Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 08:56 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 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:

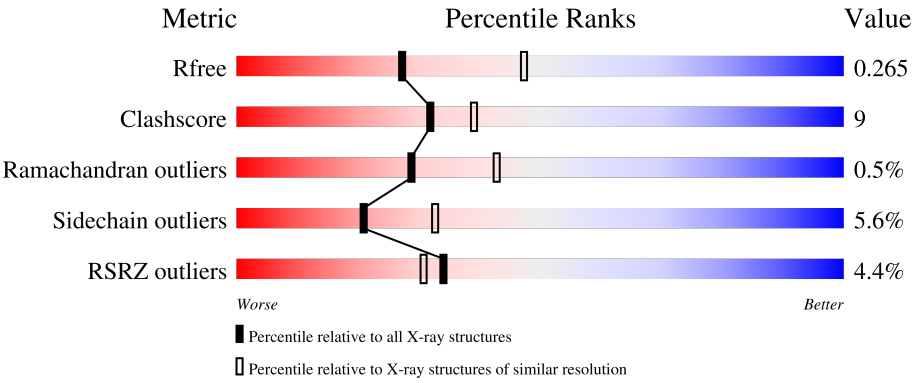
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	8% 73% 26%
1	B	466	6% 76% 23%
1	C	466	4% 82% 17%
1	D	466	% 82% 15%

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

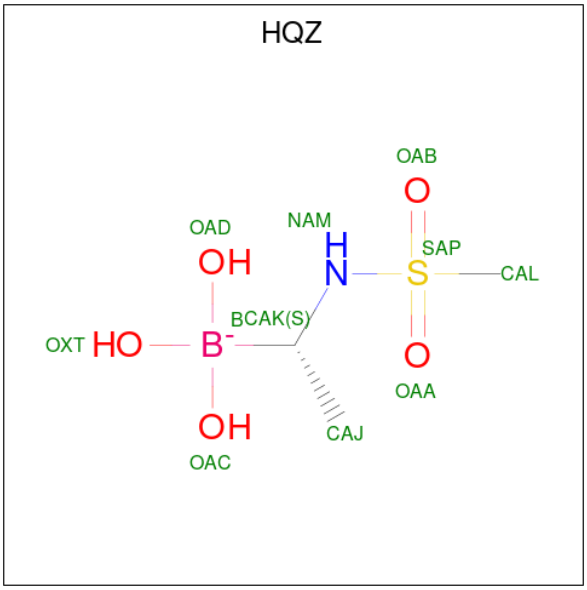
There are 5 unique types of molecules in this entry. The entry contains 13905 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-) (three-letter code: HQZ) (formula: $C_3H_{11}BNO_5S$).



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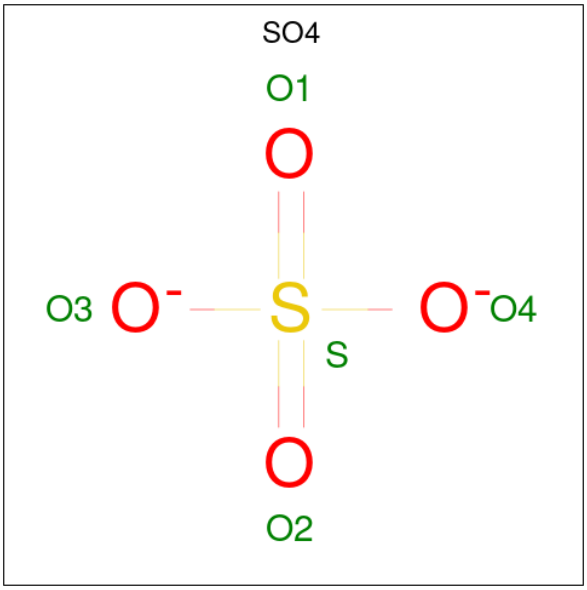
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total B C N O S 10 1 3 1 4 1	0	0
2	D	1	Total B C N O S 10 1 3 1 4 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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

- Molecule 5 is water.

