



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2017 – 08:12 PM EDT

PDB ID : 4DVX
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with MAE-II-188
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : 2012-02-23
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

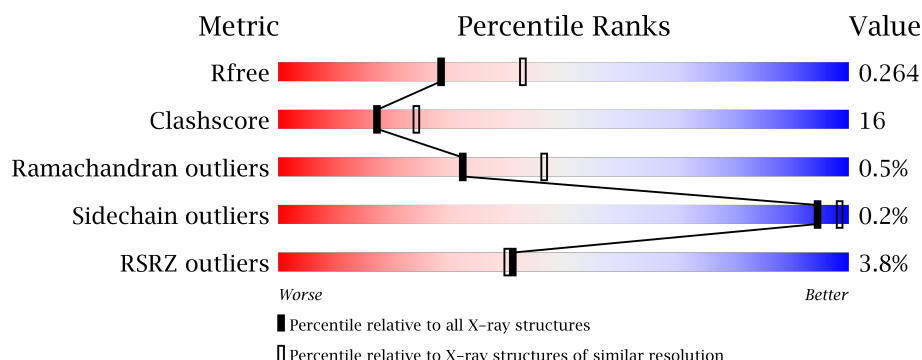
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	353	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 73%, height: 10px; background-color: green;"></div> <div style="width: 23%, height: 10px; background-color: yellow;"></div> <div style="width: 1%, height: 10px; background-color: grey;"></div> </div> </div> <div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 73% 23% . </div> </div> </div>
1	B	353	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 6%, height: 10px; background-color: red;"></div> <div style="width: 64%, height: 10px; background-color: green;"></div> <div style="width: 31%, height: 10px; background-color: yellow;"></div> <div style="width: 1%, height: 10px; background-color: grey;"></div> </div> </div> <div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 64% 31% .. </div> </div> </div>

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	NAG	A	502	-	-	-	X
2	NAG	A	506	-	-	-	X
2	NAG	A	507	-	-	-	X
2	NAG	A	510	-	-	-	X
2	NAG	B	501	-	-	-	X
2	NAG	B	510	-	-	-	X
2	NAG	B	511	-	-	-	X
3	0M5	B	512	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5826 atoms, of which 38 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.

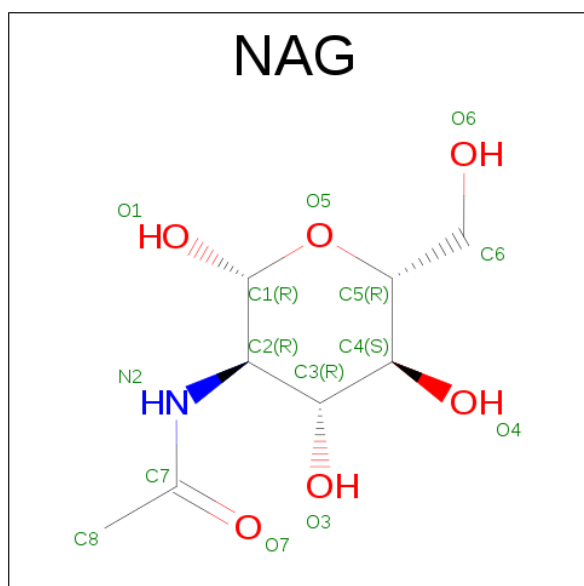
- Molecule 1 is a protein called clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	B	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
B	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



