



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 04:32 PM EDT

PDB ID : 1MU2
Title : CRYSTAL STRUCTURE OF HIV-2 REVERSE TRANSCRIPTASE
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Stammers, D.K.
Deposited on : 2002-09-23
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

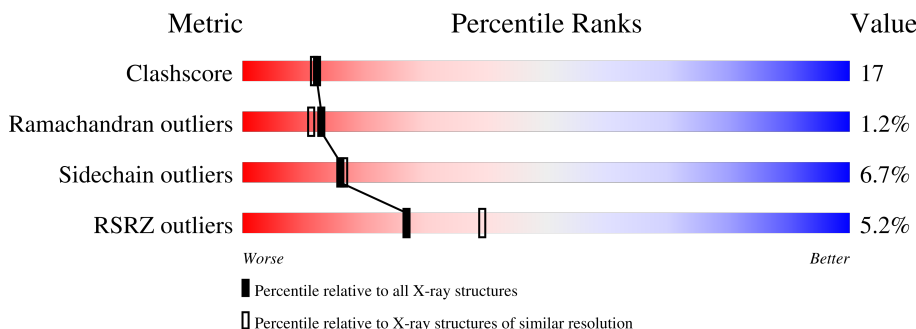
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	555	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
2	B	426	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>28%</div> <div>• 6%</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
3	SO4	A	1321	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8168 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 HIV-2 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4394	2832	742	807	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	SER	ARG	engineered mutation	UNP P04584
A	334	ASP	GLU	SEE REMARK 999	UNP P04584
A	505	VAL	SER	SEE REMARK 999	UNP P04584

- Molecule 2 is a protein called HIV-2 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3348	2171	569	599	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	284	SER	ARG	engineered mutation	UNP P04584
B	334	ASP	GLU	SEE REMARK 999	UNP P04584

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

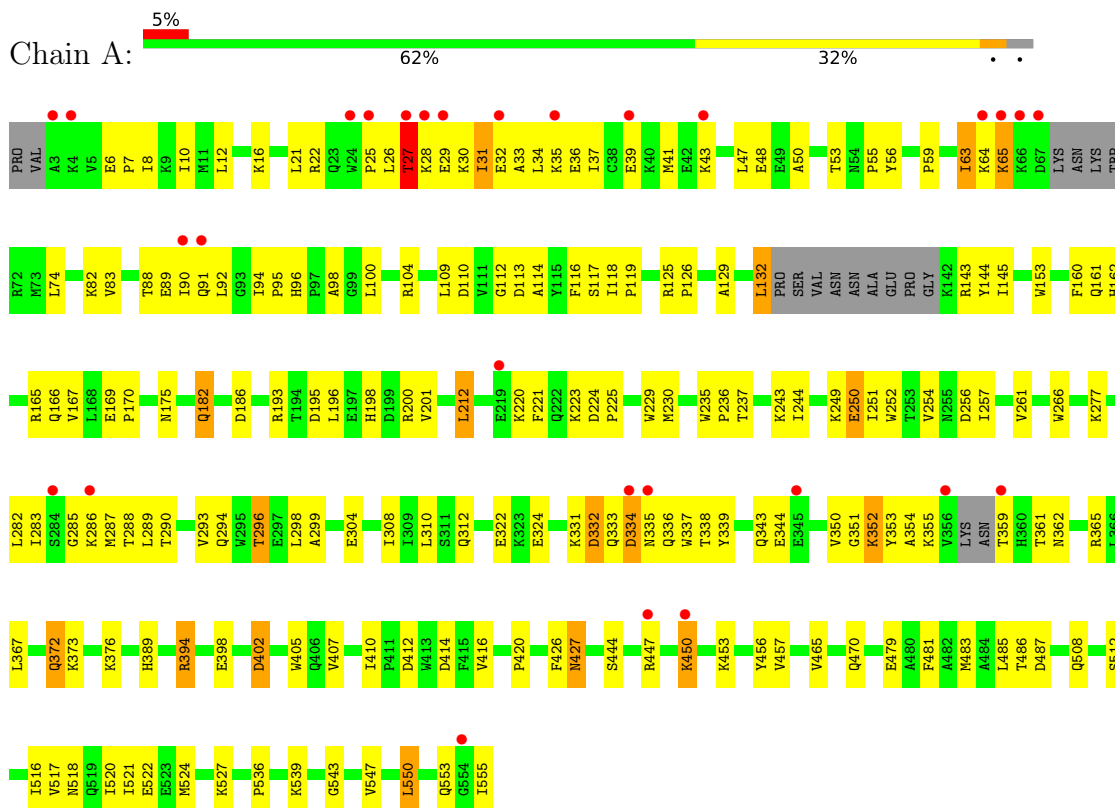
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	144	Total	O	0	0
			144	144		

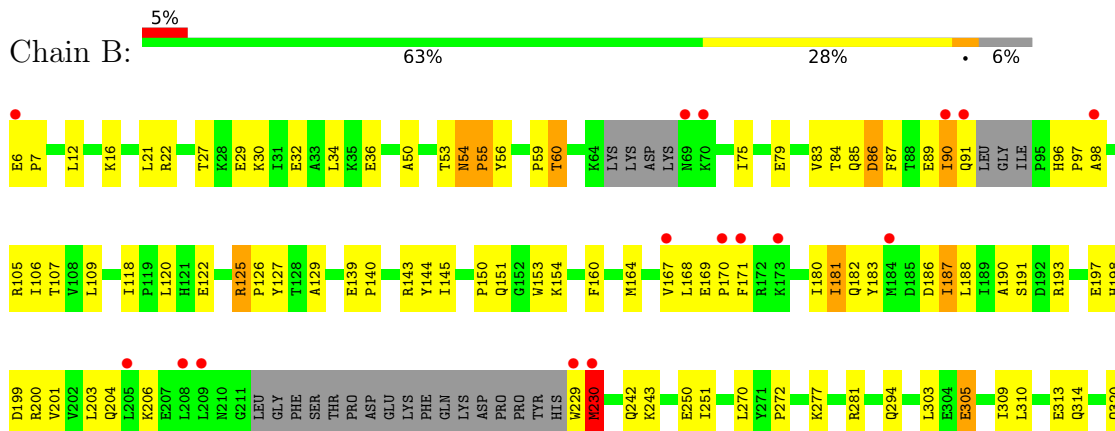
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: HIV-2 RT



- Molecule 2: HIV-2 RT





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.77Å 107.81Å 82.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.35 29.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-2.35) 100.0 (29.95-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.240 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8168	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.41	0/4500	0.66	1/6095 (0.0%)
2	B	0.43	0/3436	0.66	0/4659
All	All	0.42	0/7936	0.66	1/10754 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	MET	N-CA-C	-5.29	96.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4394	0	4424	173	0
2	B	3348	0	3374	107	0
3	A	75	0	0	5	0
3	B	35	0	0	2	0
4	A	6	0	8	0	0
4	B	24	0	32	1	0
5	A	142	0	0	5	0
5	B	144	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8168	0	7838	267	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 17.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:CG	2:B:87:PHE:H	1.49	1.12
1:A:333:GLN:HG2	1:A:336:GLN:HE21	1.21	1.04
