



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:56 PM GMT

PDB ID : 4B4X
Title : Crystal structure of a complex between Actinomadura R39 DD-peptidase and a sulfonamide boronate inhibitor
Authors : Cannella, S.E.; Sauvage, E.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.
Deposited on : 2012-08-01
Resolution : 2.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

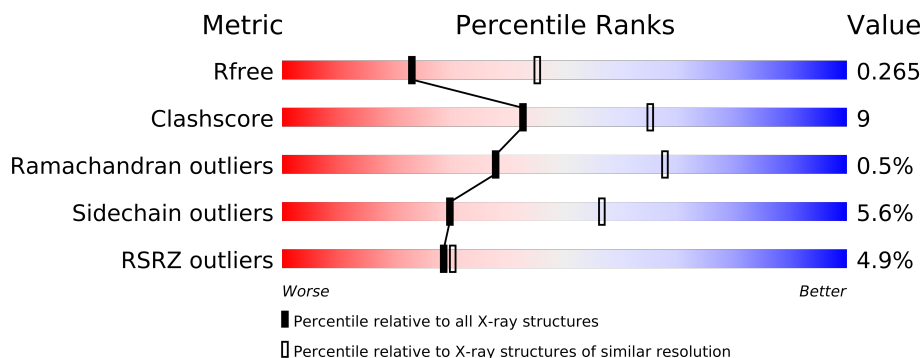
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	
1	C	466	
1	D	466	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1469	-	X
3	SO4	D	1470	-	X
4	MG	D	1472	-	X

2 Entry composition i

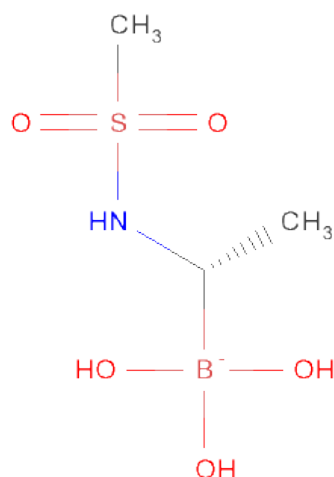
There are 5 unique types of molecules in this entry. The entry contains 13905 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	D	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			

- Molecule 2 is TRIHYDROXY{(1S)-1-[(METHYLSULFONYL)AMINO]ETHYL}BORATE (1-) (three-letter code: HQZ) (formula: C₃H₁₁BNO₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	S	0	0
			10	1	3	1	4	1		
2	B	1	Total	B	C	N	O	S	0	0
			10	1	3	1	4	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	B	C	N	O	S	0	0
			10	1	3	1	4	1		
2	D	1	Total	B	C	N	O	S	0	0
			10	1	3	1	4	1		

- 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	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		

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

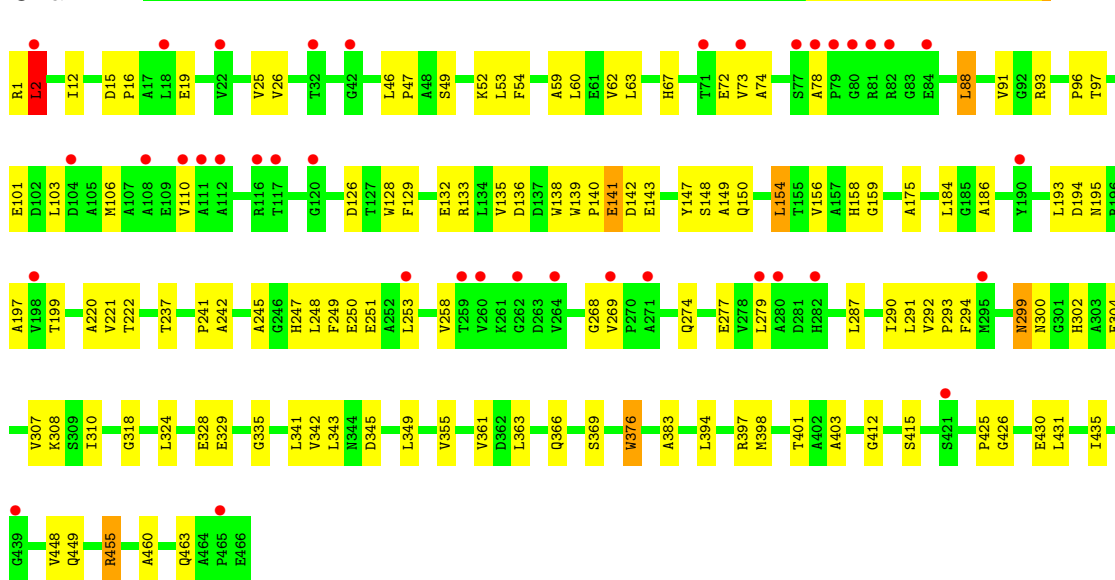
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total 92	O 92	0	0
5	B	68	Total 68	O 68	0	0
5	C	76	Total 76	O 76	0	0
5	D	111	Total 111	O 111	0	0

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 errors 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.