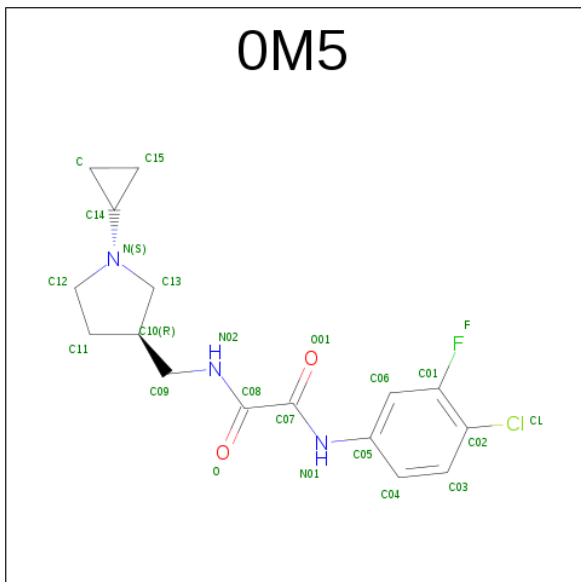
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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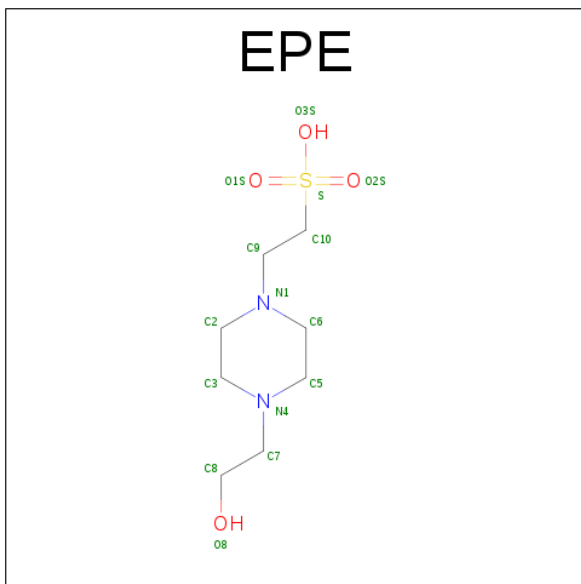
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-(4-chloro-3-fluorophenyl)-N'-{[(3R)-1-cyclopropylpyrrolidin-3-yl]methyl}ethanediamide (three-letter code: 0M5) (formula: $C_{16}H_{19}ClFN_3O_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			42	16	1	1	19	3	2		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			42	16	1	1	19	3	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

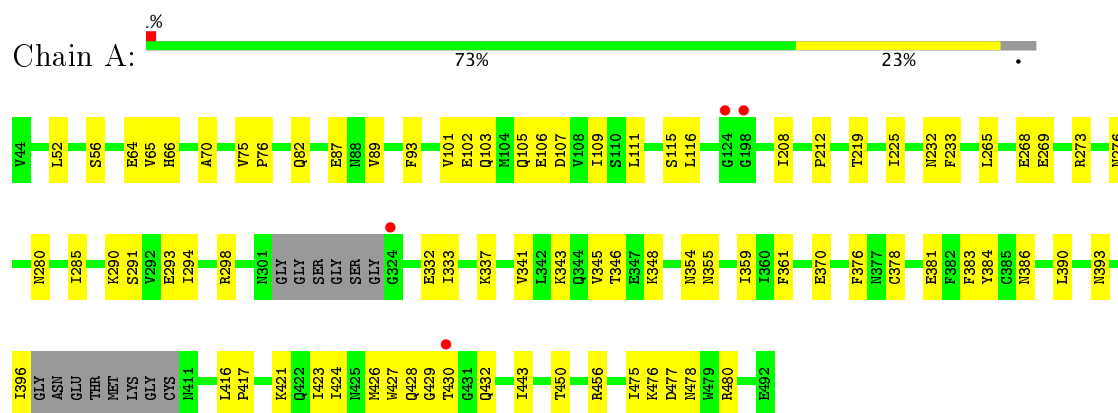
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	33	Total	O	0	0
			33	33		

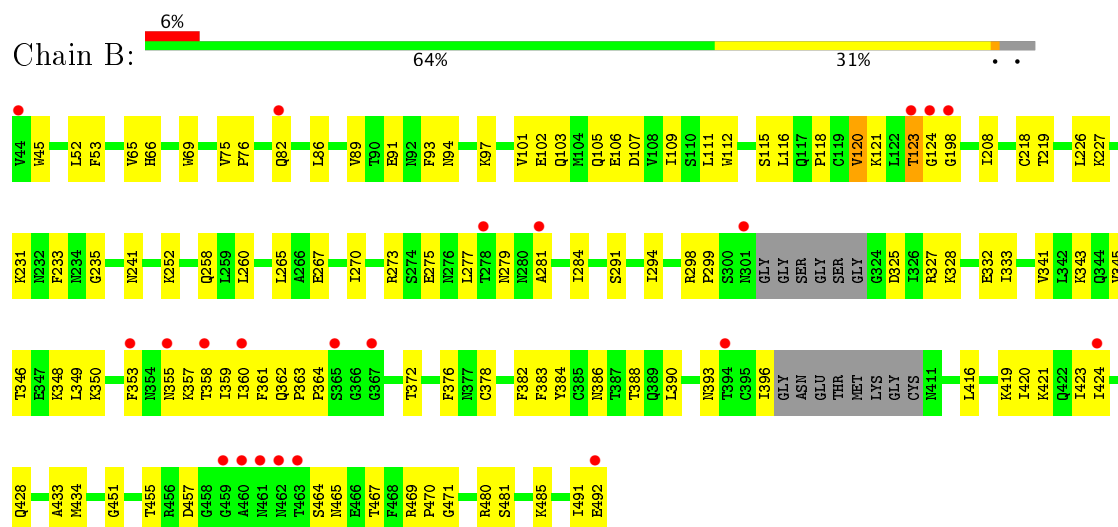
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.61Å 68.30Å 93.96Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	28.46 – 2.40 46.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.5 (28.46-2.40) 78.8 (46.96-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.200 , 0.263 0.210 , 0.264	Depositor DCC
R_{free} test set	1229 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: 0M5, EPE, NAG

