



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:25 PM UTC

PDB ID : 4B4X / pdb_00004b4x
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 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

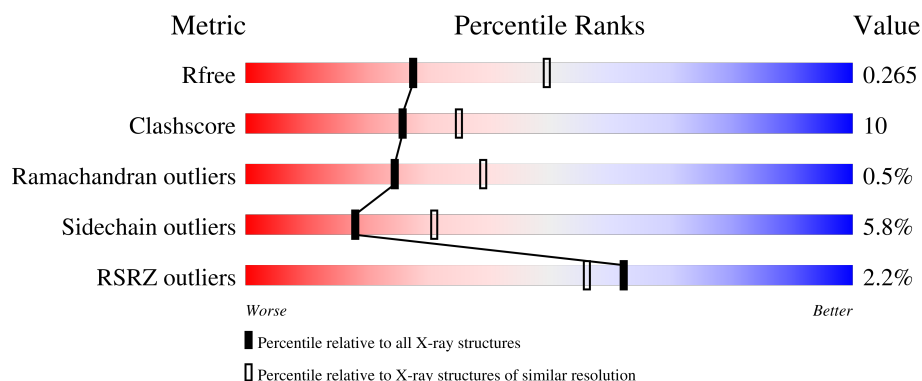
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	4% 70% 28% .
1	B	466	3% 74% 24% .
1	C	466	2% 79% 19% .
1	D	466	% 82% 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
3	SO4	A	1470	-	-	X	-
3	SO4	B	1470	-	-	X	-
3	SO4	C	1466	-	-	X	-
3	SO4	D	1470	-	-	X	-
3	SO4	D	1474	-	-	X	-

2 Entry composition [i](#)

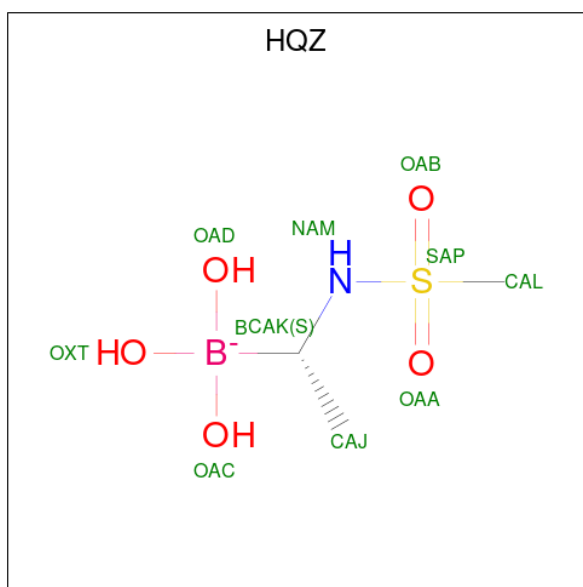
There are 5 unique types of molecules in this entry. The entry contains 13905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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-) (CCD ID: 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 (CCD ID: 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 (CCD ID: 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		

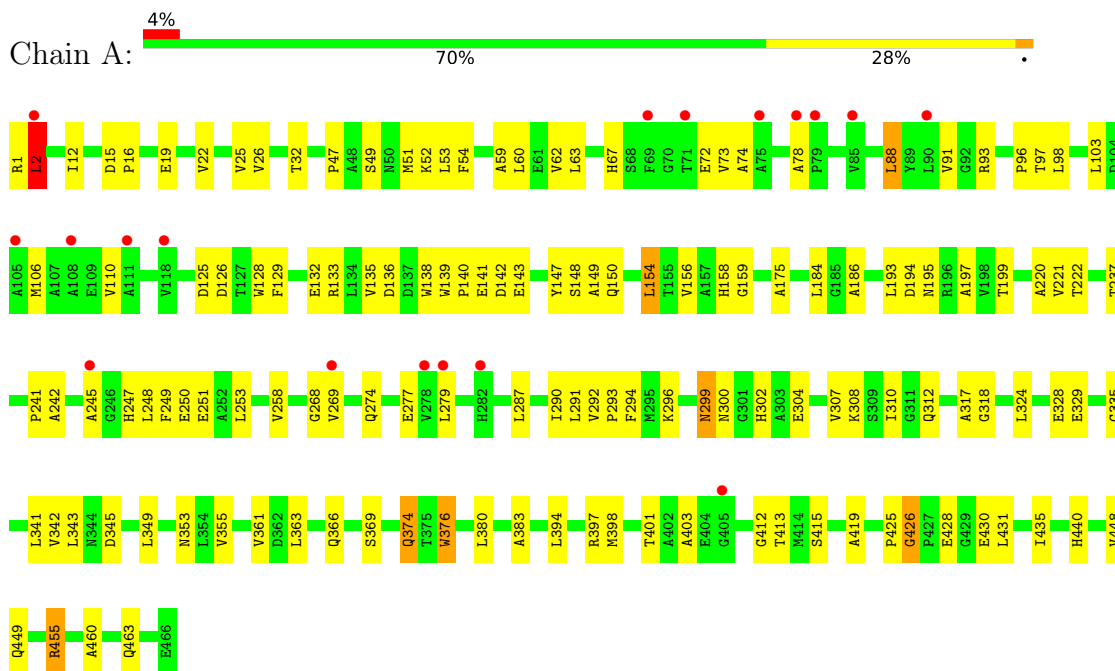
- Molecule 5 is water.