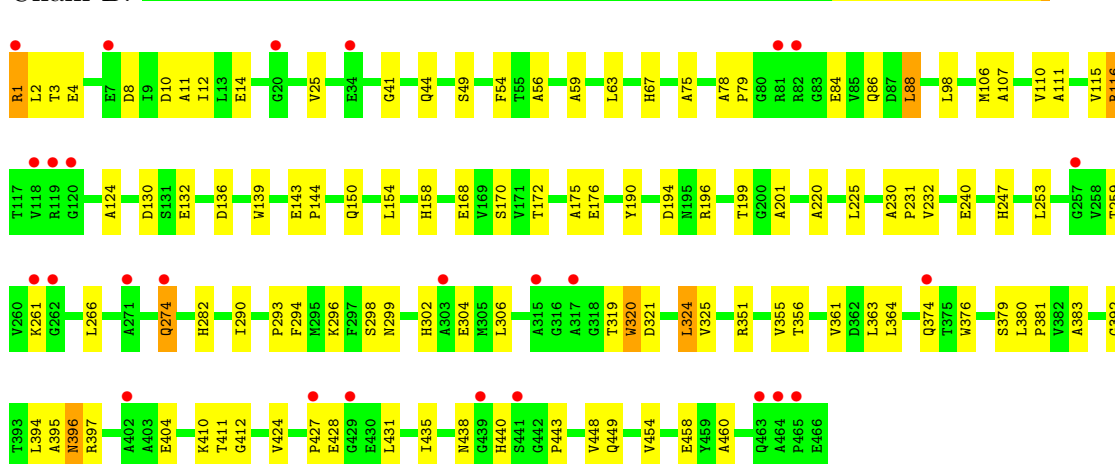
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



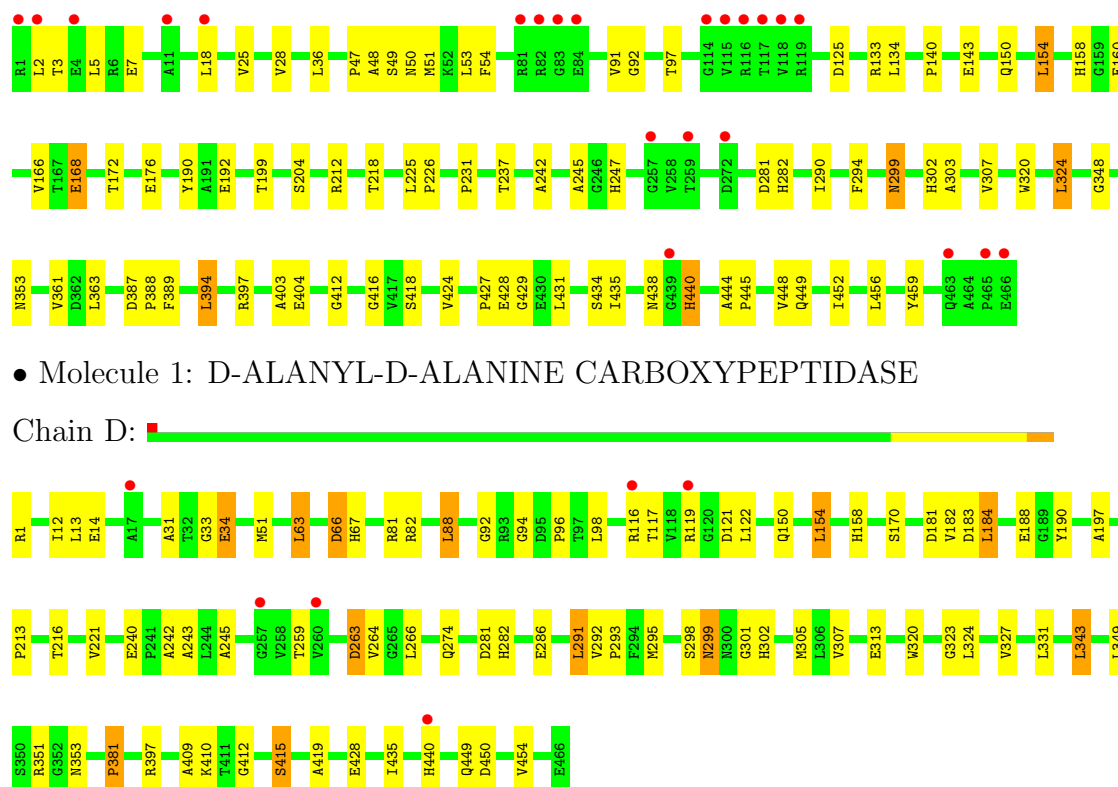
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain D:

