



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:17 AM UTC

PDB ID : 4B4Z / pdb_00004b4z
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 : 2012-08-02
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

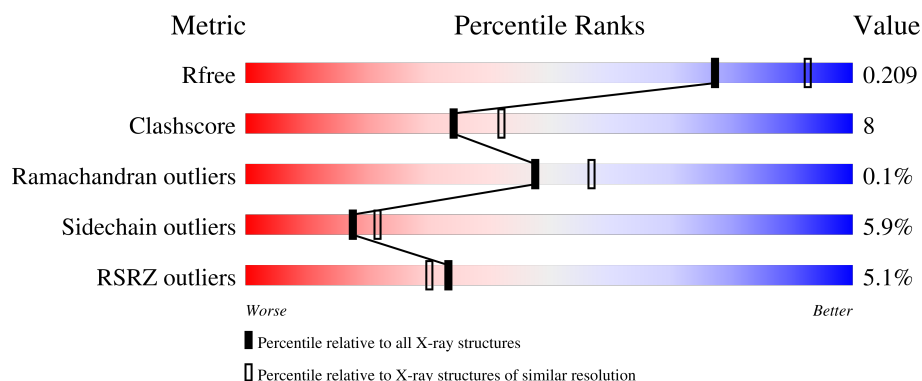
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	466	2% 85% 13% .
1	B	466	2% 84% 15% .
1	C	466	% 86% 13% .
1	D	466	15% 81% 16% ..

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
4	SO4	A	1473	-	-	X	-
4	SO4	B	1472	-	-	X	-
4	SO4	C	1472	-	-	X	-
4	SO4	D	1471	-	-	X	-

2 Entry composition [i](#)

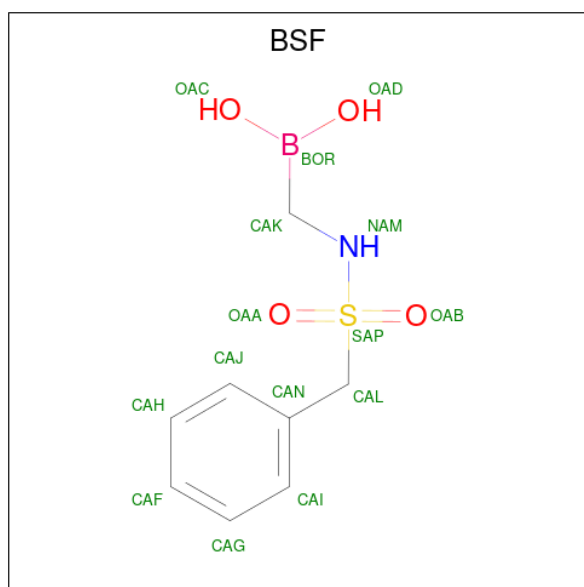
There are 5 unique types of molecules in this entry. The entry contains 14610 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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	461	Total	C	N	O	S	0	0	0
			3310	2049	556	699	6			

- Molecule 2 is {[(benzylsulfonyl)amino]methyl}boronic acid (CCD ID: BSF) (formula: C₈H₁₂BNO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		
2	B	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		

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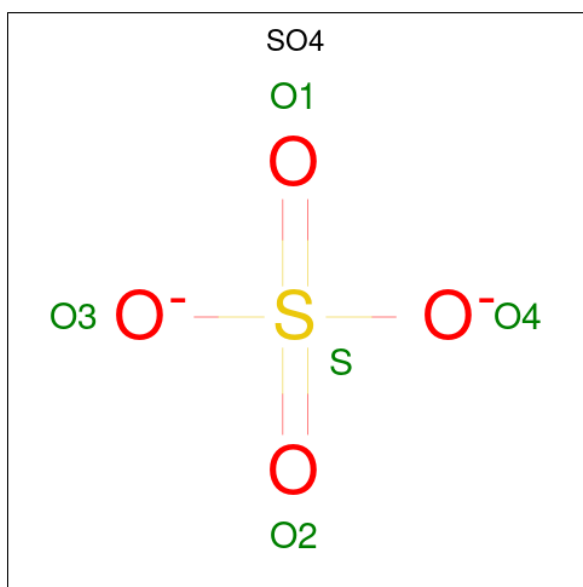
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		
2	D	1	Total	B	C	N	O	S	0	0
			13	1	8	1	2	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

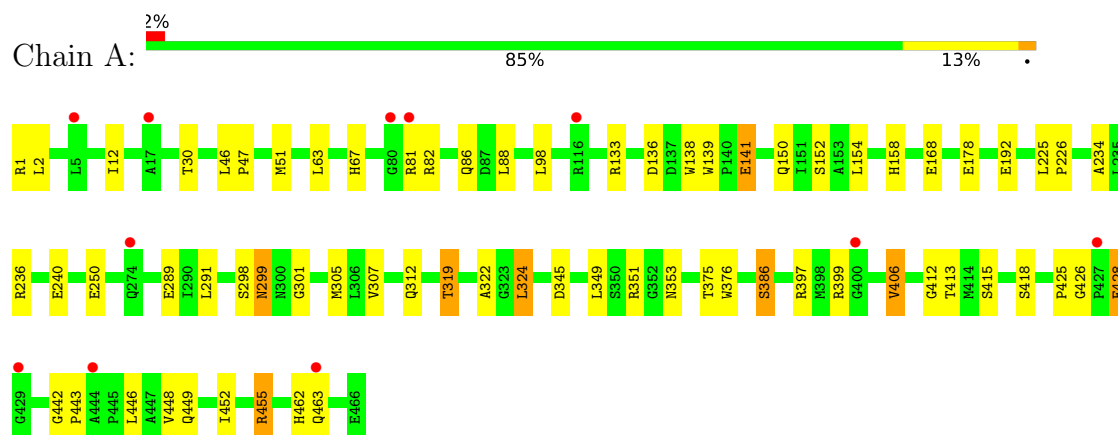
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	288	Total 288	O 288	0	0
5	B	279	Total 279	O 279	0	0
5	C	298	Total 298	O 298	0	0
5	D	208	Total 208	O 208	0	0