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	0.20	0/2709	0.38	0/3678
1	B	0.20	0/2708	0.37	0/3675
All	All	0.20	0/5417	0.38	0/7353

There are no bond length outliers.

There are no bond angle outliers.

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	2654	0	2588	66	0
1	B	2654	0	2588	105	0
2	A	154	0	143	7	0
2	B	154	0	143	3	0
3	A	23	19	19	1	0
3	B	23	19	19	2	0
4	A	15	0	17	2	0
4	B	15	0	17	4	0
5	A	63	0	0	6	0
5	B	33	0	0	7	0
All	All	5788	38	5534	174	0

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

All (174) 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:343:LYS:HE2	1:B:396:ILE:HG22	1.33	1.02
1:B:124:GLY:HA2	1:B:198:GLY:HA3	1.42	1.00
1:A:65:VAL:HG11	1:A:208:ILE:HD12	1.40	0.98
2:A:511:NAG:H83	5:A:662:HOH:O	1.72	0.90
1:B:198:GLY:O	5:B:622:HOH:O	1.94	0.85
1:B:120:VAL:HG13	1:B:434:MET:HB3	1.57	0.84
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.18	0.79
1:A:293:GLU:OE1	5:A:648:HOH:O	2.03	0.77
1:B:97:LYS:NZ	1:B:275:GLU:OE2	2.18	0.77
1:B:485:LYS:NZ	5:B:629:HOH:O	2.06	0.75
1:B:106:GLU:OE1	5:B:620:HOH:O	2.05	0.75
1:B:428:GLN:OE1	1:B:428:GLN:N	2.20	0.75
2:A:508:NAG:H82	1:B:252:LYS:HE3	1.69	0.74
1:B:124:GLY:CA	1:B:198:GLY:HA3	2.18	0.74
1:B:332:GLU:C	1:B:333:ILE:HD12	2.09	0.73
1:A:421:LYS:NZ	1:A:421:LYS:HB3	2.04	0.73
1:B:65:VAL:HG11	1:B:115:SER:HB3	1.72	0.72
1:A:346:THR:HG23	1:A:359:ILE:HB	1.72	0.72
1:B:423:ILE:C	1:B:424:ILE:HD12	2.08	0.72
1:A:480:ARG:NH2	5:A:608:HOH:O	2.22	0.71
1:A:107:ASP:OD2	4:A:513:EPE:H72	1.90	0.70
1:A:82:GLN:OE1	1:A:82:GLN:N	2.21	0.70
1:B:481:SER:N	5:B:631:HOH:O	1.82	0.69
1:A:65:VAL:CG1	1:A:208:ILE:HD12	2.19	0.69
1:A:290:LYS:HE3	1:A:337:LYS:NZ	2.07	0.69
1:A:348:LYS:NZ	5:A:661:HOH:O	2.26	0.69
1:A:343:LYS:HD3	1:A:396:ILE:HG23	1.76	0.68
1:B:390:LEU:HD11	1:B:416:LEU:HD11	1.76	0.68
1:B:294:ILE:HG13	1:B:333:ILE:HD11	1.77	0.66
1:B:121:LYS:NZ	1:B:123:THR:HG22	2.10	0.66
1:B:357:LYS:HE3	1:B:464:SER:HA	1.77	0.66
1:B:103:GLN:HB3	4:B:513:EPE:O8	1.96	0.66
1:B:233:PHE:CE2	1:B:235:GLY:HA2	2.32	0.65
1:A:333:ILE:HD12	1:A:333:ILE:N	2.13	0.64
2:A:508:NAG:C8	1:B:252:LYS:HE3	2.28	0.64
1:B:121:LYS:HZ2	1:B:123:THR:HG22	1.62	0.64
1:B:107:ASP:OD2	4:B:513:EPE:H72	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:ND2	2:A:508:NAG:H83	2.14	0.63
1:A:423:ILE:C	1:A:424:ILE:HD12	2.18	0.63
1:A:111:LEU:HD23	1:A:111:LEU:C	2.20	0.62
1:B:284:ILE:N	1:B:284:ILE:HD12	2.15	0.62
1:B:325:ASP:OD2	1:B:328:LYS:HG3	2.00	0.61
1:B:358:THR:OG1	1:B:464:SER:O	2.15	0.60
1:A:265:LEU:HD11	1:A:291:SER:OG	2.00	0.60
1:B:91:GLU:HG3	1:B:226:LEU:HD13	1.83	0.60
1:A:290:LYS:HE3	1:A:337:LYS:HZ2	1.67	0.60
1:B:376:PHE:HA	3:B:512:OM5:CL	2.39	0.60
1:B:378:CYS:HB3	1:B:383:PHE:CD1	2.38	0.59
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.84	0.59
1:B:82:GLN:H	1:B:82:GLN:CD	2.06	0.58
1:B:124:GLY:HA2	1:B:198:GLY:CA	2.24	0.58
1:A:421:LYS:NZ	1:A:423:ILE:O	2.36	0.58
1:A:424:ILE:HD12	1:A:424:ILE:N	2.18	0.58
1:B:93:PHE:HB2	1:B:233:PHE:HZ	1.69	0.58
