A]:LYS:HE2	1:C:145:MET:O	2.11	0.51
1:A:351:TYR:O	1:A:354[B]:GLN:HB3	2.11	0.51
1:B:283:ARG:HG3	1:B:351:TYR:CD1	2.45	0.51
1:C:311:ALA:C	1:C:313:PHE:H	2.17	0.51
1:A:356[B]:GLY:O	1:A:358[B]:VAL:HG23	2.11	0.50
1:B:189:LYS:HE3	5:B:1418:HOH:O	2.11	0.50
1:A:322[A]:LYS:HE2	1:B:145:MET:O	2.12	0.50
1:B:185:VAL:HG13	1:B:185:VAL:O	2.10	0.50
1:B:280:ASN:HA	1:B:352:THR:OG1	2.11	0.50
1:C:108:ARG:NH1	5:C:1291:HOH:O	2.45	0.49
1:C:310:THR:HG22	1:C:311:ALA:N	2.27	0.49
1:A:185:VAL:N	1:A:186:PRO:HD2	2.27	0.49
1:B:280:ASN:O	1:B:281:LEU:HB2	2.13	0.49
1:A:103:ASP:HB2	1:A:104:PRO:CD	2.42	0.49
1:C:124:LYS:O	4:C:516:MPD:H32	2.13	0.49
1:A:185:VAL:H	1:A:186:PRO:CD	2.25	0.49
1:C:25[A]:LEU:O	1:C:29:GLN:HG3	2.13	0.49
1:A:255[A]:SER:HA	1:A:383:ARG:HD2	1.94	0.49
1:C:184:ASN:HD22	1:C:184:ASN:H	1.60	0.49
1:A:102:TYR:CE2	1:A:108:ARG:HG3	2.47	0.49
1:A:106[B]:ASN:OD1	1:A:191:ARG:NH2	2.46	0.49
1:A:79[A]:ASN:CG	1:A:79[A]:ASN:O	2.55	0.49
1:B:92:PRO:O	1:B:164:MET:CE	2.46	0.48
1:C:100:ILE:HD13	1:C:193[B]:LYS:HD2	1.94	0.48
1:C:212[A]:GLU:OE1	5:C:1294:HOH:O	2.20	0.48
1:A:280:ASN:ND2	1:A:355[A]:TYR:N	2.62	0.48
1:B:59:PRO:CG	1:B:190:GLN:HB2	2.43	0.48
1:C:383:ARG:NH2	5:C:1780:HOH:O	2.47	0.48
1:A:346:ARG:O	4:A:504:MPD:HM1	2.14	0.47
1:B:24:ASN:HD22	1:B:252:ILE:H	1.62	0.47
1:C:271:ASN:HD22	1:C:304:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:MET:O	1:A:25[B]:LEU:HG	2.14	0.47
1:B:377:TYR:CE2	4:B:511:MPD:H32	2.50	0.47
1:C:108:ARG:HG2	1:C:108:ARG:NH1	2.29	0.47
1:B:12:GLN:C	1:B:14:ALA:N	2.72	0.47
1:C:25[B]:LEU:O	1:C:29:GLN:HG3	2.13	0.47
1:B:13:ALA:C	1:B:15:LEU:H	2.22	0.47
1:A:305:TYR:CZ	1:A:318:LYS:HE3	2.50	0.47
1:B:83:GLU:HB3	1:B:218:ALA:HB3	1.96	0.46
5:A:1559:HOH:O	1:C:133[A]:MET:HG3	2.16	0.46
1:B:100[A]:ILE:HD12	1:B:100[A]:ILE:N	2.30	0.46
1:A:104:PRO:CB	1:A:186:PRO:HB3	2.46	0.46
1:C:21:MET:O	1:C:25[B]:LEU:HG	2.16	0.46
1:C:108:ARG:NH1	1:C:111[B]:GLU:HB2	2.30	0.46
1:A:211:LEU:HD21	1:A:374:LEU:HD13	1.98	0.46
1:A:92:PRO:HG2	1:A:164:MET:HE2	1.98	0.45
1:A:92:PRO:HG2	1:A:164:MET:CE	2.47	0.45
1:A:16:ARG:O	1:A:18:GLN:N	2.44	0.45
1:B:99[B]:VAL:HG12	1:B:194:LEU:HD23	1.99	0.45
1:C:79:ASN:HB2	5:C:1260:HOH:O	2.17	0.44
1:C:351:TYR:CD2	1:C:354:GLN:HG3	2.51	0.44
1:B:24:ASN:ND2	1:B:252:ILE:H	2.16	0.44
1:C:161:GLU:C	1:C:162:LEU:HD12	2.43	0.44