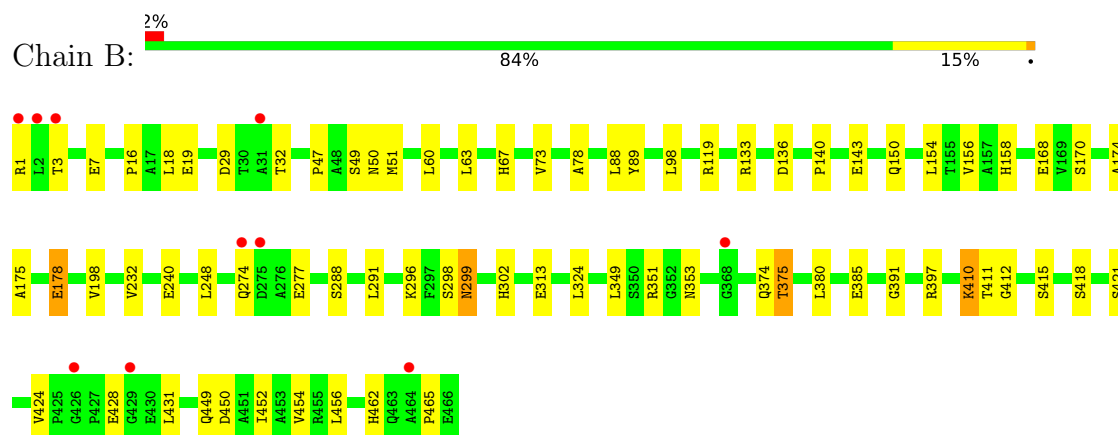
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

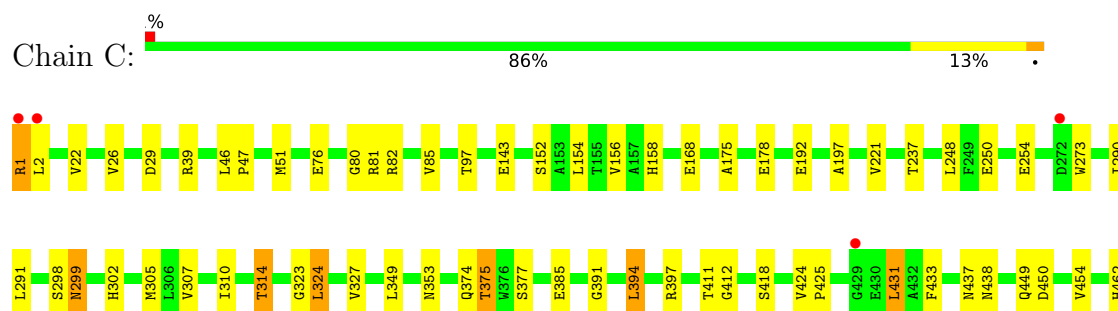
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