1:B:343:LYS:HE2	1:B:396:ILE:CG2	2.22	0.57
1:A:103:GLN:HB3	4:A:513:EPE:O8	2.04	0.57
1:B:103:GLN:OE1	4:B:513:EPE:O8	2.17	0.57
1:B:52:LEU:CD2	1:B:219:THR:HG22	2.35	0.57
1:B:260:LEU:HD12	1:B:451:GLY:HA3	1.86	0.57
1:B:45:TRP:NE1	1:B:91:GLU:OE2	2.38	0.57
1:B:65:VAL:CG1	1:B:115:SER:HB3	2.35	0.57
1:B:358:THR:OG1	1:B:465:ASN:ND2	2.38	0.57
1:B:116:LEU:HD21	1:B:208:ILE:HD11	1.87	0.57
1:B:491:ILE:HG22	1:B:492:GLU:N	2.20	0.56
1:A:354:ASN:OD1	2:A:508:NAG:H81	2.05	0.56
1:B:333:ILE:HD12	1:B:333:ILE:N	2.19	0.56
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.39	0.56
1:A:232:ASN:ND2	1:A:268:GLU:OE1	2.38	0.56
1:B:105:GLN:O	1:B:109:ILE:HG13	2.06	0.55
1:A:332:GLU:C	1:A:333:ILE:HD12	2.27	0.55
1:A:429:GLY:O	5:A:627:HOH:O	2.18	0.55
1:B:384:TYR:CE1	1:B:421:LYS:HB2	2.41	0.55
1:B:265:LEU:HD11	1:B:291:SER:OG	2.08	0.54
1:B:390:LEU:CD1	1:B:416:LEU:HD11	2.38	0.53
1:B:116:LEU:CD2	1:B:208:ILE:HD11	2.39	0.53
1:B:325:ASP:HB3	1:B:328:LYS:HG3	1.91	0.53
1:B:457:ASP:OD2	1:B:467:THR:OG1	2.24	0.53
1:A:426:MET:SD	1:A:430:THR:OG1	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:O	1:A:106:GLU:HG3	2.09	0.53
1:B:424:ILE:N	1:B:424:ILE:HD12	2.23	0.52
1:A:475:ILE:O	1:A:478:ASN:HB2	2.09	0.52
1:B:343:LYS:CE	1:B:396:ILE:HG22	2.24	0.52
1:B:231:LYS:NZ	1:B:267:GLU:OE1	2.42	0.51
1:B:386:ASN:OD1	1:B:388:THR:HG23	2.10	0.51
1:B:65:VAL:HG11	1:B:208:ILE:HD12	1.93	0.51
1:B:69:TRP:CB	1:B:111:LEU:HD13	2.41	0.51
1:A:421:LYS:HZ2	1:A:421:LYS:HB3	1.75	0.51
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.93	0.51
1:B:341:VAL:O	1:B:345:VAL:HG23	2.11	0.51
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.46	0.51
1:A:111:LEU:HD23	1:A:111:LEU:O	2.11	0.50
1:B:481:SER:OG	5:B:631:HOH:O	2.19	0.50
1:A:428:GLN:OE1	1:A:428:GLN:N	2.39	0.50
1:B:112:TRP:CE3	1:B:116:LEU:HD12	2.47	0.50
1:B:346:THR:HG22	1:B:350:LYS:HE2	1.93	0.49
1:B:198:GLY:N	5:B:622:HOH:O	2.44	0.49
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.12	0.49
1:A:116:LEU:HD12	1:A:116:LEU:N	2.27	0.49
1:A:269:GLU:HG2	2:A:505:NAG:H61	1.94	0.49
1:A:105:GLN:O	1:A:109:ILE:HG13	2.12	0.49
1:A:273:ARG:HB2	1:A:285:ILE:HB	1.95	0.49
1:A:386:ASN:HB3	1:A:417:PRO:HG2	1.94	0.48
1:B:294:ILE:O	1:B:294:ILE:HG23	2.13	0.48
1:B:118:PRO:HG3	1:B:433:ALA:HB1	1.95	0.48
1:B:86:LEU:HB3	1:B:89:VAL:HG21	1.94	0.48
1:B:102:GLU:O	1:B:106:GLU:HG3	2.13	0.48
1:A:421:LYS:HZ3	1:A:421:LYS:HB3	1.76	0.48
1:A:87:GLU:O	1:A:89:VAL:HG23	2.14	0.48
1:B:376:PHE:CA	3:B:512:OM5:CL	2.99	0.48
1:A:376:PHE:HA	3:A:512:OM5:CL	2.51	0.48
1:B:233:PHE:O	1:B:273:ARG:NH1	2.40	0.47
1:A:291:SER:O	1:A:337:LYS:HE3	2.14	0.47
1:B:481:SER:CB	5:B:631:HOH:O	2.62	0.47
2:A:508:NAG:C8	1:B:252:LYS:CE	2.92	0.47
1:A:56:SER:OG	1:A:70:ALA:HB1	2.15	0.46
1:B:357:LYS:CE	1:B:464:SER:HA	2.44	0.46
1:A:52:LEU:CD2	1:A:219:THR:HG22	2.46	0.46
1:B:53:PHE:CZ	1:B:218:CYS:HB2	2.52	0.45
1:B:241:ASN:HD22	2:B:502:NAG:H83	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:H	1:B:393:ASN:HD21	1.64	0.45