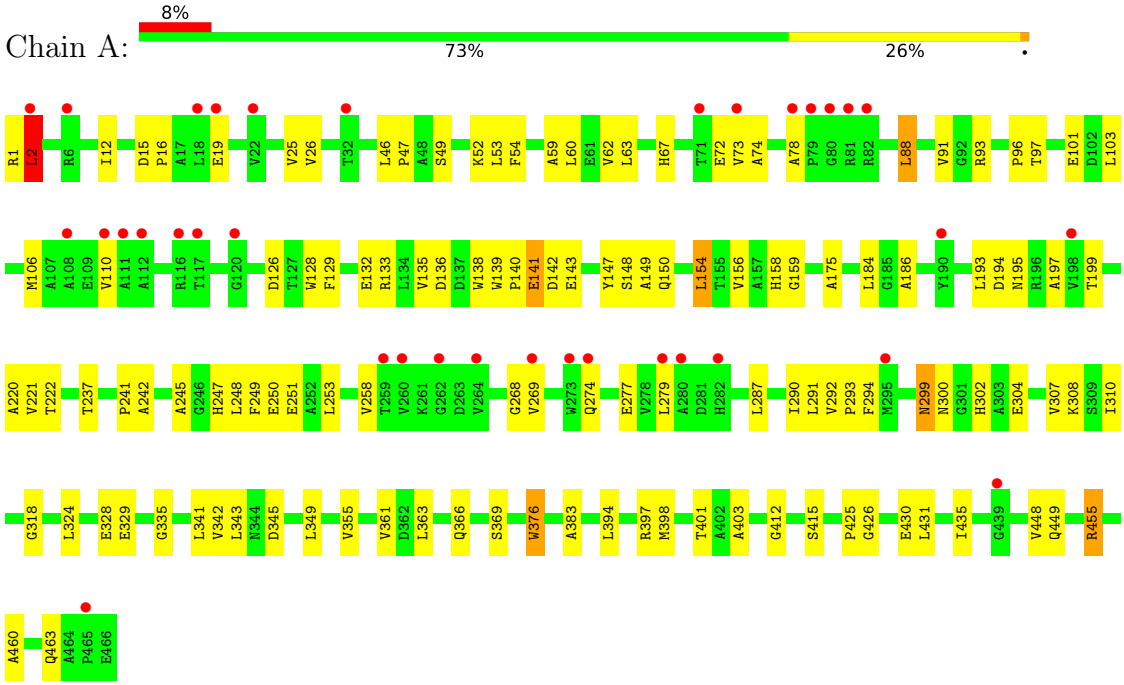
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	68	Total O 68 68	0	0
5	C	76	Total O 76 76	0	0
5	D	111	Total O 111 111	0	0

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.

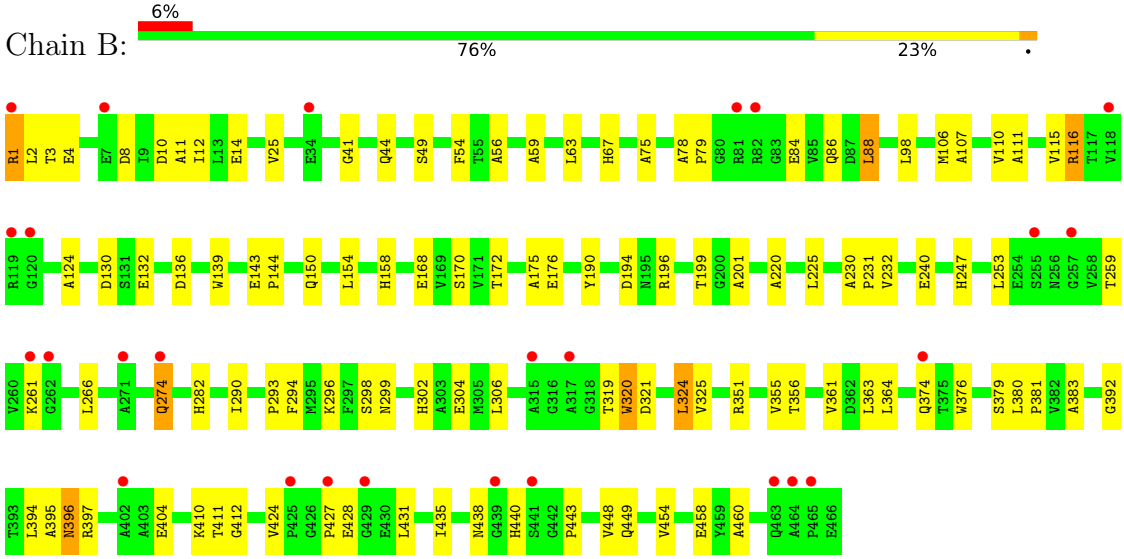
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