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

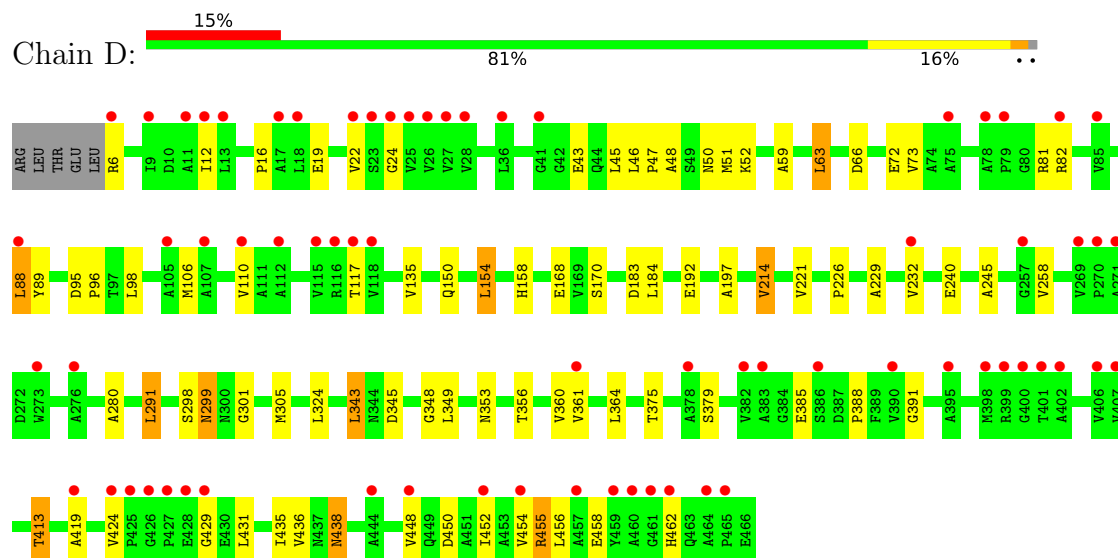


• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.12Å 90.69Å 105.73Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	35.25 – 2.20 35.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.25-2.20) 99.2 (35.25-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.260 0.206 , 0.209	Depositor DCC
R_{free} test set	4888 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14610	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: MG, BSF, 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	0.58	0/3412	0.83	0/4666
1	B	0.57	1/3403 (0.0%)	0.81	0/4656
1	C	0.60	1/3403 (0.0%)	0.82	0/4656
1	D	0.56	0/3369	0.85	1/4608 (0.0%)
All	All	0.58	2/13587 (0.0%)	0.83	1/18586 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	465	PRO	C-N	-6.80	1.23	1.33
1	B	465	PRO	C-N	-6.41	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	VAL	CB-CA-C	-6.02	101.57	111.51

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	3353	0	3199	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3344	0	3193	53	0
1	C	3344	0	3193	43	0
1	D	3310	0	3148	60	0
2	A	13	0	10	2	0
2	B	13	0	10	3	0
2	C	13	0	10	1	0
2	D	13	0	10	3	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	35	0	0	3	0
4	B	35	0	0	6	0
4	C	35	0	0	8	0
4	D	25	0	0	5	0
5	A	288	0	0	4	0
5	B	279	0	0	4	0
5	C	298	0	0	2	0
5	D	208	0	0	9	1
All	All	14610	0	12773	200	1

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 8.