1:A:65:VAL:HB	1:A:115:SER:OG	2.18	0.44
1:B:362:GLN:HB3	1:B:363:PRO:HD2	1.99	0.44
1:B:327:ARG:O	1:B:419:LYS:HA	2.18	0.44
1:B:382:PHE:O	1:B:420:ILE:HA	2.17	0.44
1:B:258:GLN:HG2	1:B:470:PRO:HB2	1.99	0.44
1:A:294:ILE:O	1:A:294:ILE:HG23	2.17	0.44
1:A:370:GLU:OE1	1:A:370:GLU:N	2.39	0.44
1:A:476:LYS:O	1:A:480:ARG:HG3	2.18	0.44
1:B:364:PRO:HG2	1:B:372:THR:HA	2.00	0.43
1:B:227:LYS:HE3	1:B:485:LYS:HE3	1.99	0.43
1:A:384:TYR:OH	1:A:424:ILE:HG23	2.17	0.43
1:A:432:GLN:N	1:A:432:GLN:OE1	2.51	0.43
1:B:345:VAL:O	1:B:349:LEU:HG	2.18	0.43
1:B:362:GLN:O	1:B:469:ARG:HG2	2.18	0.43
1:B:270:ILE:O	1:B:348:LYS:HE2	2.18	0.43
4:B:513:EPE:H51	4:B:513:EPE:H82	1.88	0.43
1:B:360:ILE:HB	1:B:467:THR:HG22	2.00	0.43
1:A:341:VAL:O	1:A:345:VAL:HG23	2.19	0.42
1:B:65:VAL:HG23	1:B:66:HIS:N	2.33	0.42
1:A:348:LYS:HD3	5:A:634:HOH:O	2.19	0.42
1:B:457:ASP:OD1	1:B:469:ARG:NH1	2.53	0.42
1:A:265:LEU:HD21	1:A:450:THR:HG22	2.01	0.42
1:B:102:GLU:O	1:B:105:GLN:HB3	2.20	0.42
1:B:360:ILE:HG23	1:B:393:ASN:ND2	2.34	0.42
1:B:363:PRO:O	1:B:469:ARG:HD2	2.18	0.42
1:B:284:ILE:CD1	1:B:284:ILE:N	2.82	0.42
1:B:346:THR:HG23	1:B:359:ILE:HB	2.01	0.42
1:B:455:THR:HG23	1:B:471:GLY:HA3	2.02	0.42
1:B:325:ASP:HB3	1:B:328:LYS:CG	2.49	0.42
1:B:491:ILE:HG22	1:B:492:GLU:H	1.84	0.42
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.85	0.42
1:B:279:ASN:C	1:B:281:ALA:H	2.23	0.42
1:A:75:VAL:HB	1:A:76:PRO:HD2	2.02	0.42
1:B:94:ASN:ND2	1:B:97:LYS:HD3	2.34	0.42
1:A:219:THR:HG23	1:A:225:ILE:CG1	2.50	0.42
1:A:427:TRP:CE3	1:A:475:ILE:HG13	2.56	0.41
1:B:353:PHE:O	1:B:357:LYS:HB2	2.20	0.41
1:A:361:PHE:O	1:A:393:ASN:ND2	2.44	0.41
1:B:75:VAL:HB	1:B:76:PRO:HD2	2.03	0.41
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:NAG:H83	2:B:510:NAG:H2	1.91	0.41
1:A:65:VAL:HG11	1:A:115:SER:HB3	2.02	0.41
1:A:65:VAL:HG23	1:A:66:HIS:N	2.36	0.41
1:A:298:ARG:HD2	1:A:298:ARG:C	2.41	0.41
1:B:69:TRP:HB2	1:B:111:LEU:HD13	2.03	0.41
1:B:361:PHE:H	1:B:393:ASN:ND2	2.19	0.41
1:B:94:ASN:HD21	1:B:97:LYS:HD3	1.86	0.40
1:B:298:ARG:HA	1:B:299:PRO:HD2	1.94	0.40
1:B:93:PHE:HB2	1:B:233:PHE:CZ	2.53	0.40
1:A:390:LEU:HD11	1:A:416:LEU:HD11	2.02	0.40
1:A:381:GLU:HG3	1:A:443:ILE:HD13	2.04	0.40
1:A:280:ASN:HB2	1:A:456:ARG:O	2.21	0.40
1:B:277:LEU:HG	2:B:501:NAG:H83	2.02	0.40
1:B:393:ASN:HA	1:B:396:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/353 (94%)	322 (97%)	10 (3%)	1 (0%)	44	60
1	B	331/353 (94%)	313 (95%)	16 (5%)	2 (1%)	28	41
All	All	664/706 (94%)	635 (96%)	26 (4%)	3 (0%)	32	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	B	355	ASN
1	B	123	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	303/311 (97%)	303 (100%)	0	100	100
1	B	303/311 (97%)	302 (100%)	1 (0%)	94	98
All	All	606/622 (97%)	605 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	120	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS
1	A	444	ASN
1	B	422	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 carbohydrates in this entry.