1:C:163[B]:THR:HG23	5:C:1108:HOH:O	2.18	0.44
1:C:103:ASP:HB2	1:C:104:PRO:HD2	1.99	0.43
1:A:133[A]:MET:HG3	5:A:1559:HOH:O	2.18	0.43
1:B:103:ASP:HB2	1:B:104:PRO:CD	2.48	0.43
1:B:133[A]:MET:HE2	1:B:135:THR:CG2	2.46	0.43
1:B:240:LEU:HB3	5:B:1460:HOH:O	2.17	0.43
1:C:244:GLN:O	1:C:245:ASN:CB	2.66	0.43
1:A:288:ILE:HG22	5:A:1718:HOH:O	2.17	0.43
1:C:311:ALA:C	1:C:313:PHE:N	2.76	0.43
1:A:352[A]:THR:CG2	1:A:357[A]:ASN:HB3	2.49	0.43
1:B:352:THR:O	1:B:355:TYR:O	2.37	0.43
1:A:307:SER:HB2	1:A:318:LYS:HA	2.00	0.43
1:C:184:ASN:H	1:C:184:ASN:ND2	2.17	0.43
1:A:24:ASN:CG	1:A:252:ILE:HB	2.43	0.42
1:A:83:GLU:HB3	1:A:218:ALA:HB3	2.01	0.42
1:B:12:GLN:O	1:B:14:ALA:N	2.53	0.42
1:B:13:ALA:C	1:B:15:LEU:N	2.76	0.42
1:B:243:GLY:N	1:B:246:GLY:O	2.45	0.42
1:B:308:GLN:NE2	1:B:345:ASN:HD21	2.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HA	1:A:377:TYR:O	2.19	0.42
1:A:19:GLN:H	1:A:19:GLN:HG2	1.68	0.42
1:B:310:THR:HG22	1:B:358:VAL:HG22	2.02	0.42
1:A:356[A]:GLY:C	1:A:358[A]:VAL:H	2.27	0.42
1:A:356[A]:GLY:C	1:A:358[A]:VAL:N	2.78	0.42
1:C:15:LEU:O	1:C:19:GLN:HG3	2.21	0.41
1:B:357:ASN:HD22	1:B:358:VAL:N	2.16	0.41
1:B:98[B]:ARG:HB2	1:B:195:GLU:HB2	2.03	0.41
1:C:108:ARG:HD2	1:C:111[A]:GLU:OE1	2.21	0.41
1:C:184:ASN:HD22	1:C:184:ASN:N	2.17	0.41
1:A:269[A]:THR:CG2	1:A:272:VAL:HB	2.46	0.41
1:A:26[B]:GLN:OE1	1:A:30:ILE:HD11	2.21	0.41
1:A:92:PRO:C	1:A:164:MET:HE3	2.43	0.41
1:C:184:ASN:HD22	1:C:184:ASN:C	2.29	0.41
1:B:59:PRO:HB2	1:B:234:GLN:OE1	2.21	0.41
1:C:127:ALA:O	1:C:128:PRO:C	2.64	0.41
1:B:311:ALA:O	1:B:312:ASN:CB	2.68	0.40
1:C:283:ARG:NH1	5:C:1626:HOH:O	2.35	0.40
1:A:46:THR:HG23	1:A:229[B]:SER:OG	2.21	0.40
1:A:49:PRO:HA	1:A:52[B]:ARG:O	2.22	0.40
1:A:92:PRO:CG	1:A:164:MET:HE2	2.52	0.40
5:A:1559:HOH:O	1:B:133[B]:MET:HG3	2.21	0.40
1:A:102:TYR:HB2	1:A:191:ARG:HB2	2.03	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	392/394 (100%)	365 (93%)	24 (6%)	3 (1%)	16	4
1	B	394/394 (100%)	371 (94%)	20 (5%)	3 (1%)	16	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	384/394 (98%)	367 (96%)	14 (4%)	3 (1%)	16	4
All	All	1170/1182 (99%)	1103 (94%)	58 (5%)	9 (1%)	16	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	PRO
1	B	12	GLN
1	B	312	ASN
1	C	245	ASN
1	A	16	ARG
1	A	185	VAL
1	B	13	ALA
1	C	356	GLY