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

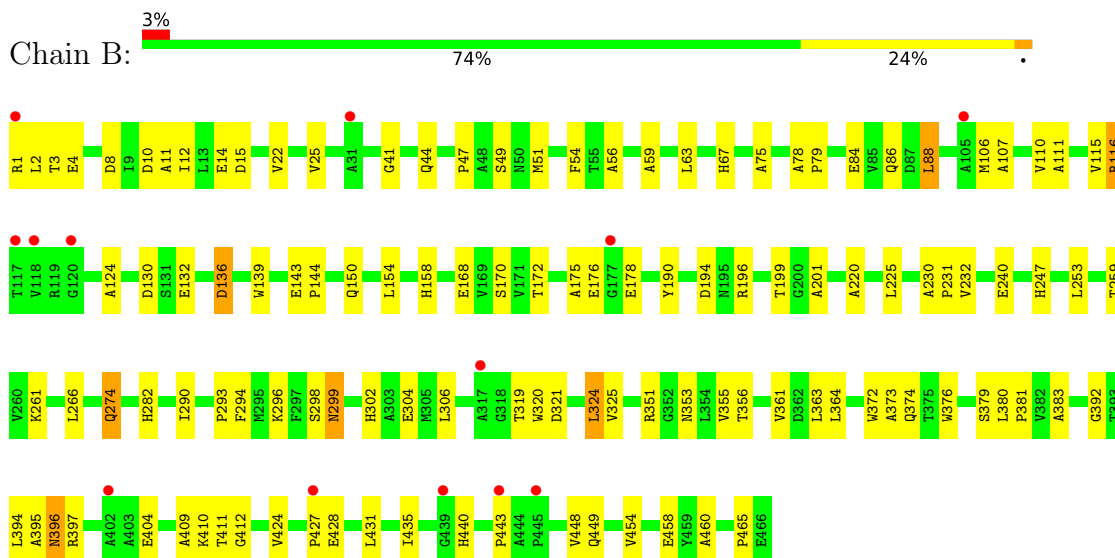
3 Residue-property plots [i](#)

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.

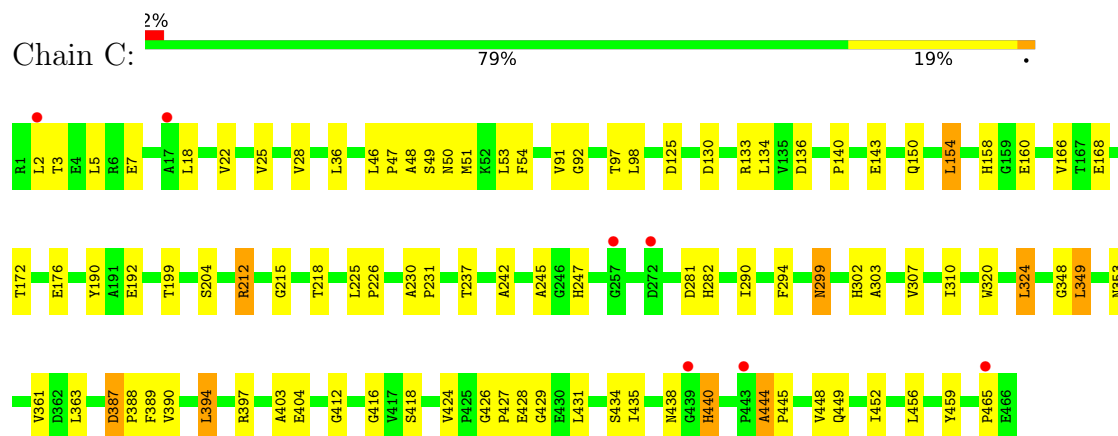
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