5.6 Ligand geometry

26 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	NAG	A	501	1	14,14,15	0.53	0	15,19,21	0.62	0
2	NAG	A	502	1	14,14,15	0.52	0	15,19,21	0.57	0
2	NAG	A	503	1	14,14,15	0.51	0	15,19,21	0.54	0
2	NAG	A	504	1	14,14,15	0.53	0	15,19,21	0.58	0
2	NAG	A	505	1	14,14,15	0.52	0	15,19,21	0.59	0
2	NAG	A	506	1	14,14,15	0.30	0	15,19,21	0.83	0
2	NAG	A	507	1	14,14,15	0.54	0	15,19,21	0.57	0
2	NAG	A	508	1	14,14,15	0.55	0	15,19,21	0.50	0
2	NAG	A	509	1	14,14,15	0.54	0	15,19,21	0.55	0
2	NAG	A	510	1	14,14,15	0.52	0	15,19,21	0.59	0
2	NAG	A	511	1	14,14,15	0.26	0	15,19,21	0.75	1 (6%)
3	0M5	A	512	-	25,25,25	2.32	11 (44%)	29,35,35	3.53	10 (34%)
4	EPE	A	513	-	15,15,15	0.78	1 (6%)	18,20,20	1.99	7 (38%)
2	NAG	B	501	1	14,14,15	0.31	0	15,19,21	0.71	1 (6%)
2	NAG	B	502	1	14,14,15	0.53	0	15,19,21	0.67	0
2	NAG	B	503	1	14,14,15	0.49	0	15,19,21	0.72	0
2	NAG	B	504	1	14,14,15	0.36	0	15,19,21	0.73	0
2	NAG	B	505	1	14,14,15	0.53	0	15,19,21	0.58	0
2	NAG	B	506	1	14,14,15	0.56	0	15,19,21	0.57	0
2	NAG	B	507	1	14,14,15	0.53	0	15,19,21	0.56	0
2	NAG	B	508	1	14,14,15	0.53	0	15,19,21	0.55	0
2	NAG	B	509	1	14,14,15	0.52	0	15,19,21	0.55	0
2	NAG	B	510	1	14,14,15	0.51	0	15,19,21	0.60	0
2	NAG	B	511	1	14,14,15	0.51	0	15,19,21	0.65	0
3	0M5	B	512	-	25,25,25	2.32	11 (44%)	29,35,35	3.52	10 (34%)
4	EPE	B	513	-	15,15,15	0.81	1 (6%)	18,20,20	2.06	6 (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
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	0/6/23/26	0/1/1/1
2	NAG	A	510	1	-	0/6/23/26	0/1/1/1
2	NAG	A	511	1	-	0/6/23/26	0/1/1/1
3	0M5	A	512	-	-	0/13/28/28	0/2/3/3
4	EPE	A	513	-	-	0/9/19/19	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1	-	0/6/23/26	0/1/1/1
2	NAG	B	510	1	-	0/6/23/26	0/1/1/1
2	NAG	B	511	1	-	0/6/23/26	0/1/1/1
3	0M5	B	512	-	-	0/13/28/28	0/2/3/3
4	EPE	B	513	-	-	0/9/19/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	512	0M5	C04-C05	2.36	1.43	1.39
3	A	512	0M5	C04-C05	2.38	1.43	1.39
3	B	512	0M5	C11-C12	2.38	1.57	1.52
3	A	512	0M5	C11-C12	2.41	1.57	1.52
3	A	512	0M5	C03-C04	2.56	1.43	1.38
3	B	512	0M5	C06-C01	2.58	1.42	1.37
3	B	512	0M5	C03-C04	2.60	1.43	1.38
3	A	512	0M5	C06-C01	2.60	1.42	1.37
4	A	513	EPE	C10-S	2.62	1.81	1.77
4	B	513	EPE	C10-S	2.64	1.81	1.77
3	B	512	0M5	C09-C10	2.64	1.56	1.51
3	A	512	0M5	C09-C10	2.68	1.56	1.51