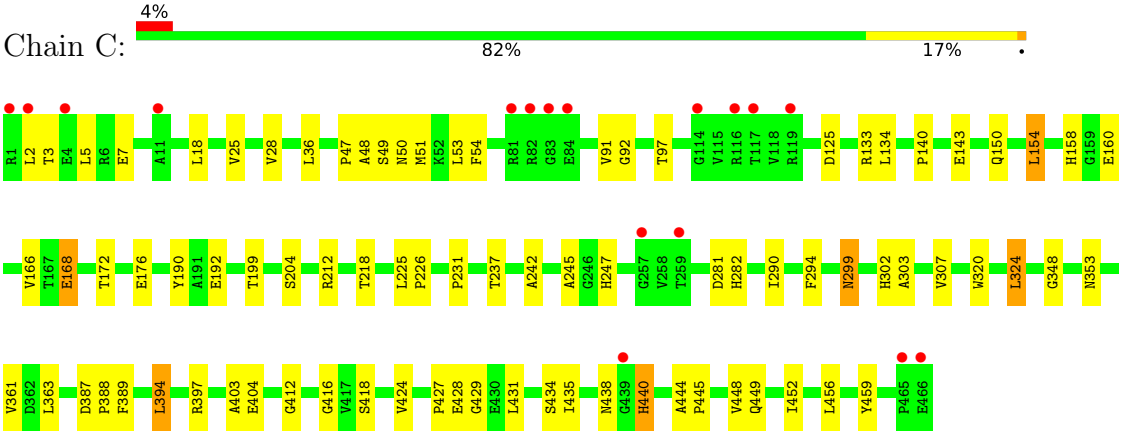
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:



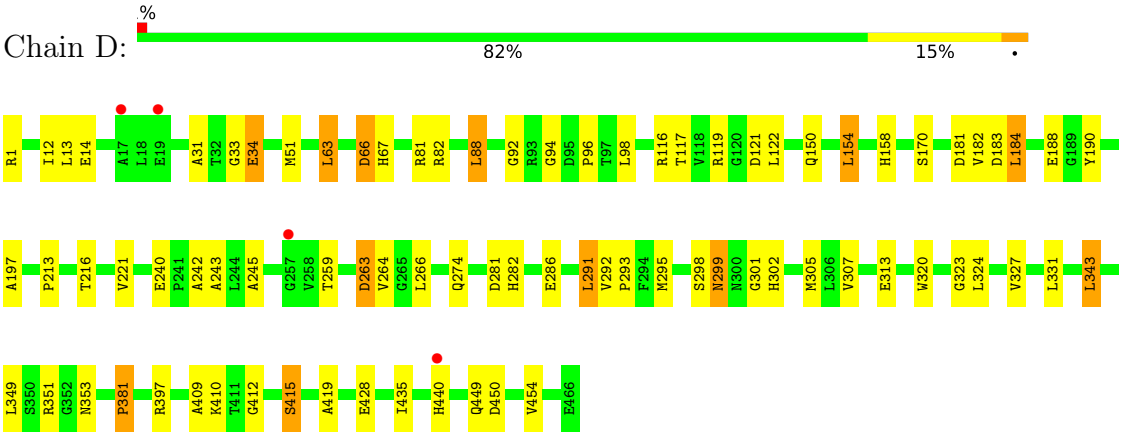
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	2825 reflections (5.05%)	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)	0.35 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HQZ, SO4, 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	0.66	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(^{o})	Ideal(^{o})
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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 9.