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



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



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 0.216 , 0.265	Depositor DCC
R_{free} test set	2888 reflections (5.06%)	wwPDB-VP
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 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	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.

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: SO4, HQZ, MG

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	0.81	0/3412	1.03	6/4666 (0.1%)
1	B	0.76	1/3403 (0.0%)	0.96	6/4656 (0.1%)
1	C	0.81	1/3403 (0.0%)	0.98	13/4656 (0.3%)
1	D	0.94	0/3412	1.03	3/4666 (0.1%)
All	All	0.83	2/13630 (0.0%)	1.00	28/18644 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	PRO	C-N	-6.72	1.24	1.33
1	C	465	PRO	C-N	-6.36	1.24	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	ALA	CA-C-N	6.42	127.87	119.84
1	C	444	ALA	C-N-CA	6.42	127.87	119.84
1	C	390	VAL	N-CA-C	-6.07	106.98	111.90
1	B	136	ASP	N-CA-C	6.05	117.88	111.28
1	C	426	GLY	CA-C-N	6.02	125.73	119.05
1	C	426	GLY	C-N-CA	6.02	125.73	119.05
1	B	178	GLU	CA-C-N	5.95	125.97	119.90
1	B	178	GLU	C-N-CA	5.95	125.97	119.90
1	A	419	ALA	N-CA-C	5.95	118.92	108.75
1	A	426	GLY	CA-C-N	5.93	127.25	119.84
1	A	426	GLY	C-N-CA	5.93	127.25	119.84
1	C	98	LEU	N-CA-C	5.79	117.49	109.15
1	C	215	GLY	N-CA-C	-5.46	107.15	114.25
1	A	317	ALA	N-CA-C	5.35	117.05	107.80
1	B	409	ALA	N-CA-C	5.30	116.91	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	GLN	N-CA-C	5.28	117.11	111.36
1	D	334	LEU	N-CA-C	-5.17	106.81	113.23
1	C	310	ILE	N-CA-C	-5.17	105.50	110.72
1	A	413	THR	N-CA-C	5.16	117.76	108.48
1	D	143	GLU	CA-C-N	-5.10	114.41	119.56
1	D	143	GLU	C-N-CA	-5.10	114.41	119.56
1	C	212	ARG	CA-C-N	5.09	125.09	119.90
1	C	212	ARG	C-N-CA	5.09	125.09	119.90
1	C	387	ASP	CA-C-N	5.03	125.05	119.32
1	C	387	ASP	C-N-CA	5.03	125.05	119.32
1	C	136	ASP	N-CA-C	5.02	117.41	111.33
1	B	15	ASP	CA-C-N	5.01	124.45	119.24
1	B	15	ASP	C-N-CA	5.01	124.45	119.24

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	3200	85	0
1	B	3344	0	3194	66	0
1	C	3344	0	3194	55	0
1	D	3353	0	3200	46	1
2	A	10	0	10	0	0
2	B	10	0	10	2	0
2	C	10	0	10	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	76	0	0	0	0
5	D	111	0	0	0	0
All	All	13905	0	12828	251	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 10.