3	B	512	0M5	C-C14	3.02	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	512	0M5	C-C14	3.03	1.55	1.49
3	B	512	0M5	C15-C14	3.10	1.55	1.49
3	A	512	0M5	C15-C14	3.13	1.55	1.49
3	B	512	0M5	C07-N01	3.73	1.44	1.35
3	A	512	0M5	C07-N01	3.77	1.44	1.35
3	A	512	0M5	C05-N01	3.77	1.49	1.41
3	B	512	0M5	C05-N01	3.80	1.49	1.41
3	B	512	0M5	C08-N02	4.18	1.41	1.33
3	A	512	0M5	C08-N02	4.20	1.41	1.33
3	A	512	0M5	C07-C08	4.74	1.60	1.53
3	B	512	0M5	C07-C08	4.78	1.60	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	512	0M5	O01-C07-C08	-5.99	114.08	121.31
3	A	512	0M5	O01-C07-C08	-5.98	114.09	121.31
3	B	512	0M5	O-C08-C07	-4.11	116.35	121.31
3	A	512	0M5	O-C08-C07	-4.09	116.38	121.31
3	A	512	0M5	C04-C05-C06	-3.36	115.72	119.66
3	B	512	0M5	C04-C05-C06	-3.33	115.75	119.66
2	B	501	NAG	O5-C1-C2	-2.49	108.01	111.47
2	A	511	NAG	O5-C1-C2	-2.18	108.45	111.47
4	A	513	EPE	C5-C6-N1	-2.02	106.55	110.63
4	A	513	EPE	C7-N4-C5	2.14	116.73	111.26
4	A	513	EPE	C7-N4-C3	2.39	117.38	111.26
4	A	513	EPE	O3S-S-C10	2.82	109.53	106.06
4	B	513	EPE	O2S-S-C10	2.85	109.24	106.79
4	B	513	EPE	O3S-S-C10	2.92	109.65	106.06
4	A	513	EPE	O2S-S-C10	2.95	109.33	106.79
3	A	512	0M5	F-C01-C02	2.98	122.06	119.04
3	B	512	0M5	F-C01-C02	3.01	122.09	119.04
3	B	512	0M5	C01-C02-CL	3.10	122.67	120.02
4	B	513	EPE	O1S-S-C10	3.10	109.46	106.79
3	A	512	0M5	C01-C02-CL	3.12	122.69	120.02
4	A	513	EPE	O1S-S-C10	3.17	109.51	106.79
4	B	513	EPE	C7-N4-C5	3.33	119.80	111.26
4	B	513	EPE	C7-N4-C3	3.59	120.45	111.26
4	B	513	EPE	C5-N4-C3	4.41	118.87	108.87
4	A	513	EPE	C5-N4-C3	4.73	119.58	108.87
3	A	512	0M5	C13-N-C14	4.93	120.71	113.95
3	B	512	0M5	C13-N-C14	4.95	120.73	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	512	0M5	C05-C06-C01	5.90	122.98	118.80
3	A	512	0M5	C05-C06-C01	5.96	123.02	118.80
3	B	512	0M5	C07-C08-N02	7.53	122.61	113.51
3	A	512	0M5	C07-C08-N02	7.54	122.62	113.51
3	A	512	0M5	C12-N-C14	8.08	121.27	113.99
3	B	512	0M5	C12-N-C14	8.09	121.28	113.99
3	A	512	0M5	C08-C07-N01	8.84	125.48	112.20
3	B	512	0M5	C08-C07-N01	8.85	125.50	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	NAG	1	0
2	A	508	NAG	5	0
2	A	511	NAG	1	0
3	A	512	0M5	1	0
4	A	513	EPE	2	0
2	B	501	NAG	1	0
2	B	502	NAG	1	0
2	B	510	NAG	1	0
3	B	512	0M5	2	0
4	B	513	EPE	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	124:GLY	C	198:GLY	N	4.32