All (235) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:299:ASN:C	1:D:299:ASN:HD22	2.12	0.52
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.91	0.52
1:D:295:MET:HE3	1:D:410:LYS:HD3	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: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: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:B:427:PRO:HD3	1:B:460:ALA:O	2.12	0.50
1:D:51:MET:HE2	1:D:353:ASN:HB3	1.92	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:D:170:SER:HB2	1:D:183:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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: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:B:396:ASN:N	1:B:396:ASN:ND2	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:274:GLN:H	1:B:274:GLN:HG2	1.60	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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:HA	1:A:16:PRO:HD2	1.90	0.42
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:A:268:GLY:O	1:A:269:VAL:C	2.57	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:33:GLY:O	1:D:34:GLU:C	2.58	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: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:C	1:A:345:ASP:OD1	2.59	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: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: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:C:403:ALA:O	1:C:404:GLU:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:HD23	1:D:88:LEU:HA	1.97	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:B:230:ALA:O	1:B:231:PRO:C	2.60	0.40
1:D:51:MET:CE	1:D:353:ASN:HB3	2.50	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: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%)	34	48
1	B	464/466 (100%)	426 (92%)	35 (8%)	3 (1%)	25	37
1	C	464/466 (100%)	436 (94%)	27 (6%)	1 (0%)	47	64
1	D	464/466 (100%)	432 (93%)	29 (6%)	3 (1%)	25	37
All	All	1856/1864 (100%)	1715 (92%)	132 (7%)	9 (0%)	29	43

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/339 (100%)	322 (95%)	17 (5%)	24	38
1	B	338/339 (100%)	317 (94%)	21 (6%)	18	29
1	C	338/339 (100%)	327 (97%)	11 (3%)	38	54
1	D	339/339 (100%)	312 (92%)	27 (8%)	12	18
All	All	1354/1356 (100%)	1278 (94%)	76 (6%)	21	33

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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

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Mol	Chain	Res	Type
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
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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	1467	-	4,4,4	0.16	0	6,6,6	0.35	0
3	SO4	D	1467	-	4,4,4	0.10	0	6,6,6	0.37	0