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.33Å 92.11Å 105.96Å 90.00° 95.90° 90.00°	Depositor
Resolution (Å)	35.13 – 2.65 35.13 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.13-2.65) 98.0 (35.13-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.268 0.218 , 0.265	Depositor DCC
R_{free} test set	2825 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.5	EDS
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 55927 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13905	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HQZ, 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	0.66	0/3412	0.73	1/4666 (0.0%)
1	B	0.60	0/3403	0.69	1/4656 (0.0%)
1	C	0.65	2/3403 (0.1%)	0.68	0/4656
1	D	0.76	0/3412	0.77	1/4666 (0.0%)
All	All	0.67	2/13630 (0.0%)	0.72	3/18644 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	GLU	CD-OE2	6.33	1.32	1.25
1	C	168	GLU	CG-CD	6.11	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	343	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	46	LEU	CA-CB-CG	5.82	128.68	115.30
1	B	98	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3353	0	3200	79	0
1	B	3344	0	3194	63	0
1	C	3344	0	3194	50	0
1	D	3353	0	3200	44	1
2	A	10	0	10	0	0
2	B	10	0	10	2	0
2	C	10	0	10	0	0
2	D	10	0	10	0	0
3	A	30	0	0	3	0
3	B	30	0	0	5	0
3	C	30	0	0	2	0
3	D	30	0	0	6	0
4	A	2	0	0	0	0
4	D	2	0	0	0	1
5	A	92	0	0	2	0
5	B	68	0	0	3	0
5	C	76	0	0	0	0
5	D	111	0	0	0	0
All	All	13905	0	12828	235	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (235) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:GLY:HA3	1:A:460:ALA:HB1	1.45	0.96
1:A:341:LEU:HD13	1:A:343:LEU:HD21	1.47	0.96
1:B:130:ASP:OD2	1:B:319:THR:HG22	1.79	0.83
1:B:168:GLU:OE2	3:B:1470:SO4:S	2.37	0.82
1:B:63:LEU:O	1:B:67:HIS:HB2	1.84	0.78
1:B:443:PRO:HB2	5:B:2062:HOH:O	1.87	0.72
1:D:158:HIS:NE2	3:D:1470:SO4:O3	2.19	0.72
1:C:158:HIS:NE2	1:C:168:GLU:OE2	2.23	0.72
1:A:78:ALA:HB2	1:A:277:GLU:HG2	1.71	0.72
1:B:321:ASP:O	1:B:325:VAL:HG23	1.92	0.70
1:B:396:ASN:N	1:B:396:ASN:HD22	1.90	0.69
1:B:168:GLU:OE2	3:B:1470:SO4:O3	2.08	0.69
1:B:150:GLN:NE2	1:B:240:GLU:H	1.89	0.69
1:A:129:PHE:HA	1:A:318:GLY:HA3	1.75	0.69
1:C:158:HIS:CE1	1:C:168:GLU:OE2	2.46	0.68
1:B:397:ARG:HH22	1:B:449:GLN:HE21	1.40	0.68
1:B:1:ARG:HD3	1:B:4:GLU:HB2	1.76	0.68
1:A:398:MET:O	1:A:401:THR:OG1	2.13	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.76	0.67
1:A:247:HIS:O	1:A:250:GLU:HB3	1.94	0.67
1:A:299:ASN:HD22	1:A:302:HIS:H	1.45	0.65
1:C:160:GLU:HG3	1:C:389:PHE:HZ	1.61	0.65
1:C:204:SER:O	1:C:226:PRO:HG3	1.97	0.65
1:C:416:GLY:HA2	1:C:440:HIS:CD2	2.31	0.64
1:A:26:VAL:HG12	1:A:361:VAL:HG21	1.78	0.64
1:A:72:GLU:HG2	1:A:91:VAL:HB	1.79	0.63
1:C:49:SER:HB2	1:C:412:GLY:HA2	1.79	0.63
1:D:150:GLN:NE2	1:D:240:GLU:H	1.97	0.62
1:D:282:HIS:NE2	3:D:1474:SO4:O2	2.29	0.62
1:C:282:HIS:NE2	3:C:1466:SO4:O4	2.26	0.62
1:C:397:ARG:HH22	1:C:449:GLN:HE21	1.48	0.62
1:A:186:ALA:HB1	1:A:248:LEU:HD11	1.82	0.61
1:A:335:GLY:HA3	1:A:366:GLN:HE21	1.66	0.61
1:C:25:VAL:HG22	1:C:435:ILE:HG23	1.82	0.60
1:A:47:PRO:HB3	1:A:355:VAL:HG21	1.83	0.60
1:B:106:MET:O	1:B:110:VAL:HG23	2.01	0.60
1:A:106:MET:O	1:A:110:VAL:HG23	2.02	0.60
1:A:1:ARG:HH12	1:A:455:ARG:HH12	1.49	0.59
1:B:294:PHE:CD1	1:B:302:HIS:HB2	2.37	0.59
1:D:190:TYR:OH	1:D:243:ALA:HB3	2.02	0.59
1:A:147:TYR:HB2	1:A:300:ASN:ND2	2.17	0.58
1:A:26:VAL:CG1	1:A:361:VAL:HG21	2.33	0.58
1:A:132:GLU:O	1:A:308:LYS:NZ	2.37	0.58
1:B:116:ARG:HD2	5:B:2021:HOH:O	2.01	0.58
1:C:299:ASN:C	1:C:299:ASN:HD22	2.07	0.57
1:A:52:LYS:HE2	1:A:299:ASN:O	2.04	0.57
1:D:150:GLN:HE22	1:D:240:GLU:H	1.51	0.57
1:B:78:ALA:HB1	1:B:79:PRO:HD2	1.87	0.57
1:A:138:TRP:HH2	1:A:304:GLU:HG3	1.68	0.57
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.87	0.56
1:D:122:LEU:HB3	1:D:264:VAL:HG22	1.88	0.56
1:A:73:VAL:HG12	1:A:88:LEU:HD22	1.87	0.56
1:C:160:GLU:HG3	1:C:389:PHE:CZ	2.40	0.55
1:D:63:LEU:O	1:D:67:HIS:HB2	2.05	0.55
1:C:225:LEU:HD12	1:C:226:PRO:HD2	1.87	0.55