All (200) 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:168:GLU:OE2	4:B:1472:SO4:S	2.02	1.17
1:C:168:GLU:OE2	4:C:1472:SO4:S	2.04	1.14
1:D:24:GLY:O	5:D:2004:HOH:O	1.66	1.10
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.37	1.05
1:C:158:HIS:NE2	4:C:1472:SO4:S	2.38	0.95
1:B:288:SER:HB2	1:B:375:THR:HG21	1.52	0.91
1:B:168:GLU:OE2	4:B:1472:SO4:O2	1.87	0.91
1:C:51:MET:HE3	1:C:353:ASN:HB3	1.55	0.86
1:C:47:PRO:HG3	1:C:51:MET:CE	2.05	0.86
1:B:168:GLU:OE2	4:B:1472:SO4:O3	1.93	0.85
1:A:150:GLN:HE22	1:A:240:GLU:H	1.26	0.84
1:A:47:PRO:HG3	1:A:51:MET:HE2	1.59	0.83
1:D:47:PRO:HG3	1:D:51:MET:HE2	1.61	0.82
1:C:158:HIS:NE2	4:C:1472:SO4:O3	2.14	0.80
1:A:319:THR:HG22	1:A:322:ALA:H	1.45	0.80
1:B:158:HIS:NE2	4:B:1472:SO4:S	2.52	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLU:OE2	4:C:1472:SO4:O3	2.00	0.78
1:B:47:PRO:HG3	1:B:51:MET:HE2	1.65	0.78
1:C:168:GLU:OE2	4:C:1472:SO4:O2	2.01	0.78
1:B:462:HIS:ND1	5:B:2268:HOH:O	2.15	0.78
1:D:50:ASN:ND2	1:D:419:ALA:HB1	2.02	0.75
1:B:150:GLN:HE22	1:B:240:GLU:H	1.35	0.73
1:C:397:ARG:HH22	1:C:449:GLN:HE21	1.37	0.73
1:D:375:THR:HG23	5:D:2174:HOH:O	1.89	0.72
1:A:150:GLN:NE2	1:A:240:GLU:H	1.87	0.71
1:A:158:HIS:NE2	4:A:1473:SO4:O1	2.23	0.70
1:B:158:HIS:NE2	4:B:1472:SO4:O3	2.23	0.69
1:B:49:SER:CB	2:B:500:BSF:CAK	2.70	0.68
1:D:298:SER:CB	2:D:500:BSF:CAK	2.73	0.67
1:D:435:ILE:HA	5:D:2004:HOH:O	1.94	0.66
1:D:73:VAL:O	5:D:2033:HOH:O	2.14	0.66
1:C:307:VAL:HG11	1:C:324:LEU:HD13	1.78	0.65
1:B:175:ALA:O	1:B:178:GLU:HG2	1.97	0.65
1:A:406:VAL:HG21	1:A:462:HIS:CE1	2.31	0.65
1:D:72:GLU:OE2	5:D:2032:HOH:O	2.15	0.64
1:D:291:LEU:HD12	1:D:379:SER:CB	2.28	0.64
1:B:150:GLN:NE2	1:B:240:GLU:H	1.94	0.64
1:A:298:SER:CB	2:A:500:BSF:CAK	2.75	0.63
1:B:51:MET:CE	1:B:353:ASN:HB3	2.27	0.63
1:C:197:ALA:HB2	1:C:221:VAL:HG12	1.80	0.63
1:C:310:ILE:O	1:C:314:THR:HB	1.99	0.62
1:D:16:PRO:O	1:D:19:GLU:HG2	2.00	0.62
1:A:136:ASP:HB3	5:A:2106:HOH:O	1.99	0.61
1:A:51:MET:HE3	1:A:353:ASN:HB3	1.83	0.61
1:A:158:HIS:CE1	4:A:1473:SO4:O1	2.53	0.61
1:D:388:PRO:HA	5:D:2180:HOH:O	2.01	0.61
1:C:47:PRO:CG	1:C:51:MET:HE2	2.21	0.60
1:D:150:GLN:HE22	1:D:240:GLU:H	1.47	0.60
1:D:150:GLN:NE2	1:D:240:GLU:H	1.98	0.60
1:B:299:ASN:HD22	1:B:302:HIS:H	1.50	0.60
1:B:397:ARG:HH22	1:B:449:GLN:HE21	1.50	0.59
1:B:351:ARG:NH2	1:B:415:SER:O	2.32	0.59
1:A:351:ARG:NH2	1:A:415:SER:O	2.31	0.59
1:B:49:SER:CB	2:B:500:BSF:HAK	2.33	0.59
1:C:158:HIS:NE2	4:C:1472:SO4:O2	2.34	0.59
1:A:397:ARG:HH22	1:A:449:GLN:HE21	1.51	0.58
1:C:51:MET:HE3	1:C:353:ASN:CB	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:CG	1:A:51:MET:HE2	2.32	0.58
1:C:152:SER:O	1:C:305:MET:HE3	2.03	0.58
1:A:51:MET:CE	1:A:353:ASN:HB3	2.34	0.58
1:D:226:PRO:HG2	1:D:229:ALA:HB2	1.87	0.57
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.86	0.56
1:A:51:MET:HE3	1:A:353:ASN:CG	2.31	0.55
1:B:49:SER:HB3	2:B:500:BSF:HAK	1.88	0.55
1:D:298:SER:CB	2:D:500:BSF:HAKA	2.36	0.55
1:C:51:MET:CE	1:C:353:ASN:HB3	2.34	0.55
1:B:136:ASP:OD2	5:B:2097:HOH:O	2.18	0.54
1:A:307:VAL:HG11	1:A:324:LEU:HD13	1.90	0.54
1:B:299:ASN:ND2	1:B:302:HIS:H	2.05	0.54
1:D:158:HIS:HE1	4:D:1471:SO4:O4	1.90	0.54
1:C:158:HIS:CE1	4:C:1472:SO4:O3	2.60	0.54
1:A:141:GLU:H	1:A:141:GLU:CD	2.15	0.54
1:D:158:HIS:CE1	4:D:1471:SO4:O4	2.60	0.54
1:C:397:ARG:NH2	1:C:449:GLN:HE21	2.05	0.53
1:D:45:LEU:HD22	1:D:438:ASN:HB2	1.90	0.53
1:B:410:LYS:HE3	5:B:2200:HOH:O	2.08	0.53
1:C:298:SER:CB	2:C:500:BSF:CAK	2.87	0.53
1:B:410:LYS:HE2	1:B:411:THR:O	2.09	0.52
1:C:397:ARG:HH22	1:C:449:GLN:NE2	2.06	0.52
1:A:168:GLU:OE2	4:A:1473:SO4:O2	2.28	0.52
1:A:386:SER:HA	1:A:399:ARG:NH2	2.25	0.52
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.91	0.51
1:D:291:LEU:HD12	1:D:379:SER:HB2	1.91	0.51
1:D:48:ALA:O	1:D:348:GLY:HA3	2.11	0.51
1:D:73:VAL:CG1	1:D:88:LEU:HD11	2.40	0.51
1:D:106:MET:O	1:D:110:VAL:HG23	2.11	0.51
1:D:436:VAL:N	5:D:2004:HOH:O	2.28	0.51
1:B:397:ARG:NH2	1:B:449:GLN:HE21	2.09	0.50
1:A:299:ASN:C	1:A:299:ASN:HD22	2.18	0.50
1:A:63:LEU:O	1:A:67:HIS:HB2	2.12	0.50
1:C:323:GLY:O	1:C:327:VAL:HG23	2.12	0.50
1:C:394:LEU:HD13	1:C:411:THR:CG2	2.41	0.50
1:A:51:MET:HE3	1:A:353:ASN:CB	2.41	0.49
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.93	0.49
1:D:301:GLY:O	1:D:305:MET:HG3	2.13	0.49
1:D:12:ILE:HG22	1:D:448:VAL:HG13	1.94	0.49
1:C:168:GLU:OE2	4:C:1472:SO4:O1	2.30	0.48
1:A:289:GLU:HG2	5:A:2215:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLY:C	1:A:428:GLU:N	2.70	0.48
