



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:40 PM BST

PDB ID : 6WAM
Title : Structure of *Acinetobacter baumannii* Cap4 SAVED/CARF-domain containing receptor
Authors : Lowey, B.; Whiteley, A.T.; Keszei, A.F.A.; Morehouse, B.R.; Antine, S.P.; Cabrera, V.; Schwede, F.; Mekalanos, J.J.; Shao, S.; Lee, A.S.Y.; Kranzusch, P.J.
Deposited on : 2020-03-25
Resolution : 2.60 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

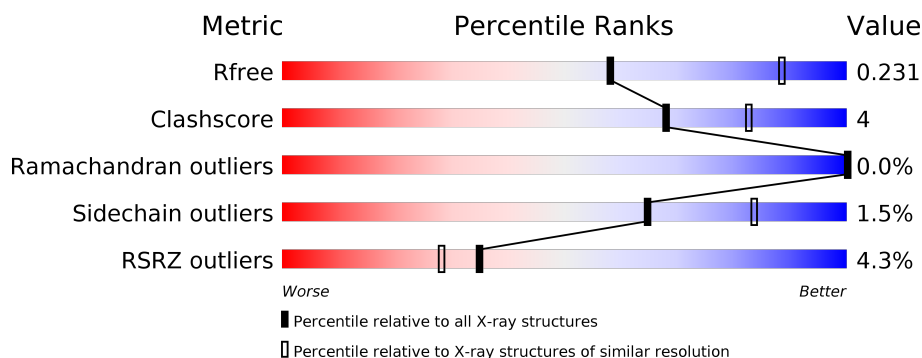
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	462	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	462	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
1	C	462	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	D	462	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	E	462	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>
1	F	462	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21147 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 SAVED domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3513	2242	592	668	11			
1	B	436	Total	C	N	O	S	0	0	0
			3504	2236	591	666	11			
1	C	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	D	437	Total	C	N	O	S	0	0	0
			3513	2242	592	668	11			
1	E	420	Total	C	N	O	S	0	0	0
			3370	2151	568	640	11			
1	F	421	Total	C	N	O	S	0	0	0
			3382	2163	569	639	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP C0VHC9
B	1	SER	-	expression tag	UNP C0VHC9
C	1	SER	-	expression tag	UNP C0VHC9
D	1	SER	-	expression tag	UNP C0VHC9
E	1	SER	-	expression tag	UNP C0VHC9
F	1	SER	-	expression tag	UNP C0VHC9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

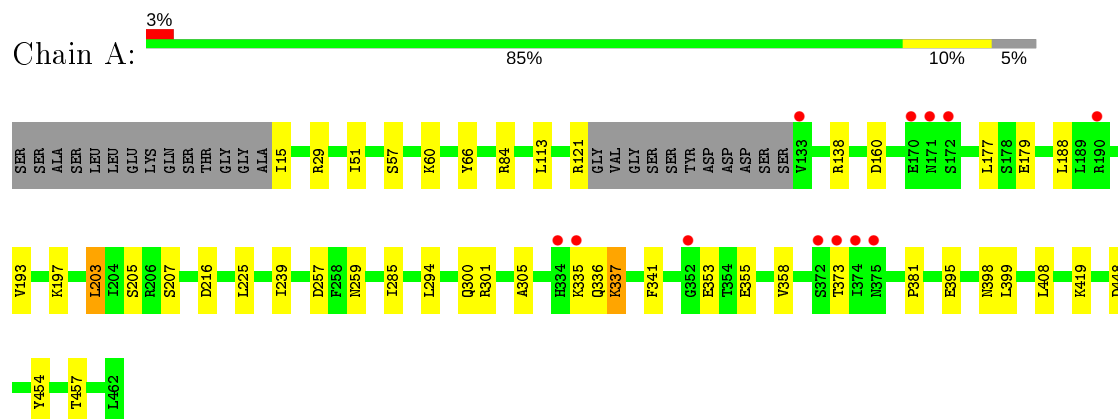
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	51	Total	O	0	0
			51	51		
3	C	52	Total	O	0	0
			52	52		
3	D	62	Total	O	0	0
			62	62		
3	E	54	Total	O	0	0
			54	54		
3	F	41	Total	O	0	0
			41	41		