All (251) 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: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
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:C:299:ASN:C	1:C:299:ASN:HD22	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:PRO:HG3	1:C:51:MET:HE2	1.81	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:51:MET:HE3	1:B:353:ASN:OD1	2.01	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: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:C:427:PRO:C	1:C:429:GLY:H	2.13	0.57
1:D:213:PRO:O	1:D:216:THR:OG1	2.23	0.57
1:D:299:ASN:C	1:D:299:ASN:HD22	2.12	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:D:12:ILE:C	1:D:14:GLU:H	2.14	0.55
1:A:47:PRO:HB3	1:A:355:VAL:CG2	2.36	0.55
1:D:295:MET:HE3	1:D:410:LYS:HD3	1.89	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
1:A:299:ASN:ND2	1:A:302:HIS:H	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:93:ARG:HG2	1:A:128:TRP:CD2	2.44	0.52
1:B:41:GLY:O	1:B:356:THR:HB	2.09	0.52
1:C:348:GLY:HA2	1:C:353:ASN:ND2	2.24	0.52
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.91	0.52
1:A:296:LYS:NZ	1:A:380:LEU:O	2.41	0.51
1:A:307:VAL:O	1:A:310:ILE:N	2.43	0.51
1:A:158:HIS:NE2	3:A:1470:SO4:O4	2.42	0.51
1:D:154:LEU:HD13	1:D:245:ALA:HB3	1.93	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:139:TRP:HB3	1:A:141:GLU:OE2	2.11	0.50
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.94	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:397:ARG:HH22	1:D:449:GLN:HE21	1.58	0.50
1:B:427:PRO:HD3	1:B:460:ALA:O	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:B:49:SER:HB2	2:B:500:HQZ:OAC	2.12	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:C:349:LEU:HD23	2:C:500:HQZ:HAL1	1.93	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:B:75:ALA:HB2	1:B:88:LEU:HD23	1.94	0.49
1:D:419:ALA:HA	1:D:435:ILE:O	2.12	0.49
1:B:296:LYS:NZ	1:B:380:LEU:O	2.30	0.49
1:B:56:ALA:HB3	1:B:376:TRP:HZ3	1.76	0.49
1:B:383:ALA:O	1:B:404:GLU:HA	2.12	0.49
1:D:184:LEU:HD22	1:D:188:GLU:OE2	2.11	0.49
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.94	0.49
1:C:307:VAL:HG11	1:C:324:LEU:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:25:VAL:HG22	1:A:435:ILE:HG23	1.96	0.47
1:D:158:HIS:CE1	3:D:1470:SO4:O1	2.67	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: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:A:268:GLY:O	1:A:269:VAL:C	2.57	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:C:361:VAL:HG23	1:C:434:SER:HB3	1.96	0.47
1:D:33:GLY:O	1:D:34:GLU:C	2.58	0.47
1:A:287:LEU:O	1:A:290:ILE:N	2.47	0.47
1:D:12:ILE:O	1:D:14:GLU:N	2.46	0.47
1:B:59:ALA:HB1	1:B:306:LEU:HD22	1.96	0.46
1:A:194:ASP:HB3	1:A:220:ALA:HA	1.97	0.46
1:B:175:ALA:O	1:B:199:THR:HB	2.14	0.46
1:A:184:LEU:HD21	1:A:193:LEU:HD13	1.98	0.46
1:B:395:ALA:C	1:B:396:ASN:HD22	2.24	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:B:383:ALA:HA	1:B:394:LEU:HB3	1.97	0.46
1:D:282:HIS:NE2	3:D:1474:SO4:O4	2.48	0.46
1:C:54:PHE:CD2	1:C:363:LEU:HD22	2.51	0.46
1:A:307:VAL:O	1:A:310:ILE:HB	2.15	0.46
1:C:299:ASN:ND2	1:C:302:HIS:H	2.12	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
1:C:403:ALA:O	1:C:404:GLU:C	2.60	0.45
1:B:230:ALA:O	1:B:231:PRO:C	2.60	0.45
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:12:ILE:HG22	1:B:448:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:H	1:B:274:GLN:HG2	1.60	0.45