1:D:6:ARG:HH11	1:D:6:ARG:HA	1.79	0.48
1:D:158:HIS:HD2	5:D:2103:HOH:O	1.95	0.48
1:D:168:GLU:OE2	4:D:1471:SO4:O3	2.31	0.48
1:D:455:ARG:HH12	1:D:458:GLU:HB2	1.79	0.48
1:A:406:VAL:HG13	1:A:425:PRO:HD2	1.96	0.48
1:B:1:ARG:NH1	1:D:429:GLY:O	2.46	0.48
1:D:22:VAL:HG11	1:D:43:GLU:HG2	1.96	0.48
1:B:51:MET:HE3	1:B:353:ASN:CG	2.38	0.48
1:B:78:ALA:HA	1:B:277:GLU:HG2	1.95	0.47
1:B:158:HIS:NE2	4:B:1472:SO4:O2	2.46	0.47
1:D:413:THR:HG23	2:D:500:BSF:OAA	2.13	0.47
1:A:133:ARG:HB3	1:A:150:GLN:HG2	1.96	0.47
1:B:133:ARG:HB3	1:B:150:GLN:HB3	1.95	0.47
1:D:6:ARG:HH22	1:D:455:ARG:HH21	1.60	0.47
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.97	0.47
1:B:63:LEU:O	1:B:67:HIS:HB2	2.15	0.47
1:B:29:ASP:HB3	1:B:32:THR:OG1	2.14	0.47
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.80	0.47
1:D:158:HIS:CE1	4:D:1471:SO4:S	3.08	0.47
1:A:386:SER:HA	1:A:399:ARG:HH21	1.79	0.47
1:A:1:ARG:HH22	1:A:455:ARG:NH2	2.14	0.46
1:A:298:SER:CB	2:A:500:BSF:HAKA	2.45	0.46
1:D:424:VAL:HB	1:D:431:LEU:HB2	1.98	0.46
1:A:86:GLN:HB3	5:A:2058:HOH:O	2.15	0.46
1:C:80:GLY:O	1:C:82:ARG:N	2.47	0.46
1:D:299:ASN:C	1:D:299:ASN:HD22	2.23	0.46
1:A:301:GLY:O	1:A:305:MET:HG3	2.16	0.46
1:D:343:LEU:HD23	1:D:343:LEU:N	2.30	0.46
1:D:385:GLU:O	1:D:391:GLY:HA3	2.15	0.46
1:B:19:GLU:OE2	5:B:2004:HOH:O	2.21	0.46
1:C:156:VAL:HG21	1:C:248:LEU:HD12	1.98	0.46
1:D:452:ILE:O	1:D:456:LEU:HG	2.15	0.46
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.98	0.46
1:C:450:ASP:O	1:C:454:VAL:HG23	2.17	0.45
1:C:425:PRO:O	1:C:462:HIS:NE2	2.46	0.45
1:A:12:ILE:HG21	1:A:452:ILE:HG13	1.99	0.45
1:B:385:GLU:O	1:B:391:GLY:HA3	2.16	0.45
1:B:450:ASP:O	1:B:454:VAL:HG23	2.16	0.45
1:C:462:HIS:HE1	5:C:2281:HOH:O	2.00	0.45
1:D:59:ALA:O	1:D:63:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:THR:O	1:D:360:VAL:HG23	2.16	0.45
1:D:458:GLU:HA	1:D:462:HIS:O	2.17	0.45
1:C:175:ALA:O	1:C:178:GLU:HB2	2.17	0.45
1:B:140:PRO:HA	1:B:143:GLU:OE2	2.17	0.44
1:D:135:VAL:HG21	1:D:345:ASP:HB3	2.00	0.44
1:D:280:ALA:O	5:D:2033:HOH:O	2.21	0.44
1:C:39:ARG:NH1	5:C:2003:HOH:O	2.42	0.44
1:D:158:HIS:NE2	4:D:1471:SO4:O3	2.44	0.44
1:D:47:PRO:CG	1:D:51:MET:HE2	2.42	0.44
1:B:170:SER:HA	1:B:232:VAL:O	2.17	0.44
1:A:81:ARG:HD3	1:B:313:GLU:OE2	2.17	0.44
1:B:298:SER:HB2	1:B:410:LYS:NZ	2.29	0.44
1:D:51:MET:HE3	1:D:353:ASN:HB3	1.98	0.44
1:B:412:GLY:O	1:B:418:SER:HA	2.17	0.44
1:C:299:ASN:HD22	1:C:302:HIS:H	1.66	0.44
1:A:152:SER:O	1:A:305:MET:HE3	2.18	0.43
1:B:288:SER:CB	1:B:375:THR:HG21	2.35	0.43
1:C:374:GLN:NE2	1:C:375:THR:HG22	2.33	0.43
1:C:97:THR:HG21	1:C:290:ILE:HG12	1.99	0.43
1:D:450:ASP:O	1:D:454:VAL:HG23	2.18	0.43
1:A:234:ALA:HB1	1:A:236:ARG:NH1	2.33	0.43
1:B:60:LEU:HD11	1:B:291:LEU:HD11	1.99	0.43
1:B:51:MET:HE3	1:B:353:ASN:HB3	1.99	0.43
1:B:298:SER:CB	1:B:410:LYS:HZ2	2.29	0.43
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.67	0.43
1:A:1:ARG:HH12	1:A:455:ARG:HH22	1.67	0.43
1:C:26:VAL:O	1:C:433:PHE:HA	2.19	0.43
1:C:76:GLU:HG3	1:C:273:TRP:CD1	2.53	0.43
1:D:343:LEU:HD23	1:D:343:LEU:H	1.83	0.43
1:C:29:ASP:HA	1:C:431:LEU:HD12	2.01	0.43
1:D:50:ASN:HD21	1:D:419:ALA:HB1	1.83	0.43
1:D:455:ARG:NH1	1:D:458:GLU:HB2	2.34	0.43
1:B:51:MET:HE2	1:B:353:ASN:HB3	2.00	0.42
1:A:138:TRP:HB3	5:A:2111:HOH:O	2.19	0.42
1:B:175:ALA:H	1:B:178:GLU:HG3	1.84	0.42
1:A:397:ARG:NH1	1:A:446:LEU:HD22	2.34	0.42
1:D:52:LYS:HE2	1:D:298:SER:C	2.45	0.42
1:D:170:SER:HB2	1:D:183:ASP:HB3	2.02	0.42
1:A:412:GLY:O	1:A:418:SER:HA	2.20	0.42
1:C:437:ASN:C	1:C:438:ASN:HD22	2.27	0.42
1:B:51:MET:HE3	1:B:353:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:ND2	1:B:421:SER:OG	2.53	0.41
1:B:73:VAL:HA	1:B:89:TYR:O	2.19	0.41
1:D:73:VAL:CG1	1:D:88:LEU:CD1	2.98	0.41
1:A:397:ARG:HH22	1:A:449:GLN:NE2	2.15	0.41
1:B:156:VAL:HG21	1:B:248:LEU:HD12	2.02	0.41
1:B:452:ILE:O	1:B:456:LEU:HG	2.20	0.41
1:B:296:LYS:NZ	1:B:380:LEU:O	2.53	0.41
1:C:143:GLU:O	1:C:237:THR:OG1	2.36	0.41
1:A:139:TRP:HB3	1:A:141:GLU:OE2	2.21	0.41
1:B:16:PRO:HA	1:B:19:GLU:HG2	2.03	0.41
1:C:385:GLU:O	1:C:391:GLY:HA3	2.21	0.41
1:C:412:GLY:O	1:C:418:SER:HA	2.20	0.41
1:D:361:VAL:HA	1:D:364:LEU:HD12	2.02	0.41
1:C:1:ARG:HD3	1:C:2:LEU:H	1.86	0.40
1:D:73:VAL:HA	1:D:89:TYR:O	2.22	0.40
1:D:154:LEU:HD13	1:D:245:ALA:HB3	2.04	0.40
1:D:95:ASP:HA	1:D:96:PRO:HD3	1.95	0.40
1:A:345:ASP:OD1	1:A:345:ASP:C	2.64	0.40
1:A:442:GLY:HA3	1:A:443:PRO:HD2	1.89	0.40
1:D:170:SER:HA	1:D:232:VAL:O	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
5:D:2197:HOH:O	5:D:2321:HOH:O[2_645]	2.06	0.14