1:A:372:GLN:HE22	2:B:400:TRP:HE1	1.08	1.00
1:A:336:GLN:HG3	1:A:352:LYS:HE3	1.47	0.95
1:A:91:GLN:HB3	1:A:161:GLN:NE2	1.80	0.94
1:A:333:GLN:HG3	1:A:334:ASP:H	1.33	0.93
2:B:60:THR:HG23	2:B:75:ILE:HG12	1.53	0.90
1:A:426:PHE:HB2	1:A:508:GLN:NE2	1.87	0.90
1:A:288:THR:HG22	1:A:290:THR:H	1.38	0.88
2:B:86:ASP:CG	2:B:87:PHE:N	2.24	0.88
1:A:91:GLN:HB3	1:A:161:GLN:HE22	1.36	0.87
2:B:90:ILE:HG13	2:B:91:GLN:HG3	1.58	0.85
1:A:465:VAL:HG21	1:A:550:LEU:HD22	1.58	0.85
1:A:333:GLN:HG2	1:A:336:GLN:NE2	1.93	0.82
1:A:389:HIS:HB3	1:A:416:VAL:HG11	1.62	0.80
2:B:90:ILE:HD11	2:B:154:LYS:HB2	1.64	0.80
1:A:96:HIS:HD2	1:A:98:ALA:H	1.30	0.79
1:A:296:THR:HG22	1:A:299:ALA:H	1.48	0.78
1:A:182:GLN:HG2	5:A:1103:HOH:O	1.85	0.77
1:A:372:GLN:NE2	2:B:400:TRP:HE1	1.82	0.77
1:A:398:GLU:OE1	2:B:360:HIS:HB3	1.88	0.74
2:B:206:LYS:HZ3	2:B:229:TRP:N	1.84	0.74
1:A:277:LYS:HB2	3:A:1305:SO4:O3	1.87	0.74
1:A:250:GLU:CD	1:A:250:GLU:H	1.90	0.74
1:A:12:LEU:HD22	1:A:83:VAL:HG12	1.70	0.73
2:B:16:LYS:HB3	2:B:83:VAL:HG13	1.70	0.73
2:B:336:GLN:HG2	2:B:355:LYS:HG2	1.69	0.73
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.54	0.71
1:A:94:ILE:HG23	1:A:230:MET:CE	2.21	0.71
2:B:12:LEU:HD22	2:B:83:VAL:HG12	1.73	0.71
1:A:221:PHE:HE2	1:A:223:LYS:HG2	1.57	0.70
1:A:426:PHE:CD2	1:A:508:GLN:HB3	2.27	0.70
1:A:296:THR:CG2	1:A:299:ALA:H	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:HB2	1:A:220:LYS:HB3	1.73	0.69
1:A:426:PHE:HE1	1:A:524:MET:HB3	1.56	0.69
1:A:10:ILE:HD13	1:A:153:TRP:HH2	1.55	0.69
2:B:6:GLU:HG3	2:B:7:PRO:HD2	1.76	0.68
2:B:109:LEU:HB2	2:B:187:ILE:HG22	1.77	0.67
1:A:296:THR:HG22	1:A:299:ALA:CB	2.25	0.66
1:A:333:GLN:HE21	1:A:336:GLN:NE2	1.93	0.66
1:A:282:LEU:HB3	1:A:293:VAL:HG11	1.77	0.65
1:A:175:ASN:HD22	1:A:193:ARG:HH22	1.43	0.65
1:A:257:ILE:O	1:A:261:VAL:HG23	1.97	0.65
1:A:332:ASP:HB2	1:A:336:GLN:HG2	1.79	0.65
1:A:224:ASP:HB3	1:A:225:PRO:HD2	1.78	0.65
1:A:339:TYR:CZ	1:A:351:GLY:HA3	2.32	0.65
1:A:8:ILE:HD11	2:B:53:THR:OG1	1.95	0.65
2:B:56:TYR:O	2:B:143:ARG:NH2	2.28	0.64
1:A:282:LEU:HB3	1:A:293:VAL:CG1	2.28	0.64
1:A:336:GLN:HG3	1:A:352:LYS:CE	2.23	0.63
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.33	0.63
1:A:10:ILE:HD13	1:A:153:TRP:CH2	2.34	0.62
1:A:95:PRO:HB2	1:A:229:TRP:HH2	1.63	0.62
1:A:29:GLU:O	1:A:32:GLU:HB3	2.00	0.62
1:A:94:ILE:HG23	1:A:230:MET:HE1	1.81	0.62
1:A:389:HIS:HB3	1:A:416:VAL:CG1	2.30	0.62
2:B:54:ASN:HD22	2:B:54:ASN:C	2.03	0.62
1:A:53:THR:HG22	1:A:53:THR:O	2.00	0.62
1:A:8:ILE:HD13	2:B:53:THR:HG23	1.81	0.61
2:B:87:PHE:O	2:B:90:ILE:HG12	1.99	0.61
1:A:91:GLN:CB	1:A:161:GLN:HE22	2.12	0.61