1:D:51:MET:HE2	1:D:353:ASN:HB3	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:OE1	1:B:304:GLU:HA	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:A:345:ASP:C	1:A:345:ASP:OD1	2.59	0.44
1:C:294:PHE:HE1	1:C:303:ALA:HB2	1.83	0.44
1:C:424:VAL:O	1:C:431:LEU:N	2.40	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:A:125:ASP:C	1:A:125:ASP:OD1	2.60	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:C:299:ASN:C	1:C:299:ASN:ND2	2.76	0.44
1:A:52:LYS:HE2	1:A:299:ASN:C	2.43	0.43
1:B:47:PRO:HG3	1:B:51:MET:HE2	1.99	0.43
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:49:SER:HB2	1:A:412:GLY:HA2	2.00	0.43
1:A:294:PHE:CD1	1:A:302:HIS:HB2	2.53	0.43
1:B:11:ALA:O	1:B:14:GLU:HB2	2.18	0.43
1:C:92:GLY:HA3	1:C:154:LEU:HG	2.01	0.43
1:A:401:THR:C	1:A:403:ALA:H	2.26	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:51:MET:HE2	1:C:51:MET:HB2	1.88	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:170:SER:HA	1:B:232:VAL:O	2.18	0.42
1:B:199:THR:HA	1:B:225:LEU:O	2.19	0.42
1:A:341:LEU:CD1	1:A:343:LEU:HD21	2.33	0.42
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:SER:CB	5:A:2074:HOH:O	2.67	0.42
1:B:296:LYS:HE2	1:B:379:SER:O	2.20	0.42
1:B:320:TRP:O	1:B:324:LEU:HB2	2.19	0.42
1:B:361:VAL:HA	1:B:364:LEU:HD12	2.01	0.42
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.93	0.42
1:B:139:TRP:CZ2	1:B:351:ARG:HD2	2.54	0.42
1:D:291:LEU:HD13	1:D:291:LEU:HA	1.93	0.42
1:A:150:GLN:NE2	1:A:241:PRO:HD3	2.34	0.42
1:A:154:LEU:HB3	1:A:242:ALA:CB	2.49	0.42
1:A:397:ARG:HH22	1:A:449:GLN:HE21	1.65	0.42
1:A:425:PRO:HA	1:A:430:GLU:HA	2.01	0.42
1:B:8:ASP:O	1:B:11:ALA:HB3	2.18	0.42
1:B:124:ALA:HB3	1:B:266:LEU:HD23	2.01	0.42
1:D:12:ILE:C	1:D:14:GLU:N	2.78	0.42
1:D:158:HIS:NE2	3:D:1470:SO4:S	2.91	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:18:LEU:HD12	1:C:448:VAL:HG21	2.01	0.42
1:B:299:ASN:HD22	1:B:299:ASN:C	2.27	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:D:345:ASP:C	1:D:345:ASP:OD1	2.62	0.42
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:C:225:LEU:HD12	1:C:226:PRO:CD	2.49	0.41
1:D:313:GLU:O	1:D:313:GLU:HG3	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:C:130:ASP:OD1	1:C:130:ASP:C	2.64	0.41
1:B:440:HIS:HB2	5:B:2004:HOH:O	2.20	0.41
1:C:230:ALA:O	1:C:231:PRO:C	2.63	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: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:C:412:GLY:O	1:C:418:SER:HA	2.20	0.41
1:D:170:SER:O	1:D:182:VAL:HA	2.21	0.41
1:B:107:ALA:HB1	1:B:253:LEU:HD23	2.01	0.41
1:B:190:TYR:HB2	1:B:247:HIS:CD2	2.56	0.41
1:C:282:HIS:CE1	3:C:1466:SO4:O3	2.74	0.41
1:D:88:LEU:HD23	1:D:88:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HG3	1:A:51:MET:HE2	2.03	0.41
1:A:54:PHE:CD1	1:A:363:LEU:HD22	2.55	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:C:166:VAL:HA	1:C:237:THR:HA	2.03	0.41
1:D:121:ASP:OD1	1:D:263:ASP:N	2.42	0.41
1:A:142:ASP:O	1:A:148:SER:HB3	2.21	0.40
1:D:51:MET:CE	1:D:353:ASN:HB3	2.50	0.40
1:A:51:MET:HE3	1:A:353:ASN:OD1	2.22	0.40
1:A:135:VAL:HG12	1:A:136:ASP:N	2.35	0.40
1:D:282:HIS:NE2	3:D:1474:SO4:S	2.86	0.40
1:A:156:VAL:HG23	1:A:245:ALA:HB2	2.04	0.40
1:B:372:TRP:O	1:B:373:ALA:C	2.64	0.40
1:C:176:GLU:HA	1:C:199:THR:HG22	2.03	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	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ASP:OD2	4:D:1472:MG:MG[2_655]	1.67	0.53