3	SO4	B	1466	-	4,4,4	0.10	0	6,6,6	0.34	0
2	HQZ	C	500	1	6,9,10	2.98	4 (66%)	7,13,16	3.96	4 (57%)
3	SO4	B	1471	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	A	1470	-	4,4,4	0.19	0	6,6,6	0.39	0
3	SO4	A	1474	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	A	1469	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	B	1469	-	4,4,4	0.18	0	6,6,6	0.20	0
2	HQZ	A	500	1	6,9,10	3.06	4 (66%)	7,13,16	3.44	2 (28%)
3	SO4	D	1468	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	B	1470	-	4,4,4	0.15	0	6,6,6	0.37	0
3	SO4	D	1470	-	4,4,4	0.17	0	6,6,6	0.37	0
3	SO4	C	1467	-	4,4,4	0.17	0	6,6,6	0.41	0
3	SO4	C	1470	-	4,4,4	0.18	0	6,6,6	0.14	0
3	SO4	D	1473	-	4,4,4	0.12	0	6,6,6	0.25	0
3	SO4	D	1474	-	4,4,4	0.19	0	6,6,6	0.42	0
3	SO4	A	1473	-	4,4,4	0.21	0	6,6,6	0.29	0
2	HQZ	D	500	1	6,9,10	2.60	4 (66%)	7,13,16	4.49	4 (57%)
3	SO4	C	1468	-	4,4,4	0.25	0	6,6,6	0.65	0
3	SO4	B	1468	-	4,4,4	0.18	0	6,6,6	0.41	0
3	SO4	A	1467	-	4,4,4	0.19	0	6,6,6	0.45	0
3	SO4	C	1466	-	4,4,4	0.25	0	6,6,6	0.27	0
2	HQZ	B	500	1	6,9,10	2.80	4 (66%)	7,13,16	4.12	3 (42%)
3	SO4	C	1469	-	4,4,4	0.18	0	6,6,6	0.19	0
3	SO4	C	1471	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	A	1468	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	D	1469	-	4,4,4	0.18	0	6,6,6	0.40	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	-	3/4/9/11	-
2	HQZ	C	500	1	-	2/4/9/11	-
2	HQZ	A	500	1	-	3/4/9/11	-
2	HQZ	B	500	1	-	4/4/9/11	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HQZ	SAP-NAM	-4.59	1.53	1.62
2	B	500	HQZ	SAP-NAM	-4.12	1.54	1.62
2	C	500	HQZ	OAB-SAP	3.92	1.50	1.43
2	A	500	HQZ	CAL-SAP	-3.87	1.66	1.75
2	A	500	HQZ	SAP-NAM	-3.85	1.54	1.62
2	A	500	HQZ	OAB-SAP	3.75	1.50	1.43
2	D	500	HQZ	CAL-SAP	-3.59	1.67	1.75
2	D	500	HQZ	SAP-NAM	-3.45	1.55	1.62
2	B	500	HQZ	CAL-SAP	-3.35	1.67	1.75
2	C	500	HQZ	CAL-SAP	-3.25	1.67	1.75
2	A	500	HQZ	OAA-SAP	3.21	1.49	1.43
2	D	500	HQZ	OAB-SAP	3.20	1.49	1.43
2	B	500	HQZ	OAB-SAP	3.14	1.49	1.43
2	B	500	HQZ	OAA-SAP	2.94	1.48	1.43
2	C	500	HQZ	OAA-SAP	2.40	1.47	1.43
2	D	500	HQZ	OAA-SAP	2.28	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HQZ	OAB-SAP-OAA	-9.75	104.83	118.85
2	D	500	HQZ	OAB-SAP-OAA	-9.51	105.17	118.85
2	C	500	HQZ	OAB-SAP-OAA	-9.28	105.51	118.85
2	A	500	HQZ	OAB-SAP-OAA	-7.56	107.98	118.85
2	D	500	HQZ	OAB-SAP-NAM	4.88	114.69	107.23
2	A	500	HQZ	OAB-SAP-NAM	4.48	114.08	107.23
2	D	500	HQZ	OAA-SAP-CAL	4.00	114.70	108.28
2	B	500	HQZ	OAA-SAP-NAM	3.58	112.70	107.23
2	D	500	HQZ	CAJ-CAK-NAM	-3.27	105.37	111.18
2	C	500	HQZ	OAB-SAP-CAL	2.99	113.07	108.28
2	C	500	HQZ	OAB-SAP-NAM	2.76	111.46	107.23
2	B	500	HQZ	OAB-SAP-CAL	2.57	112.41	108.28
2	C	500	HQZ	CAJ-CAK-NAM	-2.16	107.34	111.18