1:A:518:ASN:O	1:A:522:GLU:HG2	2.00	0.61
2:B:180:ILE:CG2	2:B:187:ILE:HD11	2.30	0.61
2:B:242:GLN:HE22	2:B:352:LYS:H	1.49	0.61
1:A:91:GLN:CB	1:A:161:GLN:NE2	2.59	0.60
1:A:361:THR:HG22	1:A:365:ARG:CZ	2.31	0.60
1:A:198:HIS:O	1:A:201:VAL:HG12	2.00	0.60
1:A:333:GLN:HG3	1:A:334:ASP:N	2.11	0.60
1:A:427:ASN:ND2	1:A:527:LYS:O	2.35	0.60
1:A:450:LYS:HB3	1:A:470:GLN:HA	1.84	0.59
2:B:122:GLU:HA	2:B:125:ARG:HG3	1.82	0.59
2:B:332:ASP:HB2	2:B:336:GLN:H	1.66	0.59
1:A:94:ILE:HG23	1:A:230:MET:HE2	1.85	0.58
1:A:353:TYR:HD1	1:A:373:LYS:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HG2	1:A:312:GLN:O	2.04	0.58
1:A:56:TYR:O	1:A:143:ARG:NH2	2.37	0.58
1:A:324:GLU:HA	1:A:324:GLU:OE2	2.03	0.58
2:B:105:ARG:NH2	2:B:199:ASP:OD1	2.37	0.58
2:B:394:ARG:HH11	2:B:415:PHE:HD2	1.51	0.58
1:A:166:GLN:NE2	3:A:1302:SO4:O4	2.36	0.57
1:A:235:TRP:HB3	1:A:236:PRO:HD2	1.86	0.57
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.88	0.56
1:A:465:VAL:HG21	1:A:550:LEU:CD2	2.32	0.56
2:B:191:SER:OG	2:B:198:HIS:HD2	1.88	0.56
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.19	0.56
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.87	0.56
1:A:8:ILE:CD1	2:B:53:THR:HG23	2.35	0.56
2:B:54:ASN:ND2	2:B:56:TYR:H	2.04	0.56
2:B:336:GLN:HG2	2:B:355:LYS:CG	2.35	0.56
1:A:35:LYS:HG2	1:A:132:LEU:HD13	1.87	0.55
1:A:96:HIS:CD2	1:A:98:ALA:H	2.17	0.55
2:B:193:ARG:NH1	2:B:201:VAL:CG2	2.70	0.55
2:B:336:GLN:CG	2:B:355:LYS:HG2	2.36	0.55
2:B:250:GLU:HG2	2:B:251:ILE:N	2.22	0.55
1:A:39:GLU:O	1:A:43:LYS:HG3	2.05	0.55
2:B:120:LEU:O	2:B:125:ARG:HD3	2.06	0.55
2:B:277:LYS:HB2	3:B:1308:SO4:O1	2.07	0.55
1:A:110:ASP:HB2	1:A:220:LYS:HD3	1.89	0.54
2:B:320:GLN:OE1	2:B:346:LYS:HE3	2.07	0.54
2:B:29:GLU:HG3	2:B:30:LYS:N	2.22	0.54
2:B:6:GLU:HG3	2:B:7:PRO:CD	2.36	0.54
2:B:305:GLU:O	2:B:309:ILE:HG12	2.08	0.54
2:B:229:TRP:O	2:B:230:MET:C	2.45	0.54
2:B:332:ASP:HB3	2:B:334:ASP:H	1.73	0.54
1:A:125:ARG:N	1:A:126:PRO:CD	2.70	0.54
2:B:50:ALA:HB2	2:B:145:ILE:HG23	1.89	0.53
2:B:394:ARG:O	2:B:398:GLU:HG3	2.08	0.53
1:A:94:ILE:HD11	1:A:266:TRP:HD1	1.74	0.53
1:A:104:ARG:HH22	1:A:195:ASP:CG	2.12	0.53
1:A:254:VAL:HG13	1:A:283:ILE:CG2	2.39	0.53
1:A:95:PRO:HB2	1:A:229:TRP:CH2	2.44	0.52
2:B:365:ARG:O	2:B:369:GLN:HG3	2.09	0.52
1:A:249:LYS:HE2	1:A:256:ASP:OD1	2.08	0.52
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.10	0.52
2:B:85:GLN:O	2:B:86:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HG3	1:A:200:ARG:HH11	1.74	0.52
1:A:296:THR:HG22	1:A:299:ALA:N	2.21	0.51
1:A:333:GLN:CG	1:A:336:GLN:HE21	2.08	0.51
2:B:385:ILE:CG2	2:B:411:PRO:HB3	2.41	0.51