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	464/466 (100%)	421 (91%)	41 (9%)	2 (0%)	30 45
1	B	464/466 (100%)	426 (92%)	35 (8%)	3 (1%)	21 34
1	C	464/466 (100%)	436 (94%)	27 (6%)	1 (0%)	43 60
1	D	464/466 (100%)	432 (93%)	29 (6%)	3 (1%)	21 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1856/1864 (100%)	1715 (92%)	132 (7%)	9 (0%)	24	39

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
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%)	317 (94%)	22 (6%)	15	27
1	B	338/339 (100%)	319 (94%)	19 (6%)	19	32
1	C	338/339 (100%)	324 (96%)	14 (4%)	27	46
1	D	339/339 (100%)	316 (93%)	23 (7%)	14	25
All	All	1354/1356 (100%)	1276 (94%)	78 (6%)	18	31

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	19	GLU
1	A	22	VAL
1	A	32	THR
1	A	88	LEU
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	154	LEU
1	A	222	THR
1	A	274	GLN
1	A	299	ASN
1	A	312	GLN
1	A	328	GLU
1	A	329	GLU
1	A	349	LEU
1	A	374	GLN
1	A	376	TRP
1	A	415	SER
1	A	428	GLU
1	A	431	LEU
1	A	440	HIS
1	A	455	ARG
1	A	463	GLN
1	B	2	LEU
1	B	3	THR
1	B	10	ASP
1	B	22	VAL
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	324	LEU
1	B	374	GLN
1	B	396	ASN
1	B	428	GLU
1	C	22	VAL
1	C	28	VAL
1	C	46	LEU
1	C	134	LEU
1	C	154	LEU
1	C	192	GLU
1	C	281	ASP

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Mol	Chain	Res	Type
1	C	299	ASN
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	394	LEU
1	C	438	ASN
1	C	440	HIS
1	D	1	ARG
1	D	28	VAL
1	D	63	LEU
1	D	77	SER
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	214	VAL
1	D	259	THR
1	D	263	ASP
1	D	274	GLN
1	D	281	ASP
1	D	289	GLU
1	D	291	LEU
1	D	299	ASN
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	440	HIS

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	50	ASN
1	A	86	GLN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	344	ASN
1	A	366	GLN
1	A	437	ASN