1	C	186	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/325 (99%)	319 (99%)	2 (1%)	78	68
1	B	321/325 (99%)	318 (99%)	3 (1%)	70	56
1	C	315/325 (97%)	312 (99%)	3 (1%)	68	52
All	All	957/975 (98%)	949 (99%)	8 (1%)	73	60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	VAL
1	A	186	PRO
1	B	106[A]	ASN
1	B	106[B]	ASN
1	B	265	GLN
1	C	184	ASN

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Mol	Chain	Res	Type
1	C	355	TYR
1	C	374	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	29	GLN
1	A	34	GLN
1	A	45	GLN
1	A	61	ASN
1	A	80	HIS
1	A	107	GLN
1	A	184	ASN
1	A	200	ASN
1	A	280	ASN
1	A	308	GLN
1	B	17	ASN
1	B	19	GLN
1	B	24	ASN
1	B	29	GLN
1	B	80	HIS
1	B	190	GLN
1	B	200	ASN
1	B	308	GLN
1	B	354	GLN
1	B	357	ASN
1	C	17	ASN
1	C	40	GLN
1	C	80	HIS
1	C	184	ASN
1	C	271	ASN
1	C	308	GLN
1	C	345	ASN
1	C	354	GLN
1	C	357	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MPD	A	505	-	7,7,7	0.49	0	9,10,10	0.49	0
4	MPD	C	512	-	7,7,7	0.55	0	9,10,10	0.43	0
4	MPD	C	515	-	7,7,7	0.46	0	9,10,10	0.54	0
4	MPD	A	504	-	7,7,7	0.49	0	9,10,10	0.50	0
4	MPD	B	510	-	7,7,7	0.44	0	9,10,10	0.50	0
4	MPD	C	517	-	7,7,7	0.48	0	9,10,10	0.51	0
4	MPD	C	514	-	7,7,7	0.49	0	9,10,10	0.52	0
4	MPD	B	513	-	7,7,7	0.47	0	9,10,10	0.45	0
4	MPD	B	508	-	7,7,7	0.60	0	9,10,10	0.58	0
4	MPD	B	502	-	7,7,7	0.51	0	9,10,10	0.49	0
4	MPD	B	506	-	7,7,7	0.52	0	9,10,10	0.44	0
4	MPD	B	511	-	7,7,7	0.52	0	9,10,10	0.45	0
4	MPD	A	509	-	7,7,7	0.43	0	9,10,10	0.42	0
4	MPD	C	516	-	7,7,7	0.44	0	9,10,10	0.51	0
4	MPD	A	501	-	7,7,7	0.40	0	9,10,10	0.49	0
4	MPD	B	507	-	7,7,7	0.46	0	9,10,10	0.47	0
4	MPD	A	503	-	7,7,7	0.55	0	9,10,10	0.50	0
4	MPD	C	518	-	7,7,7	0.48	0	9,10,10	0.55	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
4	MPD	A	505	-	-	0/5/5/5	-
4	MPD	C	512	-	-	0/5/5/5	-
4	MPD	C	515	-	-	0/5/5/5	-
4	MPD	A	504	-	-	0/5/5/5	-
4	MPD	B	510	-	-	0/5/5/5	-
4	MPD	C	517	-	-	0/5/5/5	-
4	MPD	C	514	-	-	0/5/5/5	-
4	MPD	B	513	-	-	0/5/5/5	-
4	MPD	B	508	-	-	0/5/5/5	-
4	MPD	B	502	-	-	2/5/5/5	-
4	MPD	B	506	-	-	0/5/5/5	-
4	MPD	B	511	-	-	0/5/5/5	-
4	MPD	A	509	-	-	0/5/5/5	-
4	MPD	C	516	-	-	0/5/5/5	-
4	MPD	A	501	-	-	0/5/5/5	-
4	MPD	B	507	-	-	0/5/5/5	-
4	MPD	A	503	-	-	0/5/5/5	-
4	MPD	C	518	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	502	MPD	O2-C2-C3-C4
4	B	502	MPD	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	MPD	1	0