1:A:331:LYS:HD2	1:A:420:PRO:HG2	1.91	0.51
1:A:167:VAL:HG13	1:A:212:LEU:HD23	1.93	0.51
1:A:481:PHE:CE2	1:A:485:LEU:HD11	2.46	0.51
2:B:250:GLU:CD	2:B:250:GLU:H	2.13	0.51
1:A:90:ILE:HG12	1:A:90:ILE:O	2.11	0.51
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.92	0.51
1:A:457:VAL:HB	1:A:547:VAL:HG22	1.92	0.51
1:A:333:GLN:HG2	1:A:336:GLN:HB3	1.93	0.51
1:A:352:LYS:O	1:A:373:LYS:HE2	2.11	0.50
1:A:53:THR:O	1:A:55:PRO:HD3	2.11	0.50
2:B:167:VAL:O	2:B:170:PRO:HD2	2.12	0.50
2:B:200:ARG:O	2:B:204:GLN:HG3	2.11	0.50
1:A:30:LYS:O	1:A:32:GLU:N	2.44	0.50
1:A:33:ALA:O	1:A:36:GLU:HB3	2.12	0.50
1:A:63:ILE:HD13	1:A:74:LEU:HD22	1.93	0.50
1:A:465:VAL:CG2	1:A:550:LEU:HD22	2.37	0.50
1:A:26:LEU:HB3	1:A:30:LYS:HD2	1.94	0.49
1:A:64:LYS:NZ	1:A:65:LYS:HE2	2.27	0.49
2:B:106:ILE:HG12	2:B:190:ALA:CB	2.42	0.49
2:B:370:VAL:O	2:B:374:ILE:HG13	2.12	0.49
2:B:164:MET:HE2	2:B:168:LEU:HG	1.94	0.49
1:A:285:GLY:HA3	3:A:1321:SO4:S	2.53	0.49
2:B:272:PRO:HD2	2:B:313:GLU:OE1	2.12	0.48
1:A:109:LEU:HD12	1:A:109:LEU:C	2.33	0.48
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.94	0.48
2:B:180:ILE:HG23	2:B:187:ILE:HD11	1.95	0.48
2:B:118:ILE:HD12	2:B:160:PHE:HD2	1.77	0.48
1:A:94:ILE:CG2	1:A:230:MET:HE2	2.43	0.48
2:B:243:LYS:HE3	2:B:314:GLN:HB2	1.96	0.48
2:B:394:ARG:NH1	2:B:415:PHE:HD2	2.11	0.48
1:A:162:HIS:O	1:A:166:GLN:HG3	2.14	0.48
1:A:394:ARG:NH2	5:A:1231:HOH:O	2.38	0.48
1:A:343:GLN:O	1:A:344:GLU:HB2	2.14	0.48
1:A:27:THR:O	1:A:31:ILE:HG13	2.14	0.47
1:A:143:ARG:NH1	5:A:1278:HOH:O	2.46	0.47
1:A:165:ARG:NH1	2:B:140:PRO:O	2.47	0.47
1:A:453:LYS:HG3	1:A:555:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:VAL:O	1:A:521:ILE:HG13	2.14	0.47
1:A:175:ASN:ND2	3:A:1311:SO4:O2	2.47	0.47
1:A:165:ARG:HH12	2:B:139:GLU:HG3	1.80	0.47
1:A:39:GLU:HG2	1:A:43:LYS:HE3	1.96	0.47
1:A:536:PRO:HB2	1:A:539:LYS:HG3	1.96	0.47
2:B:96:HIS:CD2	2:B:183:TYR:OH	2.68	0.47
2:B:106:ILE:HG12	2:B:190:ALA:HB2	1.97	0.47
1:A:337:TRP:CZ3	1:A:367:LEU:HD13	2.50	0.47
2:B:84:THR:HB	2:B:154:LYS:HE2	1.97	0.46
1:A:30:LYS:C	1:A:32:GLU:N	2.69	0.46
1:A:48:GLU:OE2	1:A:145:ILE:HD11	2.14	0.46
1:A:94:ILE:CD1	1:A:266:TRP:HD1	2.28	0.46
1:A:398:GLU:O	1:A:402:ASP:HB2	2.15	0.46
2:B:125:ARG:N	2:B:126:PRO:HD2	2.30	0.46
2:B:430:GLY:O	2:B:431:ASP:CB	2.63	0.46
1:A:21:LEU:HB2	1:A:59:PRO:HD3	1.98	0.46
2:B:352:LYS:HE2	2:B:429:VAL:O	2.16	0.46
1:A:310:LEU:C	1:A:312:GLN:H	2.19	0.46
1:A:88:THR:HB	2:B:54:ASN:O	2.16	0.46
1:A:244:ILE:HD12	1:A:244:ILE:N	2.31	0.46
1:A:405:TRP:CH2	2:B:417:SER:HA	2.50	0.46
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.98	0.46