1:B:150:GLN:HE22	1:B:240:GLU:H	1.54	0.55
1:A:47:PRO:HB3	1:A:355:VAL:CG2	2.36	0.55
1:D:351:ARG:NH2	1:D:415:SER:HB3	2.21	0.54
1:B:44:GLN:HA	1:B:355:VAL:O	2.07	0.54
1:A:397:ARG:HH22	1:A:449:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:ASN:ND2	1:A:302:HIS:H	2.06	0.54
1:D:213:PRO:O	1:D:216:THR:OG1	2.23	0.54
1:B:176:GLU:HG3	1:B:201:ALA:HA	1.89	0.53
1:D:94:GLY:O	1:D:96:PRO:HD3	2.08	0.53
1:C:133:ARG:HB3	1:C:150:GLN:HG2	1.90	0.53
1:D:450:ASP:O	1:D:454:VAL:HG23	2.09	0.53
1:D:351:ARG:HH21	1:D:415:SER:HB3	1.74	0.53
1:A:60:LEU:HD11	1:A:291:LEU:HD11	1.89	0.53
1:A:248:LEU:HD23	1:A:251:GLU:OE1	2.09	0.53
1:B:168:GLU:OE2	3:B:1470:SO4:O2	2.27	0.52
1:C:2:LEU:HD22	1:C:36:LEU:HD22	1.91	0.52
1:B:49:SER:HB2	1:B:412:GLY:HA2	1.91	0.52
1:B:41:GLY:O	1:B:356:THR:HB	2.09	0.52
1:A:93:ARG:HG2	1:A:128:TRP:CD2	2.44	0.52
1:C:348:GLY:HA2	1:C:353:ASN:ND2	2.24	0.52
1:D:299:ASN:HD22	1:D:299:ASN:C	2.12	0.52
1:D:295:MET:HE3	1:D:410:LYS:HD3	1.91	0.52
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.91	0.52
1:C:427:PRO:C	1:C:429:GLY:H	2.13	0.52
1:A:307:VAL:O	1:A:310:ILE:N	2.43	0.51
1:D:154:LEU:HD13	1:D:245:ALA:HB3	1.93	0.51
1:A:158:HIS:NE2	3:A:1470:SO4:O4	2.42	0.51
1:B:194:ASP:HB3	1:B:220:ALA:HA	1.93	0.51
1:D:381:PRO:HG2	1:D:409:ALA:O	2.12	0.50
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.94	0.50
1:A:139:TRP:HB3	1:A:141:GLU:OE2	2.11	0.50
1:D:12:ILE:C	1:D:14:GLU:H	2.14	0.50
1:D:397:ARG:HH22	1:D:449:GLN:HE21	1.58	0.50
1:A:103:LEU:HB3	1:A:249:PHE:HD1	1.75	0.50
1:C:91:VAL:HA	1:C:125:ASP:HB3	1.93	0.50
1:D:51:MET:HE2	1:D:353:ASN:HB3	1.92	0.50
1:B:427:PRO:HD3	1:B:460:ALA:O	2.12	0.50
1:B:49:SER:HB2	2:B:500:HQZ:OAC	2.12	0.50
1:A:63:LEU:O	1:A:67:HIS:HB2	2.12	0.50
1:A:253:LEU:HB3	1:A:258:VAL:HB	1.94	0.50
1:A:292:VAL:HB	1:A:293:PRO:HD3	1.94	0.49
1:D:66:ASP:HA	1:D:286:GLU:HB3	1.94	0.49
1:D:170:SER:HB2	1:D:183:ASP:HB2	1.95	0.49
1:A:307:VAL:HG11	1:A:324:LEU:CD1	2.43	0.49
1:D:419:ALA:HA	1:D:435:ILE:O	2.12	0.49
1:B:75:ALA:HB2	1:B:88:LEU:HD23	1.94	0.49
1:B:56:ALA:HB3	1:B:376:TRP:HZ3	1.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:184:LEU:HD22	1:D:188:GLU:OE2	2.11	0.49
1:B:383:ALA:O	1:B:404:GLU:HA	2.12	0.49
1:C:307:VAL:HG11	1:C:324:LEU:HD13	1.94	0.49
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.94	0.49
1:D:412:GLY:HA3	1:D:419:ALA:HB3	1.95	0.49
1:A:149:ALA:HA	1:A:237:THR:HG21	1.95	0.49
1:A:383:ALA:HB3	1:A:403:ALA:O	2.13	0.49
1:D:92:GLY:HA3	1:D:154:LEU:HB2	1.95	0.48
1:A:193:LEU:HD11	1:A:195:ASN:HB2	1.94	0.48
1:C:294:PHE:CE1	1:C:303:ALA:HB2	2.48	0.48
1:A:62:VAL:HG11	1:A:310:ILE:HG23	1.95	0.48
1:A:140:PRO:HA	1:A:143:GLU:HG3	1.96	0.48
1:A:307:VAL:HA	1:A:310:ILE:HD12	1.95	0.48
1:B:25:VAL:HG22	1:B:435:ILE:HG23	1.96	0.47
1:A:341:LEU:O	1:A:342:VAL:HG23	2.14	0.47
1:C:212:ARG:HG3	1:C:218:THR:O	2.15	0.47
1:D:158:HIS:CE1	3:D:1470:SO4:O1	2.67	0.47
1:A:25:VAL:HG22	1:A:435:ILE:HG23	1.96	0.47
1:D:327:VAL:O	1:D:331:LEU:HG	2.14	0.47
1:B:172:THR:HG22	1:B:231:PRO:HB3	1.96	0.47
1:B:296:LYS:NZ	1:B:380:LEU:O	2.30	0.47
1:A:88:LEU:HD21	1:A:279:LEU:HD12	1.96	0.47
1:A:292:VAL:HB	1:A:293:PRO:CD	2.45	0.47
1:C:361:VAL:HG23	1:C:434:SER:HB3	1.96	0.47
1:B:282:HIS:NE2	3:B:1471:SO4:O4	2.48	0.47
1:C:140:PRO:HA	1:C:143:GLU:HG3	1.97	0.47
1:D:12:ILE:O	1:D:14:GLU:N	2.46	0.47
1:A:287:LEU:O	1:A:290:ILE:N	2.47	0.47
1:B:59:ALA:HB1	1:B:306:LEU:HD22	1.96	0.46
1:B:175:ALA:O	1:B:199:THR:HB	2.14	0.46
1:A:194:ASP:HB3	1:A:220:ALA:HA	1.97	0.46
1:A:184:LEU:HD21	1:A:193:LEU:HD13	1.98	0.46
1:A:96:PRO:HG2	1:A:97:THR:HG23	1.96	0.46
1:A:126:ASP:HB3	1:A:154:LEU:HB2	1.97	0.46
1:D:282:HIS:NE2	3:D:1474:SO4:O4	2.48	0.46
1:B:383:ALA:HA	1:B:394:LEU:HB3	1.97	0.46
1:B:396:ASN:N	1:B:396:ASN:ND2	2.61	0.46
1:C:54:PHE:CD2	1:C:363:LEU:HD22	2.51	0.46
1:C:299:ASN:ND2	1:C:302:HIS:H	2.12	0.46
1:A:307:VAL:O	1:A:310:ILE:HB	2.15	0.46
1:B:1:ARG:CZ	1:D:428:GLU:HG2	2.46	0.46
1:C:50:ASN:O	1:C:53:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:5:LEU:HD22	1:C:459:TYR:CG	2.52	0.45