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%)	450 (97%)	14 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	464/466 (100%)	449 (97%)	14 (3%)	1 (0%)	43	51
1	C	464/466 (100%)	450 (97%)	13 (3%)	1 (0%)	43	51
1	D	459/466 (98%)	440 (96%)	19 (4%)	0	100	100
All	All	1851/1864 (99%)	1789 (97%)	60 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	ARG
1	B	174	ALA

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%)	314 (93%)	25 (7%)	13	14
1	B	338/339 (100%)	322 (95%)	16 (5%)	23	31
1	C	338/339 (100%)	321 (95%)	17 (5%)	22	28
1	D	334/339 (98%)	313 (94%)	21 (6%)	16	19
All	All	1349/1356 (100%)	1270 (94%)	79 (6%)	18	22

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	30	THR
1	A	46	LEU
1	A	82	ARG
1	A	88	LEU
1	A	98	LEU
1	A	141	GLU
1	A	154	LEU
1	A	178	GLU

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Mol	Chain	Res	Type
1	A	192	GLU
1	A	250	GLU
1	A	291	LEU
1	A	299	ASN
1	A	312	GLN
1	A	319	THR
1	A	324	LEU
1	A	349	LEU
1	A	375	THR
1	A	376	TRP
1	A	386	SER
1	A	406	VAL
1	A	413	THR
1	A	428	GLU
1	A	455	ARG
1	A	463	GLN
1	B	3	THR
1	B	7	GLU
1	B	18	LEU
1	B	88	LEU
1	B	98	LEU
1	B	154	LEU
1	B	178	GLU
1	B	198	VAL
1	B	274	GLN
1	B	299	ASN
1	B	324	LEU
1	B	349	LEU
1	B	374	GLN
1	B	375	THR
1	B	410	LYS
1	B	428	GLU
1	C	1	ARG
1	C	22	VAL
1	C	46	LEU
1	C	85	VAL
1	C	154	LEU
1	C	192	GLU
1	C	250	GLU
1	C	254	GLU
1	C	291	LEU
1	C	299	ASN

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Mol	Chain	Res	Type
1	C	314	THR
1	C	324	LEU
1	C	349	LEU
1	C	375	THR
1	C	377	SER
1	C	394	LEU
1	C	431	LEU
1	D	46	LEU
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	117	THR
1	D	154	LEU
1	D	184	LEU
1	D	192	GLU
1	D	214	VAL
1	D	258	VAL
1	D	291	LEU
1	D	299	ASN
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	413	THR
1	D	438	ASN
1	D	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	50	ASN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	366	GLN
1	A	396	ASN
1	A	437	ASN
1	A	449	GLN
1	A	462	HIS