2:B:83:VAL:HG12	2:B:83:VAL:O	2.15	0.46
1:A:41:MET:HB2	1:A:47:LEU:HD12	1.98	0.46
1:A:129:ALA:HA	1:A:144:TYR:O	2.15	0.46
1:A:285:GLY:HA3	3:A:1321:SO4:O3	2.16	0.46
1:A:335:ASN:O	1:A:354:ALA:HA	2.16	0.46
2:B:54:ASN:HD22	2:B:56:TYR:H	1.63	0.46
2:B:171:PHE:HZ	2:B:201:VAL:HG13	1.80	0.46
2:B:385:ILE:HG21	2:B:411:PRO:HB3	1.96	0.46
1:A:196:LEU:HG	1:A:200:ARG:HH21	1.81	0.45
1:A:350:VAL:HG12	1:A:351:GLY:N	2.31	0.45
1:A:447:ARG:O	1:A:450:LYS:HE3	2.16	0.45
2:B:21:LEU:HB2	2:B:59:PRO:HD3	1.97	0.45
2:B:109:LEU:HB2	2:B:187:ILE:CG2	2.45	0.45
1:A:257:ILE:HG13	1:A:293:VAL:HG21	1.99	0.45
1:A:113:ASP:HB3	1:A:116:PHE:CD2	2.51	0.45
2:B:396:ILE:HD12	2:B:396:ILE:N	2.32	0.45
1:A:90:ILE:HG23	1:A:161:GLN:NE2	2.32	0.45
2:B:358:ASN:HD21	2:B:360:HIS:CE1	2.35	0.45
1:A:426:PHE:CE1	1:A:524:MET:HB3	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:O	1:A:547:VAL:HG23	2.17	0.44
2:B:250:GLU:CG	2:B:251:ILE:N	2.79	0.44
2:B:424:LEU:O	2:B:427:ASN:HB2	2.17	0.44
1:A:252:TRP:O	1:A:293:VAL:HG23	2.18	0.44
1:A:25:PRO:O	1:A:26:LEU:HD23	2.17	0.44
1:A:376:LYS:NZ	4:B:1403:GOL:O2	2.50	0.44
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.65	0.44
2:B:417:SER:O	2:B:419:PRO:HD3	2.18	0.44
1:A:33:ALA:O	1:A:37:ILE:HG13	2.17	0.44
1:A:110:ASP:CB	1:A:220:LYS:HD3	2.48	0.44
2:B:320:GLN:C	2:B:322:GLU:H	2.20	0.44
2:B:193:ARG:HB3	2:B:197:GLU:HB2	2.00	0.44
1:A:92:LEU:HD23	2:B:22:ARG:NH1	2.33	0.44
1:A:250:GLU:CD	1:A:250:GLU:N	2.65	0.44
1:A:293:VAL:HG12	1:A:294:GLN:N	2.33	0.44
1:A:112:GLY:O	1:A:113:ASP:C	2.55	0.43
2:B:395:GLU:HB2	5:B:1022:HOH:O	2.17	0.43
2:B:430:GLY:O	2:B:431:ASP:HB2	2.16	0.43
2:B:183:TYR:CD2	2:B:379:LEU:HD22	2.53	0.43
2:B:129:ALA:HA	2:B:144:TYR:O	2.19	0.43
1:A:486:THR:HG22	1:A:487:ASP:OD2	2.18	0.43
2:B:79:GLU:OE2	2:B:79:GLU:HA	2.19	0.43
1:A:332:ASP:HB2	1:A:336:GLN:CG	2.47	0.43
1:A:405:TRP:CZ3	2:B:417:SER:HA	2.53	0.43
2:B:393:GLU:HB3	2:B:396:ILE:HD13	2.01	0.42
1:A:359:THR:O	1:A:512:SER:HA	2.19	0.42
2:B:331:LYS:HG2	2:B:335:ASN:HA	2.01	0.42
1:A:30:LYS:C	1:A:32:GLU:H	2.22	0.42
1:A:331:LYS:CG	1:A:420:PRO:HG2	2.49	0.42
1:A:516:ILE:HG23	1:A:517:VAL:N	2.34	0.42
2:B:22:ARG:HG2	3:B:1317:SO4:O4	2.19	0.42
1:A:92:LEU:CD2	2:B:22:ARG:HH12	2.33	0.42
1:A:94:ILE:CD1	1:A:266:TRP:CD1	3.03	0.42
1:A:289:LEU:HA	1:A:289:LEU:HD12	1.82	0.42
1:A:50:ALA:HB2	1:A:145:ILE:HG23	1.99	0.42
1:A:196:LEU:HG	1:A:200:ARG:NH2	2.34	0.42
1:A:479:GLU:O	1:A:483:MET:HG3	2.20	0.42
1:A:83:VAL:HG12	1:A:83:VAL:O	2.20	0.42
2:B:171:PHE:CZ	2:B:201:VAL:HG13	2.55	0.42
1:A:456:TYR:C	1:A:456:TYR:CD2	2.93	0.42