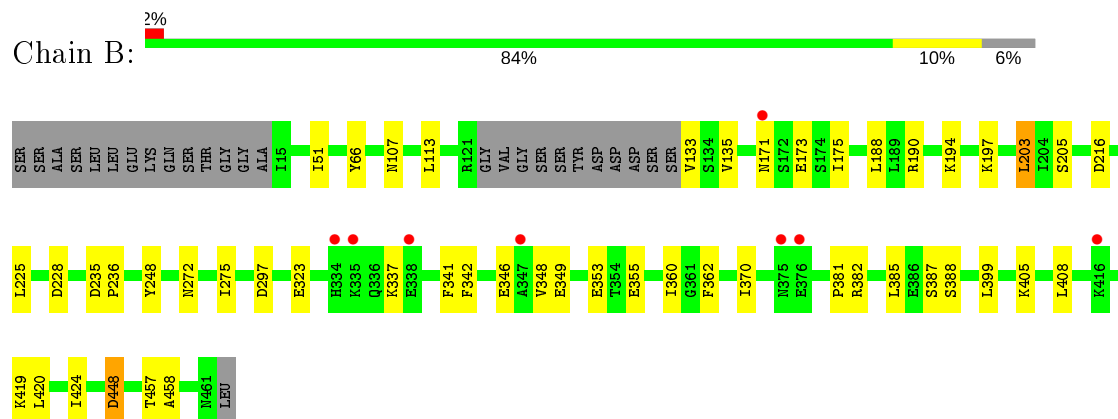
3 Residue-property plots [i](#)

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.

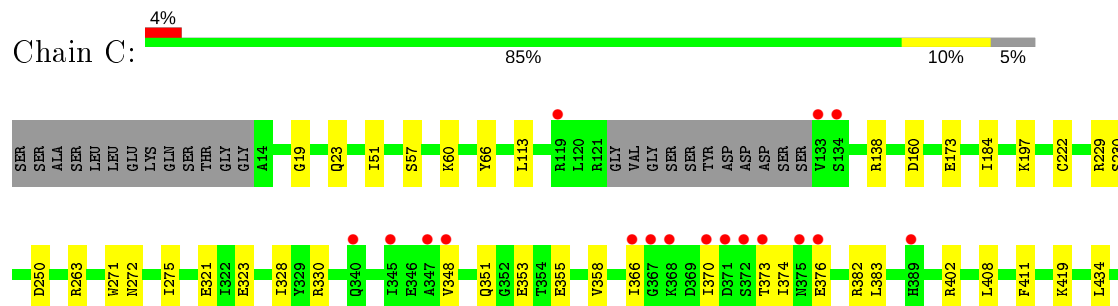
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein

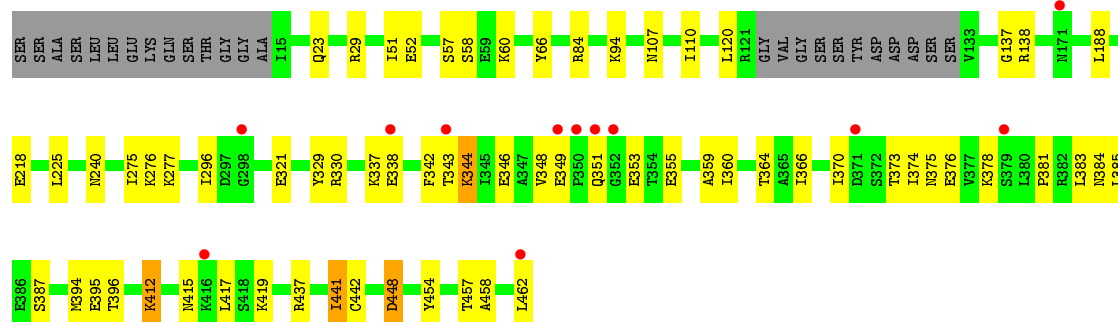
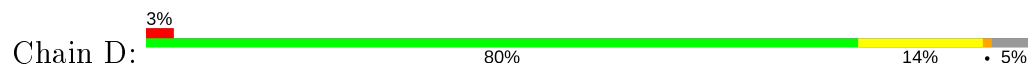