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Mol	Chain	Res	Type
1	A	463	GLN
1	B	44	GLN
1	B	50	ASN
1	B	150	GLN
1	B	299	ASN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	50	ASN
1	C	299	ASN
1	C	366	GLN
1	C	437	ASN
1	C	449	GLN
1	D	50	ASN
1	D	67	HIS
1	D	150	GLN
1	D	299	ASN
1	D	302	HIS
1	D	366	GLN
1	D	437	ASN
1	D	449	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	1467	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	D	1468	-	4,4,4	0.21	0	6,6,6	0.20	0
2	BSF	D	500	1	11,13,15	0.78	0	15,17,20	2.58	3 (20%)
4	SO4	B	1471	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	D	1469	-	4,4,4	0.31	0	6,6,6	0.20	0
4	SO4	D	1467	-	4,4,4	0.24	0	6,6,6	0.20	0
4	SO4	A	1467	-	4,4,4	0.22	0	6,6,6	0.28	0
4	SO4	A	1469	-	4,4,4	0.27	0	6,6,6	0.31	0
4	SO4	C	1466	-	4,4,4	0.25	0	6,6,6	0.29	0
2	BSF	C	500	1	11,13,15	0.93	0	15,17,20	2.19	2 (13%)
4	SO4	D	1470	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	C	1469	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	C	1470	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	C	1472	-	4,4,4	0.33	0	6,6,6	0.57	0
4	SO4	C	1471	-	4,4,4	0.25	0	6,6,6	0.14	0
4	SO4	A	1470	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	C	1468	-	4,4,4	0.31	0	6,6,6	0.13	0
4	SO4	B	1470	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	B	1466	-	4,4,4	0.26	0	6,6,6	0.26	0
4	SO4	D	1471	-	4,4,4	0.31	0	6,6,6	0.27	0
4	SO4	A	1471	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	B	1467	-	4,4,4	0.23	0	6,6,6	0.20	0
4	SO4	B	1468	-	4,4,4	0.25	0	6,6,6	0.12	0
2	BSF	B	500	1	11,13,15	0.98	0	15,17,20	2.12	1 (6%)
4	SO4	B	1472	-	4,4,4	0.36	0	6,6,6	0.62	0
4	SO4	A	1472	-	4,4,4	0.21	0	6,6,6	0.09	0
4	SO4	A	1473	-	4,4,4	0.67	0	6,6,6	0.37	0
4	SO4	B	1469	-	4,4,4	0.23	0	6,6,6	0.20	0
4	SO4	A	1468	-	4,4,4	0.24	0	6,6,6	0.10	0
2	BSF	A	500	1	11,13,15	0.79	0	15,17,20	1.71	2 (13%)

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	BSF	D	500	1	-	0/8/9/11	0/1/1/1
2	BSF	A	500	1	-	0/8/9/11	0/1/1/1
2	BSF	B	500	1	-	0/8/9/11	0/1/1/1
2	BSF	C	500	1	-	2/8/9/11	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	BSF	OAB-SAP-OAA	-8.60	107.31	119.34
2	C	500	BSF	OAB-SAP-OAA	-7.80	108.43	119.34
2	B	500	BSF	OAB-SAP-OAA	-7.80	108.44	119.34
2	A	500	BSF	OAB-SAP-OAA	-5.47	111.69	119.34
2	D	500	BSF	CAN-CAL-SAP	-3.21	105.91	112.44
2	C	500	BSF	OAA-SAP-CAL	2.24	111.77	108.33
2	A	500	BSF	OAB-SAP-CAL	2.15	111.64	108.33
2	D	500	BSF	CAJ-CAN-CAI	2.12	121.39	118.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	BSF	CAN-CAL-SAP-OAA
2	C	500	BSF	CAN-CAL-SAP-NAM

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	BSF	3	0
2	C	500	BSF	1	0
4	C	1472	SO4	8	0
4	D	1471	SO4	5	0
2	B	500	BSF	3	0
4	B	1472	SO4	6	0
4	A	1473	SO4	3	0
2	A	500	BSF	2	0