4	B	511	MPD	1	0
4	C	516	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	370/394 (93%)	0.80	58 (15%) 5 5	8, 23, 52, 73	24 (6%)
1	B	374/394 (94%)	0.64	61 (16%) 4 5	7, 20, 56, 73	22 (5%)
1	C	371/394 (94%)	0.68	55 (14%) 5 6	7, 22, 55, 67	15 (4%)
All	All	1115/1182 (94%)	0.70	174 (15%) 5 5	7, 22, 55, 73	61 (5%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	PHE	9.1
1	A	355[A]	TYR	8.6
1	A	185	VAL	8.5
1	A	353[A]	LEU	8.4
1	B	36	TYR	7.8
1	B	355	TYR	7.8
1	A	36	TYR	7.7
1	C	279	ALA	7.7
1	C	313	PHE	7.5
1	B	311	ALA	7.3
1	B	313	PHE	6.7
1	A	312	ASN	6.6
1	B	13	ALA	6.6
1	B	15	LEU	6.5
1	B	312	ASN	6.5
1	C	14	ALA	6.4
1	C	355	TYR	6.4
1	C	353	LEU	6.3
1	A	354[A]	GLN	6.2
1	A	15	LEU	6.1
1	C	384	THR	6.0
1	C	36	TYR	5.9
1	C	312	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	281	LEU	5.9
1	B	186	PRO	5.9
1	B	188	SER	5.7
1	B	14	ALA	5.6
1	A	184	ASN	5.6
1	A	186	PRO	5.6
1	A	384	THR	5.5
1	C	356	GLY	5.4
1	B	185	VAL	5.2
1	A	311	ALA	5.1
1	B	384	THR	5.1
1	C	25[A]	LEU	5.0
1	C	311	ALA	5.0
1	A	25[A]	LEU	5.0
1	B	25[A]	LEU	5.0
1	C	15	LEU	5.0
1	B	357	ASN	5.0
1	A	356[A]	GLY	4.9
1	B	164	MET	4.9
1	C	243	GLY	4.9
1	B	247	TYR	4.7
1	C	244	GLN	4.7
1	C	281	LEU	4.7
1	C	186	PRO	4.6
1	C	17	ASN	4.6
1	B	189	LYS	4.6
1	A	351	TYR	4.5
1	C	357	ASN	4.5
1	B	353	LEU	4.5
1	B	12	GLN	4.5
1	B	187	GLN	4.5
1	B	356	GLY	4.4
1	C	185	VAL	4.4
1	A	20	ALA	4.4
1	B	243	GLY	4.4
1	B	62	VAL	4.4
1	B	248	ILE	4.4
1	C	16	ARG	4.3
1	A	242	VAL	4.2
1	B	242	VAL	4.2
1	A	248	ILE	4.2
1	A	247	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	314	SER	4.0
1	B	314	SER	4.0
1	B	239	GLN	4.0
1	C	62	VAL	4.0
1	B	16	ARG	3.9
1	B	11	GLN	3.9
1	C	280	ASN	3.9
1	A	246	GLY	3.8
1	B	23	ALA	3.8
1	B	18	GLN	3.8
1	B	354	GLN	3.7
1	A	243	GLY	3.7
1	B	244	GLN	3.6
1	A	23	ALA	3.6
1	A	314	SER	3.6
1	B	20	ALA	3.6
1	B	240	LEU	3.5
1	B	351	TYR	3.5
1	A	17	ASN	3.5
1	A	16	ARG	3.5
1	C	352	THR	3.4
1	C	18	GLN	3.4
1	C	21	MET	3.4
1	A	62	VAL	3.4
1	A	187	GLN	3.4
1	A	310	THR	3.4
1	C	354	GLN	3.3
1	B	281	LEU	3.3
1	C	383	ARG	3.3
1	B	22	ALA	3.3
1	B	383	ARG	3.3
1	A	245	ASN	3.3
1	A	382	SER	3.2
1	C	315	ASP	3.2
1	A	357[A]	ASN	3.1
1	A	244	GLN	3.1
1	B	184	ASN	3.1
1	A	52[A]	ARG	3.1
1	B	21	MET	3.1
1	A	18	GLN	3.1
1	B	352	THR	3.1
1	A	183	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	3.0
1	C	107	GLN	2.9