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	339/353 (96%)	-0.03	4 (1%) 79 77	47, 65, 109, 133	0
1	B	339/353 (96%)	0.33	22 (6%) 20 18	51, 80, 131, 166	0
All	All	678/706 (96%)	0.15	26 (3%) 41 40	47, 71, 122, 166	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	GLY	7.2
1	B	394	THR	5.5
1	B	492	GLU	4.7
1	B	44	VAL	4.6
1	A	198	GLY	4.5
1	B	123	THR	3.7
1	A	430	THR	3.6
1	B	462	ASN	3.3
1	A	324	GLY	3.3
1	B	301	ASN	3.2
1	B	461	ASN	3.0
1	B	353	PHE	3.0
1	B	459	GLY	2.8
1	B	198	GLY	2.8
1	B	82	GLN	2.8
1	B	281	ALA	2.7
1	B	365	SER	2.6
1	A	124	GLY	2.6
1	B	460	ALA	2.4
1	B	367	GLY	2.3
1	B	278	THR	2.3
1	B	360	ILE	2.3
1	B	355	ASN	2.2
1	B	358	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	424	ILE	2.2
1	B	463	THR	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	510	14/15	0.67	0.54	13.12	119,147,162,167	0
2	NAG	B	511	14/15	0.76	0.30	10.21	92,103,113,114	0
2	NAG	A	506	14/15	0.79	0.48	7.96	37,49,60,63	0
2	NAG	A	502	14/15	0.77	0.54	7.28	121,139,158,160	0
2	NAG	A	507	14/15	0.69	0.30	5.36	78,107,127,136	0
2	NAG	B	501	14/15	0.86	0.38	4.19	34,43,46,46	0
3	0M5	B	512	23/23	0.82	0.30	3.72	48,74,127,129	0
2	NAG	B	510	14/15	0.56	0.62	3.41	153,163,175,178	0
4	EPE	A	513	15/15	0.94	0.22	1.95	59,68,75,77	0
2	NAG	B	506	14/15	0.90	0.17	0.60	66,89,108,117	0
4	EPE	B	513	15/15	0.96	0.18	0.39	58,70,83,83	0
3	0M5	A	512	23/23	0.95	0.18	0.28	48,74,127,129	0
2	NAG	A	508	14/15	0.95	0.16	0.01	54,60,72,86	0
2	NAG	B	505	14/15	0.85	0.17	-0.05	92,103,109,113	0
2	NAG	A	505	14/15	0.92	0.15	-0.23	74,78,90,90	0
2	NAG	A	501	14/15	0.93	0.14	-0.52	76,83,95,99	0
2	NAG	B	503	14/15	0.94	0.16	-0.74	45,56,63,64	0
2	NAG	B	509	14/15	0.90	0.15	-0.92	63,85,91,92	0
2	NAG	A	503	14/15	0.97	0.10	-1.99	48,60,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	504	14/15	0.85	0.43	-	24,33,39,42	0
2	NAG	B	502	14/15	0.78	0.24	-	112,135,140,143	0
2	NAG	A	509	14/15	0.91	0.14	-	76,87,96,100	0
2	NAG	A	511	14/15	0.81	0.43	-	45,55,60,64	0
2	NAG	B	508	14/15	0.40	0.81	-	137,152,162,166	0
2	NAG	B	507	14/15	0.79	0.29	-	83,110,127,129	0
2	NAG	A	504	14/15	0.93	0.15	-	65,75,83,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.