1:C:97:THR:HG21	1:C:290:ILE:HG12	1.99	0.45
1:B:454:VAL:O	1:B:458:GLU:HG3	2.16	0.45
1:B:274:GLN:H	1:B:274:GLN:HG2	1.60	0.45
1:B:12:ILE:HG22	1:B:448:VAL:HG13	1.99	0.45
1:A:369:SER:HB2	5:A:2074:HOH:O	2.15	0.45
1:B:290:ILE:O	1:B:293:PRO:HD2	2.17	0.45
1:B:304:GLU:HA	1:B:304:GLU:OE1	2.17	0.45
1:A:59:ALA:O	1:A:63:LEU:HB2	2.17	0.45
1:B:143:GLU:N	1:B:144:PRO:CD	2.80	0.45
1:C:424:VAL:O	1:C:431:LEU:N	2.40	0.44
1:C:294:PHE:HE1	1:C:303:ALA:HB2	1.83	0.44
1:C:242:ALA:O	1:C:245:ALA:HB3	2.17	0.44
1:D:242:ALA:HB3	1:D:266:LEU:HD21	1.99	0.44
1:B:49:SER:CB	2:B:500:HQZ:OAC	2.65	0.44
1:B:111:ALA:HA	1:B:115:VAL:O	2.17	0.44
1:B:381:PRO:HB2	1:B:394:LEU:HD12	1.99	0.44
1:C:190:TYR:HB2	1:C:247:HIS:CD2	2.53	0.44
1:A:175:ALA:O	1:A:199:THR:HB	2.18	0.44
1:B:54:PHE:CD2	1:B:363:LEU:HD22	2.53	0.43
1:A:1:ARG:NH2	1:A:455:ARG:HH22	2.15	0.43
1:C:48:ALA:O	1:C:348:GLY:HA3	2.18	0.43
1:B:158:HIS:NE2	3:B:1470:SO4:O3	2.49	0.43
1:A:53:LEU:HD22	1:A:376:TRP:CH2	2.53	0.43
1:A:294:PHE:CD1	1:A:302:HIS:HB2	2.53	0.43
1:C:92:GLY:HA3	1:C:154:LEU:HG	2.01	0.43
1:A:49:SER:HB2	1:A:412:GLY:HA2	2.00	0.43
1:B:11:ALA:O	1:B:14:GLU:HB2	2.18	0.43
1:C:416:GLY:HA2	1:C:440:HIS:HD2	1.82	0.43
1:D:197:ALA:HB2	1:D:221:VAL:HG12	2.00	0.43
1:D:307:VAL:HG13	1:D:323:GLY:HA3	2.00	0.43
1:C:3:THR:O	1:C:7:GLU:HG3	2.19	0.43
1:B:410:LYS:HE3	1:B:411:THR:O	2.19	0.43
1:B:199:THR:HA	1:B:225:LEU:O	2.19	0.42
1:B:170:SER:HA	1:B:232:VAL:O	2.18	0.42
1:A:341:LEU:CD1	1:A:343:LEU:HD21	2.33	0.42
1:B:296:LYS:HE2	1:B:379:SER:O	2.20	0.42
1:A:369:SER:CB	5:A:2074:HOH:O	2.67	0.42
1:B:361:VAL:HA	1:B:364:LEU:HD12	2.01	0.42
1:B:320:TRP:O	1:B:324:LEU:HB2	2.19	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.90	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:TRP:CZ2	1:B:351:ARG:HD2	2.54	0.42
1:D:291:LEU:HA	1:D:291:LEU:HD13	1.93	0.42
1:A:268:GLY:O	1:A:269:VAL:C	2.57	0.42
1:D:158:HIS:NE2	3:D:1470:SO4:S	2.91	0.42
1:A:397:ARG:HH22	1:A:449:GLN:HE21	1.65	0.42
1:A:154:LEU:HB3	1:A:242:ALA:CB	2.49	0.42
1:B:8:ASP:O	1:B:11:ALA:HB3	2.18	0.42
1:D:33:GLY:O	1:D:34:GLU:C	2.58	0.42
1:B:124:ALA:HB3	1:B:266:LEU:HD23	2.01	0.42
1:A:425:PRO:HA	1:A:430:GLU:HA	2.01	0.42
1:A:150:GLN:NE2	1:A:241:PRO:HD3	2.34	0.42
1:C:18:LEU:HD12	1:C:448:VAL:HG21	2.01	0.42
1:A:133:ARG:N	3:A:1469:SO4:O1	2.53	0.42
1:B:424:VAL:HB	1:B:431:LEU:HB2	2.02	0.42
1:C:452:ILE:O	1:C:456:LEU:HG	2.19	0.42
1:D:301:GLY:O	1:D:305:MET:HG3	2.20	0.42
1:B:395:ALA:C	1:B:396:ASN:HD22	2.24	0.41
1:C:394:LEU:HD12	1:C:397:ARG:HD3	2.02	0.41
1:A:294:PHE:HD1	1:A:302:HIS:HB2	1.85	0.41
1:A:345:ASP:OD1	1:A:345:ASP:C	2.59	0.41
1:C:225:LEU:HD12	1:C:226:PRO:CD	2.49	0.41
1:D:313:GLU:HG3	1:D:313:GLU:O	2.19	0.41
1:A:394:LEU:HD23	1:A:397:ARG:HD3	2.01	0.41
1:C:5:LEU:HD22	1:C:459:TYR:CD1	2.55	0.41
1:B:440:HIS:HB2	5:B:2004:HOH:O	2.20	0.41
1:C:444:ALA:HA	1:C:445:PRO:HD3	1.84	0.41
1:D:292:VAL:HB	1:D:293:PRO:CD	2.51	0.41
1:C:412:GLY:O	1:C:418:SER:HA	2.20	0.41
1:A:1:ARG:O	1:A:2:LEU:HB2	2.20	0.41
1:A:158:HIS:NE2	3:A:1470:SO4:O2	2.54	0.41
1:D:170:SER:O	1:D:182:VAL:HA	2.21	0.41
1:C:282:HIS:CE1	3:C:1466:SO4:O3	2.74	0.41
1:B:190:TYR:HB2	1:B:247:HIS:CD2	2.56	0.41
1:B:107:ALA:HB1	1:B:253:LEU:HD23	2.01	0.41
1:D:88:LEU:HA	1:D:88:LEU:HD23	1.97	0.41
1:C:403:ALA:O	1:C:404:GLU:C	2.60	0.41
1:A:74:ALA:O	1:A:88:LEU:HD23	2.21	0.41
1:A:139:TRP:HA	1:A:140:PRO:HD3	1.98	0.41
1:D:121:ASP:OD1	1:D:263:ASP:N	2.42	0.41
1:C:166:VAL:HA	1:C:237:THR:HA	2.03	0.41
1:A:54:PHE:CD1	1:A:363:LEU:HD22	2.55	0.41
1:D:51:MET:CE	1:D:353:ASN:HB3	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:230:ALA:O	1:B:231:PRO:C	2.60	0.40
1:A:142:ASP:O	1:A:148:SER:HB3	2.21	0.40
1:D:282:HIS:NE2	3:D:1474:SO4:S	2.86	0.40
1:A:135:VAL:HG12	1:A:136:ASP:N	2.35	0.40
1:C:176:GLU:HA	1:C:199:THR:HG22	2.03	0.40
1:A:156:VAL:HG23	1:A:245:ALA:HB2	2.04	0.40
1:C:387:ASP:HA	1:C:388:PRO:HD3	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:181:ASP:OD2	4:D:1472:MG:MG[2.655]	1.67	0.53