2:B:339:TYR:CE1	2:B:351:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:ILE:HA	2:B:386:PRO:HD3	1.84	0.41
1:A:457:VAL:CG2	1:A:547:VAL:HG22	2.50	0.41
1:A:82:LYS:HE3	1:A:82:LYS:HB2	1.82	0.41
1:A:250:GLU:CG	1:A:251:ILE:H	2.33	0.41
1:A:520:ILE:O	1:A:524:MET:HG3	2.20	0.41
2:B:12:LEU:HD11	2:B:127:TYR:CZ	2.55	0.41
2:B:86:ASP:OD2	2:B:87:PHE:N	2.43	0.41
2:B:181:ILE:O	2:B:181:ILE:HG12	2.15	0.41
1:A:41:MET:HE3	1:A:47:LEU:HD11	2.01	0.41
2:B:96:HIS:HD2	2:B:183:TYR:OH	2.02	0.41
1:A:161:GLN:HG3	5:A:1227:HOH:O	2.21	0.41
1:A:331:LYS:CD	1:A:420:PRO:HG2	2.50	0.41
1:A:453:LYS:HE3	1:A:555:ILE:HG12	2.03	0.41
1:A:304:GLU:O	1:A:308:ILE:HG13	2.21	0.41
1:A:361:THR:HB	1:A:362:ASN:H	1.67	0.41
1:A:444:SER:OG	1:A:555:ILE:HG21	2.21	0.41
1:A:338:THR:CG2	1:A:352:LYS:HZ3	2.33	0.41
1:A:16:LYS:HB3	1:A:83:VAL:HG13	2.01	0.41
1:A:36:GLU:O	1:A:39:GLU:HB3	2.21	0.41
2:B:181:ILE:HD11	2:B:183:TYR:CE2	2.56	0.41
2:B:343:GLN:O	2:B:344:GLU:HB2	2.20	0.41
1:A:457:VAL:CB	1:A:547:VAL:HG22	2.51	0.40
2:B:182:GLN:HG3	2:B:186:ASP:O	2.21	0.40
1:A:64:LYS:O	1:A:65:LYS:C	2.59	0.40
2:B:83:VAL:O	2:B:83:VAL:CG1	2.70	0.40
1:A:6:GLU:HA	1:A:7:PRO:HD3	1.97	0.40
1:A:298:LEU:HG	5:A:1111:HOH:O	2.21	0.40
1:A:118:ILE:HA	1:A:119:PRO:HD2	1.92	0.40
2:B:54:ASN:HD22	2:B:55:PRO:N	2.20	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	530/555 (96%)	489 (92%)	36 (7%)	5 (1%)	17	17
2	B	394/426 (92%)	372 (94%)	16 (4%)	6 (2%)	10	8
All	All	924/981 (94%)	861 (93%)	52 (6%)	11 (1%)	13	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	286	LYS
2	B	230	MET
1	A	65	LYS
2	B	90	ILE
1	A	31	ILE
1	A	355	LYS
2	B	86	ASP
2	B	98	ALA
2	B	321	GLU
2	B	358	ASN

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	477/492 (97%)	447 (94%)	30 (6%)	18	19
2	B	363/385 (94%)	337 (93%)	26 (7%)	14	14
All	All	840/877 (96%)	784 (93%)	56 (7%)	16	17

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	27	THR
1	A	28	LYS
1	A	34	LEU
1	A	63	ILE

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Mol	Chain	Res	Type
1	A	89	GLU
1	A	100	LEU
1	A	117	SER
1	A	132	LEU
1	A	182	GLN
1	A	186	ASP
1	A	212	LEU
1	A	237	THR
1	A	250	GLU
1	A	296	THR
1	A	322	GLU
1	A	332	ASP
1	A	334	ASP
1	A	352	LYS
1	A	372	GLN
1	A	394	ARG
1	A	402	ASP
1	A	407	VAL
1	A	410	ILE
1	A	412	ASP
1	A	414	ASP
1	A	427	ASN
1	A	450	LYS
1	A	550	LEU
1	A	553	GLN
2	B	32	GLU
2	B	34	LEU
2	B	36	GLU
2	B	54	ASN
2	B	55	PRO
2	B	60	THR
2	B	89	GLU
2	B	125	ARG
2	B	151	GLN
2	B	181	ILE
2	B	187	ILE
2	B	188	LEU
2	B	203	LEU
2	B	230	MET
2	B	270	LEU
2	B	281	ARG
2	B	294	GLN

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Mol	Chain	Res	Type
2	B	303	LEU
2	B	305	GLU
2	B	310	LEU