1	B	33	GLN	2.9
1	C	20	ALA	2.9
1	B	245	ASN	2.9
1	A	22	ALA	2.9
1	B	246	GLY	2.9
1	A	19	GLN	2.8
1	C	316	THR	2.8
1	A	188	SER	2.8
1	C	269	THR	2.8
1	A	280	ASN	2.8
1	A	21	MET	2.8
1	C	310	THR	2.8
1	A	81	ALA	2.7
1	B	382	SER	2.7
1	A	315	ASP	2.7
1	C	33	GLN	2.7
1	A	33	GLN	2.6
1	B	280	ASN	2.6
1	B	310	THR	2.6
1	C	248	ILE	2.6
1	B	241	PRO	2.6
1	A	174	GLU	2.6
1	C	242	VAL	2.6
1	B	19	GLN	2.6
1	C	382	SER	2.6
1	B	238[A]	ASP	2.6
1	C	26	GLN	2.5
1	C	277[A]	GLN	2.5
1	C	270	PRO	2.5
1	B	252	ILE	2.5
1	C	245	ASN	2.4
1	A	347	ASP	2.4
1	B	26[A]	GLN	2.4
1	C	187	GLN	2.4
1	A	249	LEU	2.4
1	C	247	TYR	2.4
1	C	272	VAL	2.4
1	A	316	THR	2.3
1	C	23	ALA	2.3
1	C	246	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	251	LEU	2.3
1	B	249	LEU	2.3
1	B	30	ILE	2.3
1	C	191	ARG	2.3
1	A	269[A]	THR	2.2
1	B	17	ASN	2.2
1	C	351	TYR	2.2
1	A	352[A]	THR	2.2
1	A	61	ASN	2.2
1	C	19	GLN	2.2
1	B	27	ALA	2.2
1	C	367	VAL	2.1
1	B	251	LEU	2.1
1	C	189	LYS	2.1
1	A	279	ALA	2.1
1	A	27	ALA	2.1
1	B	315	ASP	2.1
1	A	30	ILE	2.1
1	C	184	ASN	2.0
1	C	369[A]	GLN	2.0
1	B	61	ASN	2.0
1	A	34	GLN	2.0
1	A	283	ARG	2.0
1	A	383	ARG	2.0
1	B	279	ALA	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
4	MPD	A	504	8/8	0.64	0.34	65,65,66,66	0
4	MPD	C	514	8/8	0.67	0.37	60,61,61,61	0
4	MPD	C	515	8/8	0.69	0.29	65,65,66,67	0
4	MPD	C	516	8/8	0.69	0.29	61,61,62,62	0
4	MPD	C	517	8/8	0.71	0.29	66,66,67,67	0
4	MPD	B	513	8/8	0.75	0.25	64,64,65,65	0
4	MPD	B	510	8/8	0.76	0.27	61,62,62,63	0
4	MPD	B	507	8/8	0.76	0.23	63,63,64,64	0
4	MPD	B	502	8/8	0.77	0.20	41,42,45,47	0
4	MPD	A	509	8/8	0.80	0.25	63,64,64,64	0
4	MPD	C	512	8/8	0.80	0.28	63,63,63,64	0
4	MPD	B	506	8/8	0.80	0.25	61,62,63,63	0
4	MPD	A	503	8/8	0.81	0.19	42,43,45,46	0
4	MPD	B	511	8/8	0.81	0.23	49,50,50,50	0
4	MPD	A	505	8/8	0.82	0.23	66,66,67,67	0
4	MPD	B	508	8/8	0.84	0.17	35,37,37,39	0
4	MPD	A	501	8/8	0.85	0.16	30,32,33,33	0
4	MPD	C	518	8/8	0.86	0.18	45,45,47,48	0
3	NA	B	701	1/1	0.92	0.11	32,32,32,32	0
3	NA	B	706	1/1	0.93	0.30	40,40,40,40	0
3	NA	C	707	1/1	0.95	0.12	30,30,30,30	0
2	CL	A	602	1/1	0.96	0.10	30,30,30,30	0
3	NA	A	703	1/1	0.96	0.09	27,27,27,27	0
3	NA	A	704	1/1	0.96	0.12	39,39,39,39	0
3	NA	B	702	1/1	0.97	0.10	28,28,28,28	0
3	NA	A	705	1/1	0.98	0.04	27,27,27,27	0
2	CL	B	601	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.