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	464/466 (100%)	421 (91%)	41 (9%)	2 (0%)	43	74
1	B	464/466 (100%)	426 (92%)	35 (8%)	3 (1%)	33	63
1	C	464/466 (100%)	436 (94%)	27 (6%)	1 (0%)	56	84
1	D	464/466 (100%)	432 (93%)	29 (6%)	3 (1%)	33	63
All	All	1856/1864 (100%)	1715 (92%)	132 (7%)	9 (0%)	38	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	SER
1	C	428	GLU
1	D	13	LEU
1	D	31	ALA
1	A	2	LEU
1	B	392	GLY
1	D	34	GLU

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Mol	Chain	Res	Type
1	B	86	GLN
1	A	159	GLY

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	339/339 (100%)	322 (95%)	17 (5%)	34	63
1	B	338/339 (100%)	317 (94%)	21 (6%)	26	51
1	C	338/339 (100%)	327 (97%)	11 (3%)	50	80
1	D	339/339 (100%)	312 (92%)	27 (8%)	17	35
All	All	1354/1356 (100%)	1278 (94%)	76 (6%)	30	56

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	19	GLU
1	A	88	LEU
1	A	101	GLU
1	A	141	GLU
1	A	154	LEU
1	A	222	THR
1	A	274	GLN
1	A	299	ASN
1	A	328	GLU
1	A	329	GLU
1	A	349	LEU
1	A	376	TRP
1	A	415	SER
1	A	431	LEU
1	A	455	ARG
1	A	463	GLN
1	B	1	ARG
1	B	2	LEU
1	B	3	THR

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Mol	Chain	Res	Type
1	B	10	ASP
1	B	84	GLU
1	B	88	LEU
1	B	116	ARG
1	B	132	GLU
1	B	136	ASP
1	B	154	LEU
1	B	196	ARG
1	B	259	THR
1	B	261	LYS
1	B	274	GLN
1	B	299	ASN
1	B	320	TRP
1	B	324	LEU
1	B	374	GLN
1	B	396	ASN
1	B	428	GLU
1	B	438	ASN
1	C	28	VAL
1	C	134	LEU
1	C	154	LEU
1	C	192	GLU
1	C	281	ASP
1	C	299	ASN
1	C	320	TRP
1	C	324	LEU
1	C	394	LEU
1	C	438	ASN
1	C	440	HIS
1	D	1	ARG
1	D	63	LEU
1	D	66	ASP
1	D	81	ARG
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU
1	D	116	ARG
1	D	117	THR
1	D	119	ARG
1	D	154	LEU
1	D	184	LEU
1	D	259	THR

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Mol	Chain	Res	Type
1	D	263	ASP
1	D	274	GLN
1	D	281	ASP
1	D	291	LEU
1	D	298	SER
1	D	299	ASN
1	D	302	HIS
1	D	320	TRP
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	381	PRO
1	D	415	SER
1	D	440	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	344	ASN
1	A	366	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	150	GLN
1	B	247	HIS
1	B	299	ASN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	C	44	GLN
1	C	299	ASN
1	C	302	HIS
1	C	366	GLN
1	C	437	ASN
1	C	440	HIS
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN

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Mol	Chain	Res	Type
1	D	86	GLN
1	D	150	GLN
1	D	299	ASN
1	D	302	HIS
1	D	344	ASN
1	D	437	ASN
1	D	449	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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	$\# Z > 2$
3	SO4	A	1467	-	4,4,4	0.23	0	6,6,6	0.70	0
3	SO4	A	1468	-	4,4,4	0.08	0	6,6,6	0.07	0
3	SO4	A	1469	-	4,4,4	0.23	0	6,6,6	0.34	0
3	SO4	A	1470	-	4,4,4	0.19	0	6,6,6	0.32	0
3	SO4	A	1473	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	A	1474	-	4,4,4	0.18	0	6,6,6	0.31	0
2	HQZ	A	500	1	9,9,10	2.24	5 (55%)	12,13,16	3.35	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	1466	-	4,4,4	0.14	0	6,6,6	0.28	0
3	SO4	B	1467	-	4,4,4	0.08	0	6,6,6	0.31	0
3	SO4	B	1468	-	4,4,4	0.11	0	6,6,6	0.25	0
3	SO4	B	1469	-	4,4,4	0.17	0	6,6,6	0.25	0
3	SO4	B	1470	-	4,4,4	0.28	0	6,6,6	0.38	0
3	SO4	B	1471	-	4,4,4	0.24	0	6,6,6	0.20	0
2	HQZ	B	500	1	9,9,10	2.14	5 (55%)	12,13,16	3.44	5 (41%)
3	SO4	C	1466	-	4,4,4	0.34	0	6,6,6	0.25	0
3	SO4	C	1467	-	4,4,4	0.07	0	6,6,6	0.27	0
3	SO4	C	1468	-	4,4,4	0.20	0	6,6,6	0.60	0
3	SO4	C	1469	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	C	1470	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	C	1471	-	4,4,4	0.12	0	6,6,6	0.16	0
2	HQZ	C	500	1	9,9,10	2.19	4 (44%)	12,13,16	3.29	5 (41%)
3	SO4	D	1467	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	D	1468	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	D	1469	-	4,4,4	0.26	0	6,6,6	0.33	0
3	SO4	D	1470	-	4,4,4	0.11	0	6,6,6	0.45	0
3	SO4	D	1473	-	4,4,4	0.08	0	6,6,6	0.22	0
3	SO4	D	1474	-	4,4,4	0.21	0	6,6,6	0.37	0
2	HQZ	D	500	1	9,9,10	2.13	4 (44%)	12,13,16	3.55	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1467	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1468	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1469	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1470	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1473	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1474	-	-	0/0/0/0	0/0/0/0
2	HQZ	A	500	1	-	0/4/9/11	0/0/0/0
3	SO4	B	1466	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1467	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1468	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1469	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1470	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1471	-	-	0/0/0/0	0/0/0/0
2	HQZ	B	500	1	-	0/4/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	1466	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1467	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1468	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1469	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1470	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1471	-	-	0/0/0/0	0/0/0/0
2	HQZ	C	500	1	-	0/4/9/11	0/0/0/0
3	SO4	D	1467	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1468	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1469	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1470	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1473	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1474	-	-	0/0/0/0	0/0/0/0
2	HQZ	D	500	1	-	0/4/9/11	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HQZ	B-CAK	3.54	1.61	1.57
2	C	500	HQZ	SAP-NAM	-3.26	1.53	1.62
2	C	500	HQZ	OAB-SAP	3.12	1.50	1.43
2	A	500	HQZ	OAB-SAP	2.98	1.50	1.43
2	B	500	HQZ	B-CAK	2.97	1.61	1.57
2	A	500	HQZ	CAL-SAP	-2.94	1.66	1.75
2	B	500	HQZ	SAP-NAM	-2.93	1.54	1.62
2	C	500	HQZ	B-CAK	2.85	1.60	1.57
2	A	500	HQZ	SAP-NAM	-2.74	1.54	1.62
2	D	500	HQZ	CAL-SAP	-2.72	1.67	1.75
2	A	500	HQZ	B-CAK	2.69	1.60	1.57
2	A	500	HQZ	OAA-SAP	2.56	1.49	1.43
2	D	500	HQZ	OAB-SAP	2.55	1.49	1.43
2	B	500	HQZ	CAL-SAP	-2.53	1.67	1.75
2	B	500	HQZ	OAB-SAP	2.50	1.49	1.43
2	D	500	HQZ	SAP-NAM	-2.46	1.55	1.62
2	C	500	HQZ	CAL-SAP	-2.45	1.67	1.75
2	B	500	HQZ	OAA-SAP	2.34	1.48	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HQZ	OAB-SAP-OAA	-8.26	104.83	118.74
2	D	500	HQZ	OAB-SAP-OAA	-8.06	105.17	118.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HQZ	OAB-SAP-OAA	-7.86	105.51	118.74
2	A	500	HQZ	OAD-B-CAK	-6.73	106.88	121.13