2	B	330	GLN
2	B	332	ASP
2	B	358	ASN
2	B	395	GLU
2	B	413	TRP
2	B	431	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	121	HIS
1	A	161	GLN
1	A	175	ASN
1	A	182	GLN
1	A	210	ASN
1	A	245	GLN
1	A	258	GLN
1	A	314	GLN
1	A	336	GLN
1	A	342	HIS
1	A	360	HIS
1	A	372	GLN
1	A	399	GLN
1	A	508	GLN
1	A	519	GLN
1	A	544	ASN
2	B	54	ASN
2	B	96	HIS
2	B	161	GLN
2	B	182	GLN
2	B	198	HIS
2	B	204	GLN
2	B	210	ASN
2	B	242	GLN
2	B	294	GLN
2	B	358	ASN
2	B	399	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

27 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	SO4	A	1315	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	A	1306	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	B	1314	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	A	1319	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	A	1302	-	4,4,4	0.31	0	6,6,6	0.34	0
3	SO4	A	1303	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	A	1311	-	4,4,4	0.27	0	6,6,6	0.14	0
3	SO4	A	1321	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	A	1313	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	A	1304	-	4,4,4	0.32	0	6,6,6	0.09	0
4	GOL	A	1400	-	5,5,5	0.87	0	5,5,5	0.24	0
3	SO4	A	1318	-	4,4,4	0.28	0	6,6,6	0.06	0
4	GOL	B	1402	-	5,5,5	0.62	0	5,5,5	0.17	0
3	SO4	A	1305	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	B	1309	-	4,4,4	0.25	0	6,6,6	0.13	0
4	GOL	B	1401	-	5,5,5	0.70	0	5,5,5	0.24	0
3	SO4	A	1301	-	4,4,4	0.25	0	6,6,6	0.11	0
4	GOL	B	1403	-	5,5,5	0.73	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	1404	-	5,5,5	1.08	0	5,5,5	0.32	0
3	SO4	B	1317	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	B	1308	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	A	1316	-	4,4,4	0.30	0	6,6,6	0.15	0
3	SO4	A	1300	-	4,4,4	0.35	0	6,6,6	0.21	0
3	SO4	B	1320	-	4,4,4	0.28	0	6,6,6	0.08	0
3	SO4	B	1310	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	A	1312	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	B	1307	-	4,4,4	0.31	0	6,6,6	0.23	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	GOL	B	1403	-	-	4/4/4/4	-
4	GOL	B	1404	-	-	4/4/4/4	-
4	GOL	A	1400	-	-	2/4/4/4	-
4	GOL	B	1402	-	-	0/4/4/4	-
4	GOL	B	1401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1401	GOL	O1-C1-C2-C3
4	B	1403	GOL	O1-C1-C2-C3
4	B	1403	GOL	C1-C2-C3-O3
4	B	1401	GOL	O1-C1-C2-O2
4	A	1400	GOL	O1-C1-C2-C3
4	B	1404	GOL	O1-C1-C2-C3
4	B	1404	GOL	C1-C2-C3-O3
4	B	1403	GOL	O1-C1-C2-O2
4	B	1403	GOL	O2-C2-C3-O3
4	B	1404	GOL	O1-C1-C2-O2
4	B	1404	GOL	O2-C2-C3-O3
4	A	1400	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	SO4	1	0