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%)	-0.05	11 (2%) 59 56	19, 30, 55, 75	0
1	B	466/466 (100%)	0.06	10 (2%) 63 60	20, 32, 54, 74	0
1	C	466/466 (100%)	-0.16	4 (0%) 81 79	18, 28, 47, 66	0
1	D	461/466 (98%)	0.79	69 (14%) 5 4	20, 40, 69, 81	0
All	All	1859/1864 (99%)	0.16	94 (5%) 33 30	18, 32, 60, 81	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	GLY	4.2
1	D	378	ALA	4.1
1	D	112	ALA	4.0
1	D	41	GLY	3.9
1	D	12	ILE	3.9
1	D	9	ILE	3.8
1	D	425	PRO	3.7
1	D	17	ALA	3.6
1	A	429	GLY	3.6
1	A	427	PRO	3.4
1	D	118	VAL	3.3
1	D	390	VAL	3.3
1	D	448	VAL	3.3
1	D	11	ALA	3.3
1	B	429	GLY	3.2
1	D	407	VAL	3.1
1	D	26	VAL	3.1
1	D	465	PRO	3.1
1	D	105	ALA	3.0
1	D	426	GLY	3.0
1	D	36	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	273	TRP	2.9
1	D	402	ALA	2.9
1	C	429	GLY	2.9
1	D	18	LEU	2.9
1	D	269	VAL	2.8
1	D	6	ARG	2.8
1	D	444	ALA	2.8
1	D	386	SER	2.8
1	B	274	GLN	2.7
1	C	272	ASP	2.7
1	D	22	VAL	2.7
1	D	452	ILE	2.7
1	B	2	LEU	2.7
1	B	464	ALA	2.6
1	B	275	ASP	2.6
1	D	27	VAL	2.6
1	D	276	ALA	2.6
1	D	424	VAL	2.6
1	A	80	GLY	2.6
1	D	406	VAL	2.6
1	D	427	PRO	2.6
1	D	462	HIS	2.6
1	D	28	VAL	2.5
1	A	17	ALA	2.5
1	D	78	ALA	2.5
1	D	454	VAL	2.5
1	D	395	ALA	2.5
1	D	13	LEU	2.5
1	D	461	GLY	2.5
1	C	2	LEU	2.4
1	D	459	TYR	2.4
1	D	79	PRO	2.4
1	A	444	ALA	2.4
1	D	271	ALA	2.4
1	D	464	ALA	2.3
1	D	115	VAL	2.3
1	D	24	GLY	2.3
1	D	429	GLY	2.3
1	D	457	ALA	2.3
1	D	428	GLU	2.3
1	D	75	ALA	2.3
1	D	117	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	460	ALA	2.3
1	D	232	VAL	2.3
1	A	400	GLY	2.2
1	D	398	MET	2.2
1	D	401	THR	2.2
1	A	5	LEU	2.2
1	D	23	SER	2.2
1	D	25	VAL	2.2
1	D	85	VAL	2.2
1	B	3	THR	2.2
1	B	31	ALA	2.2
1	D	82	ARG	2.2
1	D	270	PRO	2.2
1	B	368	GLY	2.2
1	D	107	ALA	2.2
1	D	361	VAL	2.1
1	D	116	ARG	2.1
1	A	274	GLN	2.1
1	A	463	GLN	2.1
1	B	1	ARG	2.1
1	D	399	ARG	2.1
1	D	382	VAL	2.1
1	D	257	GLY	2.1
1	A	81	ARG	2.1
1	D	110	VAL	2.1
1	B	426	GLY	2.1
1	D	383	ALA	2.0
1	D	88	LEU	2.0
1	C	1	ARG	2.0
1	D	419	ALA	2.0
1	A	116	ARG	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	1471	5/5	0.39	0.20	74,76,76,76	0
4	SO4	A	1473	5/5	0.49	0.17	84,85,86,86	0
4	SO4	D	1470	5/5	0.51	0.22	119,119,119,119	0
4	SO4	A	1472	5/5	0.65	0.13	98,98,98,98	0
4	SO4	C	1469	5/5	0.65	0.18	99,100,100,100	0
4	SO4	D	1467	5/5	0.67	0.15	78,79,79,79	0
4	SO4	A	1470	5/5	0.73	0.19	110,111,111,111	0
4	SO4	B	1469	5/5	0.73	0.16	84,84,85,85	0
4	SO4	B	1471	5/5	0.75	0.14	80,81,81,81	0
4	SO4	A	1471	5/5	0.80	0.09	94,94,94,94	0
4	SO4	B	1470	5/5	0.82	0.10	82,82,83,83	0
3	MG	A	611	1/1	0.83	0.13	54,54,54,54	0
4	SO4	C	1471	5/5	0.85	0.17	88,88,88,88	0
4	SO4	A	1468	5/5	0.88	0.10	76,76,76,76	0
4	SO4	D	1468	5/5	0.88	0.10	67,68,68,68	0
2	BSF	D	500	13/15	0.90	0.12	36,41,43,44	0
2	BSF	A	500	13/15	0.90	0.13	30,44,46,47	0
4	SO4	B	1466	5/5	0.91	0.12	53,53,53,54	0
4	SO4	B	1472	5/5	0.92	0.12	31,34,36,37	0
4	SO4	B	1467	5/5	0.92	0.09	64,64,64,64	0
4	SO4	C	1470	5/5	0.92	0.16	55,56,57,57	0
3	MG	D	610	1/1	0.92	0.09	40,40,40,40	0
3	MG	A	610	1/1	0.93	0.06	37,37,37,37	0
4	SO4	C	1467	5/5	0.94	0.08	59,59,60,60	0
4	SO4	A	1469	5/5	0.94	0.15	48,49,51,51	0
2	BSF	B	500	13/15	0.95	0.10	25,29,40,40	0
4	SO4	A	1467	5/5	0.96	0.09	37,38,38,39	0
4	SO4	C	1472	5/5	0.96	0.09	33,35,37,38	0
3	MG	D	611	1/1	0.96	0.11	42,42,42,42	0
4	SO4	B	1468	5/5	0.97	0.12	38,39,39,40	0
4	SO4	C	1466	5/5	0.97	0.07	40,40,42,42	0
4	SO4	D	1469	5/5	0.97	0.10	35,35,37,38	0
2	BSF	C	500	13/15	0.97	0.09	21,25,39,39	0
4	SO4	C	1468	5/5	0.97	0.11	36,38,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.