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Mol	Chain	Res	Type
1	A	449	GLN
1	B	44	GLN
1	B	150	GLN
1	B	247	HIS
1	B	256	ASN
1	B	299	ASN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	C	44	GLN
1	C	247	HIS
1	C	299	ASN
1	C	302	HIS
1	C	366	GLN
1	C	396	ASN
1	C	437	ASN
1	C	440	HIS
1	C	449	GLN
1	D	44	GLN
1	D	150	GLN
1	D	299	ASN
1	D	302	HIS
1	D	437	ASN
1	D	449	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 oligosaccharides 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	1469	-	4,4,4	0.22	0	6,6,6	0.25	0
3	SO4	C	1470	-	4,4,4	0.29	0	6,6,6	0.13	0
2	HQZ	A	500	1	6,9,10	3.21	4 (66%)	6,13,16	3.92	2 (33%)
3	SO4	B	1468	-	4,4,4	0.30	0	6,6,6	0.41	0
3	SO4	B	1466	-	4,4,4	0.21	0	6,6,6	0.30	0
3	SO4	B	1467	-	4,4,4	0.28	0	6,6,6	0.32	0
3	SO4	C	1471	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	D	1470	-	4,4,4	0.28	0	6,6,6	0.32	0
3	SO4	C	1467	-	4,4,4	0.29	0	6,6,6	0.42	0
3	SO4	C	1469	-	4,4,4	0.29	0	6,6,6	0.19	0
3	SO4	A	1474	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	B	1471	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	D	1473	-	4,4,4	0.24	0	6,6,6	0.25	0
2	HQZ	C	500	1	6,9,10	3.11	4 (66%)	6,13,16	4.46	3 (50%)
3	SO4	D	1467	-	4,4,4	0.21	0	6,6,6	0.38	0
3	SO4	D	1469	-	4,4,4	0.26	0	6,6,6	0.41	0
3	SO4	B	1470	-	4,4,4	0.22	0	6,6,6	0.36	0
3	SO4	C	1468	-	4,4,4	0.35	0	6,6,6	0.65	0
3	SO4	C	1466	-	4,4,4	0.35	0	6,6,6	0.25	0
3	SO4	A	1468	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	D	1468	-	4,4,4	0.37	0	6,6,6	0.13	0
3	SO4	A	1467	-	4,4,4	0.29	0	6,6,6	0.44	0
2	HQZ	D	500	1	6,9,10	2.72	4 (66%)	6,13,16	4.97	3 (50%)
2	HQZ	B	500	1	6,9,10	2.92	4 (66%)	6,13,16	4.76	3 (50%)
3	SO4	B	1469	-	4,4,4	0.29	0	6,6,6	0.23	0
3	SO4	A	1470	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	D	1474	-	4,4,4	0.30	0	6,6,6	0.30	0
3	SO4	A	1473	-	4,4,4	0.31	0	6,6,6	0.29	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
2	HQZ	D	500	1	-	2/4/9/11	-
2	HQZ	A	500	1	-	2/4/9/11	-
2	HQZ	C	500	1	-	2/4/9/11	-
2	HQZ	B	500	1	-	2/4/9/11	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HQZ	SAP-NAM	-4.65	1.53	1.62
2	C	500	HQZ	OAB-SAP	4.18	1.50	1.43
2	B	500	HQZ	SAP-NAM	-4.16	1.54	1.62
2	A	500	HQZ	CAL-SAP	-4.07	1.66	1.75
2	A	500	HQZ	OAB-SAP	4.00	1.50	1.43
2	A	500	HQZ	SAP-NAM	-3.88	1.54	1.62
2	D	500	HQZ	CAL-SAP	-3.78	1.67	1.75
2	B	500	HQZ	CAL-SAP	-3.53	1.67	1.75
2	D	500	HQZ	SAP-NAM	-3.47	1.55	1.62
2	C	500	HQZ	CAL-SAP	-3.42	1.67	1.75
2	A	500	HQZ	OAA-SAP	3.42	1.49	1.43
2	D	500	HQZ	OAB-SAP	3.41	1.49	1.43
2	B	500	HQZ	OAB-SAP	3.35	1.49	1.43
2	B	500	HQZ	OAA-SAP	3.13	1.48	1.43
2	C	500	HQZ	OAA-SAP	2.55	1.47	1.43
2	D	500	HQZ	OAA-SAP	2.43	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HQZ	OAB-SAP-OAA	-10.47	104.83	118.87
2	D	500	HQZ	OAB-SAP-OAA	-10.22	105.17	118.87
2	C	500	HQZ	OAB-SAP-OAA	-9.97	105.51	118.87
2	A	500	HQZ	OAB-SAP-OAA	-8.12	107.98	118.87
2	D	500	HQZ	OAB-SAP-NAM	5.19	114.69	107.29
2	A	500	HQZ	OAB-SAP-NAM	4.76	114.08	107.29
2	D	500	HQZ	OAA-SAP-CAL	4.07	114.70	108.26
2	B	500	HQZ	OAA-SAP-NAM	3.79	112.70	107.29
2	C	500	HQZ	OAB-SAP-CAL	3.04	113.07	108.26
2	C	500	HQZ	OAB-SAP-NAM	2.92	111.46	107.29
2	B	500	HQZ	OAB-SAP-CAL	2.62	112.41	108.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HQZ	CAK-NAM-SAP-OAA
2	C	500	HQZ	CAK-NAM-SAP-OAA
2	D	500	HQZ	CAK-NAM-SAP-OAA
2	A	500	HQZ	CAJ-CAK-NAM-SAP
2	C	500	HQZ	CAK-NAM-SAP-CAL
2	A	500	HQZ	CAK-NAM-SAP-OAA
2	B	500	HQZ	CAK-NAM-SAP-CAL
2	D	500	HQZ	CAK-NAM-SAP-CAL