3	A	1311	SO4	1	0
3	A	1321	SO4	2	0
3	A	1305	SO4	1	0
4	B	1403	GOL	1	0
3	B	1317	SO4	1	0
3	B	1308	SO4	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	538/555 (96%)	0.00	28 (5%)	27 39	26, 52, 101, 149	0
2	B	402/426 (94%)	-0.04	21 (5%)	27 39	25, 43, 93, 135	0
All	All	940/981 (95%)	-0.02	49 (5%)	27 39	25, 48, 99, 149	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	6.9
1	A	24	TRP	6.8
2	B	356	VAL	5.2
1	A	334	ASP	5.1
1	A	65	LYS	4.7
1	A	64	LYS	4.5
1	A	359	THR	4.3
1	A	356	VAL	4.3
1	A	66	LYS	4.2
2	B	355	LYS	4.2
2	B	360	HIS	4.0
1	A	25	PRO	3.8
2	B	90	ILE	3.8
1	A	43	LYS	3.8
1	A	335	ASN	3.8
1	A	284	SER	3.6
2	B	70	LYS	3.6
1	A	554	GLY	3.6
2	B	91	GLN	3.5
1	A	28	LYS	3.5
1	A	32	GLU	3.1
2	B	230	MET	3.1
2	B	229	TRP	3.0
2	B	69	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	3	ALA	2.9
1	A	29	GLU	2.9
2	B	357	LYS	2.8
1	A	345	GLU	2.8
2	B	171	PHE	2.8
2	B	358	ASN	2.8
1	A	219	GLU	2.8
1	A	27	THR	2.8
2	B	98	ALA	2.7
1	A	91	GLN	2.6
2	B	173	LYS	2.6
2	B	6	GLU	2.6
2	B	205	LEU	2.5
1	A	90	ILE	2.5
2	B	208	LEU	2.5
2	B	184	MET	2.4
1	A	35	LYS	2.3
2	B	170	PRO	2.2
1	A	447	ARG	2.1
1	A	286	LYS	2.1
1	A	450	LYS	2.1
1	A	39	GLU	2.1
2	B	167	VAL	2.1
1	A	4	LYS	2.0
2	B	209	LEU	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 monosaccharides 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(\AA^2)	Q<0.9
4	GOL	B	1404	6/6	0.78	0.21	61,61,80,81	0
3	SO4	A	1321	5/5	0.84	0.31	135,135,144,149	0
3	SO4	B	1320	5/5	0.85	0.16	127,134,138,141	0
3	SO4	A	1311	5/5	0.85	0.22	109,111,120,122	0
3	SO4	A	1305	5/5	0.86	0.32	122,125,133,144	0
3	SO4	B	1314	5/5	0.86	0.17	105,118,125,127	0
4	GOL	B	1403	6/6	0.89	0.18	68,78,85,93	0
3	SO4	B	1317	5/5	0.89	0.37	141,146,150,155	0
4	GOL	B	1402	6/6	0.90	0.22	65,76,80,103	0
3	SO4	A	1316	5/5	0.90	0.17	81,88,102,117	0
3	SO4	A	1319	5/5	0.90	0.23	99,108,119,128	0
4	GOL	B	1401	6/6	0.92	0.32	34,52,56,87	0
4	GOL	A	1400	6/6	0.93	0.17	39,60,69,81	0
3	SO4	B	1310	5/5	0.93	0.22	127,132,136,138	0
3	SO4	A	1302	5/5	0.93	0.17	65,84,103,114	0
3	SO4	A	1304	5/5	0.93	0.15	85,87,105,108	0
3	SO4	A	1312	5/5	0.93	0.28	100,107,112,118	0
3	SO4	B	1309	5/5	0.94	0.13	93,95,100,103	0
3	SO4	B	1307	5/5	0.94	0.16	92,94,101,112	0
3	SO4	A	1318	5/5	0.95	0.20	102,108,112,120	0
3	SO4	A	1303	5/5	0.95	0.17	99,102,111,112	0
3	SO4	A	1315	5/5	0.96	0.14	71,79,85,87	0
3	SO4	A	1306	5/5	0.97	0.17	113,117,125,128	0
3	SO4	B	1308	5/5	0.97	0.11	73,80,88,96	0
3	SO4	A	1300	5/5	0.98	0.08	63,65,77,77	0
3	SO4	A	1301	5/5	0.98	0.07	77,88,101,107	0
3	SO4	A	1313	5/5	0.99	0.13	66,75,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.