There are no chirality outliers.

All (12) 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	C	500	HQZ	CAK-NAM-SAP-CAL
2	D	500	HQZ	CAK-NAM-SAP-OAA

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

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1471	SO4	1	0
3	A	1470	SO4	2	0
3	A	1469	SO4	1	0
3	B	1470	SO4	4	0
3	D	1470	SO4	3	0
3	D	1474	SO4	3	0
3	C	1466	SO4	2	0
2	B	500	HQZ	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, 95^{th} 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%)	0.52	35 (7%)	14	11	38, 55, 73, 87	0
1	B	466/466 (100%)	0.30	26 (5%)	24	21	38, 56, 78, 91	0
1	C	466/466 (100%)	0.06	17 (3%)	42	39	26, 48, 72, 90	0
1	D	466/466 (100%)	-0.16	4 (0%)	84	83	18, 34, 55, 78	0
All	All	1864/1864 (100%)	0.18	82 (4%)	34	31	18, 51, 73, 91	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	6.5
1	A	279	LEU	5.8
1	B	317	ALA	5.1
1	A	282	HIS	4.6
1	B	464	ALA	4.5
1	B	439	GLY	4.4
1	B	118	VAL	4.2
1	A	71	THR	4.2
1	C	466	GLU	4.1
1	A	116	ARG	4.1
1	C	2	LEU	4.0
1	A	82	ARG	3.9
1	B	81	ARG	3.9
1	C	465	PRO	3.9
1	A	259	THR	3.8
1	A	81	ARG	3.8
1	B	465	PRO	3.8
1	A	78	ALA	3.7
1	A	111	ALA	3.6
1	B	271	ALA	3.5
1	B	441	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	1	ARG	3.4
1	B	120	GLY	3.4
1	C	439	GLY	3.3
1	B	262	GLY	3.3
1	C	119	ARG	3.3
1	A	79	PRO	3.2
1	A	280	ALA	3.2
1	A	262	GLY	3.1
1	A	117	THR	3.0
1	C	82	ARG	2.9
1	B	7	GLU	2.9
1	A	112	ALA	2.9
1	C	81	ARG	2.9
1	B	402	ALA	2.9
1	B	1	ARG	2.8
1	B	274	GLN	2.8
1	C	257	GLY	2.8
1	C	117	THR	2.7
1	B	427	PRO	2.7
1	C	114	GLY	2.7
1	A	198	VAL	2.7
1	B	261	LYS	2.6
1	D	257	GLY	2.6
1	B	257	GLY	2.6
1	D	17	ALA	2.6
1	C	259	THR	2.6
1	A	80	GLY	2.6
1	A	2	LEU	2.5
1	A	439	GLY	2.5
1	B	119	ARG	2.5
1	B	34	GLU	2.4
1	A	260	VAL	2.4
1	A	73	VAL	2.4
1	C	84	GLU	2.4
1	A	190	TYR	2.3
1	B	374	GLN	2.3
1	A	465	PRO	2.3
1	A	295	MET	2.2
1	A	18	LEU	2.2
1	C	11	ALA	2.2
1	C	116	ARG	2.2
1	B	429	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	440	HIS	2.2
1	A	6	ARG	2.2
1	A	269	VAL	2.2
1	A	120	GLY	2.1
1	B	82	ARG	2.1
1	C	4	GLU	2.1
1	A	22	VAL	2.1
1	A	110	VAL	2.1
1	C	83	GLY	2.1
1	A	19	GLU	2.1
1	A	32	THR	2.1
1	A	273	TRP	2.1
1	B	255	SER	2.1
1	D	19	GLU	2.1
1	A	264	VAL	2.1
1	B	463	GLN	2.1
1	A	274	GLN	2.0
1	B	425	PRO	2.0
1	B	315	ALA	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 monosaccharides 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, 95^{th} 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	1468	5/5	0.78	0.20	114,114,114,115	0
3	SO4	A	1473	5/5	0.80	0.24	100,101,101,102	0
3	SO4	B	1469	5/5	0.81	0.22	99,99,100,100	0
3	SO4	A	1470	5/5	0.84	0.18	109,109,110,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	1470	5/5	0.87	0.17	77,78,79,79	0
3	SO4	A	1469	5/5	0.89	0.28	121,122,122,122	0
3	SO4	B	1466	5/5	0.92	0.26	74,76,77,77	0
3	SO4	A	1467	5/5	0.92	0.30	61,62,62,62	0
3	SO4	B	1470	5/5	0.92	0.18	79,79,80,81	0
3	SO4	A	1474	5/5	0.92	0.14	88,88,89,89	0
3	SO4	D	1473	5/5	0.93	0.16	78,78,78,79	0
3	SO4	C	1471	5/5	0.94	0.21	84,85,86,86	0
4	MG	D	1471	1/1	0.94	0.19	10,10,10,10	0
3	SO4	D	1469	5/5	0.95	0.16	63,63,64,65	0
3	SO4	B	1467	5/5	0.95	0.09	70,71,72,72	0
2	HQZ	B	500	10/11	0.96	0.16	42,46,49,50	0
3	SO4	B	1471	5/5	0.96	0.13	108,108,108,108	0
3	SO4	C	1469	5/5	0.96	0.11	73,74,75,75	0
2	HQZ	A	500	10/11	0.96	0.19	39,41,43,47	0
3	SO4	D	1468	5/5	0.97	0.07	61,61,61,62	0
3	SO4	C	1466	5/5	0.97	0.10	65,66,67,68	0
3	SO4	B	1468	5/5	0.97	0.20	59,59,62,63	0
3	SO4	C	1470	5/5	0.97	0.09	61,61,62,63	0
3	SO4	D	1474	5/5	0.97	0.12	61,63,64,65	0
2	HQZ	C	500	10/11	0.97	0.13	34,37,38,39	0
3	SO4	C	1468	5/5	0.98	0.13	51,52,53,54	0
3	SO4	C	1467	5/5	0.98	0.07	59,61,63,64	0
4	MG	A	1471	1/1	0.98	0.19	33,33,33,33	0
4	MG	A	1472	1/1	0.98	0.22	36,36,36,36	0
3	SO4	D	1467	5/5	0.98	0.09	48,48,51,51	0
2	HQZ	D	500	10/11	0.99	0.17	21,25,25,29	0
4	MG	D	1472	1/1	0.99	0.27	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.