2	A	500	HQZ	OAB-SAP-OAA	-6.39	107.98	118.74
2	B	500	HQZ	OAD-B-CAK	-6.34	107.69	121.13
2	D	500	HQZ	OAC-B-CAK	-5.98	108.46	121.13
2	A	500	HQZ	OAC-B-CAK	-5.67	109.11	121.13
2	C	500	HQZ	OAC-B-CAK	-5.46	109.57	121.13
2	C	500	HQZ	OAD-B-CAK	-4.71	111.16	121.13
2	D	500	HQZ	OAD-B-CAK	-4.23	112.16	121.13
2	D	500	HQZ	OAB-SAP-NAM	3.90	114.69	107.41
2	B	500	HQZ	OAC-B-CAK	-3.64	113.42	121.13
2	A	500	HQZ	OAB-SAP-NAM	3.57	114.08	107.41
2	D	500	HQZ	OAA-SAP-CAL	3.28	114.70	108.44
2	B	500	HQZ	OAA-SAP-NAM	2.83	112.70	107.41
2	C	500	HQZ	OAB-SAP-CAL	2.43	113.07	108.44
2	C	500	HQZ	OAB-SAP-NAM	2.17	111.46	107.41
2	B	500	HQZ	OAB-SAP-CAL	2.08	112.41	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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	466/466 (100%)	0.61	38 (8%)	12 12	38, 55, 73, 87	0
1	B	466/466 (100%)	0.34	26 (5%)	24 24	38, 56, 78, 91	0
1	C	466/466 (100%)	0.12	22 (4%)	30 32	26, 48, 72, 90	0
1	D	466/466 (100%)	-0.10	6 (1%)	74 78	18, 34, 55, 78	0
All	All	1864/1864 (100%)	0.24	92 (4%)	28 30	18, 51, 73, 91	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	6.4
1	A	108	ALA	6.1
1	B	317	ALA	4.6
1	B	464	ALA	4.6
1	A	71	THR	4.6
1	C	465	PRO	4.4
1	B	81	ARG	4.4
1	A	282	HIS	4.3
1	A	116	ARG	4.3
1	A	78	ALA	4.3
1	B	439	GLY	4.2
1	C	466	GLU	4.2
1	A	81	ARG	4.0
1	B	465	PRO	3.8
1	B	118	VAL	3.8
1	C	2	LEU	3.7
1	A	111	ALA	3.6
1	B	271	ALA	3.5
1	B	441	SER	3.5
1	A	280	ALA	3.5
1	A	198	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	259	THR	3.5
1	A	82	ARG	3.4
1	C	1	ARG	3.3
1	C	81	ARG	3.3
1	C	119	ARG	3.3
1	A	79	PRO	3.2
1	C	117	THR	3.2
1	B	261	LYS	3.1
1	B	262	GLY	3.1
1	B	402	ALA	3.0
1	B	7	GLU	3.0
1	A	260	VAL	3.0
1	A	18	LEU	3.0
1	A	465	PRO	3.0
1	A	2	LEU	2.9
1	A	117	THR	2.9
1	C	257	GLY	2.9
1	C	114	GLY	2.9
1	B	274	GLN	2.9
1	A	112	ALA	2.8
1	A	262	GLY	2.8
1	D	17	ALA	2.7
1	C	439	GLY	2.7
1	A	80	GLY	2.7
1	C	82	ARG	2.7
1	A	439	GLY	2.7
1	B	427	PRO	2.7
1	C	259	THR	2.7
1	A	110	VAL	2.6
1	C	18	LEU	2.6
1	C	84	GLU	2.6
1	D	260	VAL	2.6
1	D	257	GLY	2.5
1	B	82	ARG	2.5
1	C	272	ASP	2.5
1	A	269	VAL	2.5
1	A	295	MET	2.5
1	B	120	GLY	2.5
1	B	119	ARG	2.4
1	A	73	VAL	2.4
1	B	257	GLY	2.4
1	B	34	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	190	TYR	2.3
1	C	116	ARG	2.3
1	A	84	GLU	2.3
1	B	20	GLY	2.3
1	A	32	THR	2.3
1	A	264	VAL	2.3
1	A	120	GLY	2.3
1	D	440	HIS	2.2
1	A	421	SER	2.2
1	B	1	ARG	2.2
1	C	463	GLN	2.2
1	A	22	VAL	2.2
1	C	118	VAL	2.2
1	C	115	VAL	2.2
1	B	429	GLY	2.1
1	C	4	GLU	2.1
1	D	116	ARG	2.1
1	B	315	ALA	2.1
1	A	77	SER	2.1
1	B	374	GLN	2.1
1	D	119	ARG	2.1
1	C	11	ALA	2.1
1	A	271	ALA	2.0
1	B	463	GLN	2.0
1	A	104	ASP	2.0
1	B	303	ALA	2.0
1	A	42	GLY	2.0
1	C	83	GLY	2.0
1	A	253	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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	D	1472	1/1	0.26	4.33	2,2,2,2	0
3	SO4	A	1469	5/5	0.28	3.38	121,122,122,122	0
3	SO4	D	1470	5/5	0.16	2.11	77,78,79,79	0
4	MG	D	1471	1/1	0.18	1.94	10,10,10,10	0
3	SO4	C	1471	5/5	0.19	1.48	84,85,86,86	0
3	SO4	D	1469	5/5	0.15	1.32	63,63,64,65	0
3	SO4	B	1466	5/5	0.26	0.96	74,76,77,77	0
3	SO4	A	1470	5/5	0.18	0.66	109,109,110,111	0
3	SO4	A	1468	5/5	0.19	0.57	114,114,114,115	0
4	MG	A	1472	1/1	0.20	0.53	36,36,36,36	0
3	SO4	A	1473	5/5	0.22	0.37	100,101,101,102	0
3	SO4	B	1468	5/5	0.20	0.08	59,59,62,63	0
4	MG	A	1471	1/1	0.20	-0.04	33,33,33,33	0
3	SO4	B	1470	5/5	0.17	-0.05	79,79,80,81	0
3	SO4	B	1469	5/5	0.17	-0.34	99,99,100,100	0
3	SO4	D	1473	5/5	0.14	-0.53	78,78,78,79	0
2	HQZ	D	500	10/11	0.16	-0.54	21,25,25,29	0
2	HQZ	A	500	10/11	0.18	-0.55	39,41,43,47	0
2	HQZ	C	500	10/11	0.14	-0.80	34,37,38,39	0
3	SO4	A	1467	5/5	0.26	-0.86	61,62,62,62	0
3	SO4	A	1474	5/5	0.13	-0.97	88,88,89,89	0
3	SO4	C	1468	5/5	0.11	-1.04	51,52,53,54	0
3	SO4	B	1471	5/5	0.13	-1.45	108,108,108,108	0
3	SO4	D	1474	5/5	0.12	-1.51	61,63,64,65	0
3	SO4	C	1470	5/5	0.09	-1.70	61,61,62,63	0
2	HQZ	B	500	10/11	0.17	-1.74	42,46,49,50	0
3	SO4	D	1467	5/5	0.09	-1.95	48,48,51,51	0
3	SO4	C	1469	5/5	0.10	-2.48	73,74,75,75	0
3	SO4	C	1467	5/5	0.07	-2.61	59,61,63,64	0
3	SO4	C	1466	5/5	0.09	-2.79	65,66,67,68	0
3	SO4	B	1467	5/5	0.09	-3.08	70,71,72,72	0
3	SO4	D	1468	5/5	0.07	-3.94	61,61,61,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.