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1469	SO4	1	0
3	D	1470	SO4	3	0
3	B	1471	SO4	1	0
2	C	500	HQZ	1	0
3	B	1470	SO4	4	0
3	C	1466	SO4	2	0
2	B	500	HQZ	2	0
3	A	1470	SO4	2	0
3	D	1474	SO4	3	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	466/466 (100%)	0.60	18 (3%) 43 35	38, 55, 73, 87	0
1	B	466/466 (100%)	0.36	13 (2%) 55 48	38, 56, 78, 91	0
1	C	466/466 (100%)	0.02	7 (1%) 72 67	26, 48, 72, 90	0
1	D	466/466 (100%)	-0.27	3 (0%) 85 83	18, 34, 55, 78	0
All	All	1864/1864 (100%)	0.18	41 (2%) 62 56	18, 51, 73, 91	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	4.5
1	A	71	THR	3.8
1	C	272	ASP	3.7
1	B	445	PRO	3.7
1	D	17	ALA	3.6
1	B	317	ALA	3.3
1	A	2	LEU	3.1
1	C	465	PRO	3.0
1	A	105	ALA	3.0
1	A	282	HIS	2.9
1	A	78	ALA	2.9
1	A	269	VAL	2.9
1	D	440	HIS	2.9
1	B	120	GLY	2.9
1	A	405	GLY	2.8
1	A	85	VAL	2.8
1	A	118	VAL	2.8
1	B	439	GLY	2.7
1	B	443	PRO	2.6
1	B	118	VAL	2.5
1	B	105	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	2	LEU	2.4
1	B	402	ALA	2.4
1	C	257	GLY	2.3
1	A	75	ALA	2.3
1	B	177	GLY	2.3
1	A	79	PRO	2.2
1	B	1	ARG	2.2
1	A	278	VAL	2.2
1	B	31	ALA	2.1
1	B	427	PRO	2.1
1	A	279	LEU	2.1
1	D	377	SER	2.1
1	A	111	ALA	2.1
1	A	245	ALA	2.1
1	C	17	ALA	2.1
1	C	443	PRO	2.1
1	B	117	THR	2.0
1	A	69	PHE	2.0
1	A	90	LEU	2.0
1	C	439	GLY	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
3	SO4	A	1473	5/5	0.61	0.17	100,101,101,102	0
3	SO4	A	1468	5/5	0.78	0.10	114,114,114,115	0
3	SO4	B	1469	5/5	0.79	0.13	99,99,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	1470	5/5	0.79	0.10	77,78,79,79	0
3	SO4	A	1470	5/5	0.81	0.11	109,109,110,111	0
3	SO4	A	1469	5/5	0.82	0.09	121,122,122,122	0
3	SO4	C	1471	5/5	0.83	0.17	84,85,86,86	0
3	SO4	A	1467	5/5	0.84	0.19	61,62,62,62	0
3	SO4	B	1466	5/5	0.85	0.20	74,76,77,77	0
3	SO4	A	1474	5/5	0.86	0.11	88,88,89,89	0
3	SO4	B	1470	5/5	0.86	0.12	79,79,80,81	0
3	SO4	D	1473	5/5	0.88	0.14	78,78,78,79	0
3	SO4	B	1467	5/5	0.90	0.08	70,71,72,72	0
3	SO4	B	1471	5/5	0.91	0.11	108,108,108,108	0
3	SO4	B	1468	5/5	0.91	0.16	59,59,62,63	0
3	SO4	C	1469	5/5	0.92	0.09	73,74,75,75	0
3	SO4	D	1469	5/5	0.93	0.12	63,63,64,65	0
3	SO4	D	1474	5/5	0.93	0.11	61,63,64,65	0
2	HQZ	C	500	10/11	0.94	0.10	34,37,38,39	0
3	SO4	C	1467	5/5	0.94	0.07	59,61,63,64	0
3	SO4	D	1467	5/5	0.95	0.10	48,48,51,51	0
3	SO4	D	1468	5/5	0.95	0.09	61,61,61,62	0
2	HQZ	B	500	10/11	0.95	0.10	42,46,49,50	0
2	HQZ	A	500	10/11	0.95	0.11	39,41,43,47	0
3	SO4	C	1470	5/5	0.95	0.09	61,61,62,63	0
3	SO4	C	1466	5/5	0.95	0.07	65,66,67,68	0
3	SO4	C	1468	5/5	0.96	0.14	51,52,53,54	0
4	MG	D	1471	1/1	0.96	0.13	10,10,10,10	0
4	MG	A	1471	1/1	0.98	0.11	33,33,33,33	0
2	HQZ	D	500	10/11	0.98	0.07	21,25,25,29	0
4	MG	A	1472	1/1	0.99	0.13	36,36,36,36	0
4	MG	D	1472	1/1	1.00	0.15	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.