- Molecule 1: SAVED domain-containing protein

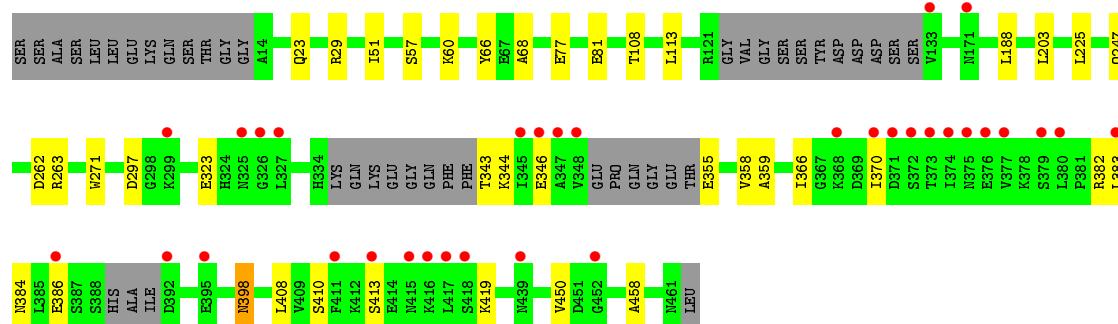
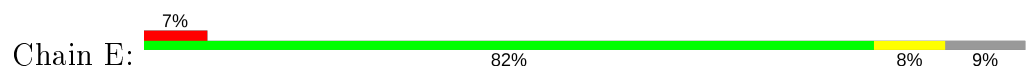




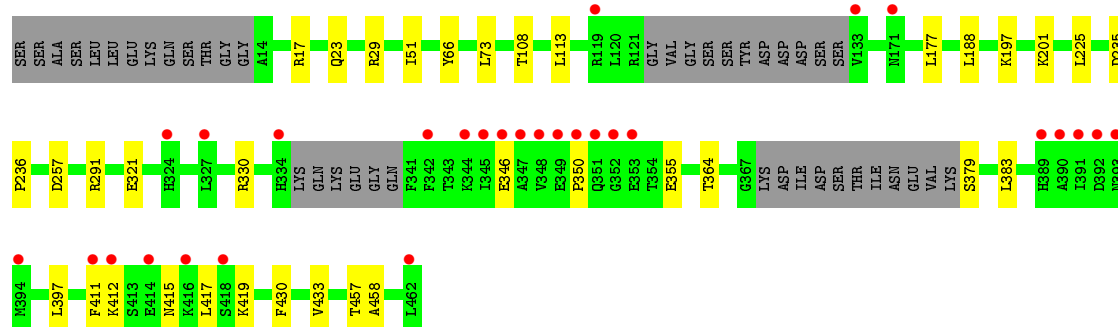
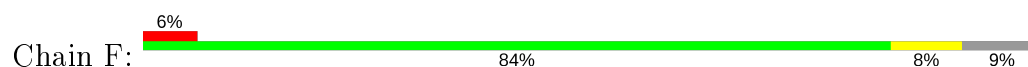
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.72Å 111.38Å 173.30Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	39.60 – 2.60 39.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (39.60-2.60) 86.3 (39.60-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.194 , 0.229 0.193 , 0.231	Depositor DCC
R_{free} test set	1993 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21147	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

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	0.28	0/3588	0.45	0/4849
1	B	0.29	0/3579	0.45	0/4838
1	C	0.28	0/3593	0.45	0/4856
1	D	0.29	0/3588	0.46	0/4849
1	E	0.28	0/3438	0.45	0/4645
1	F	0.28	0/3455	0.46	0/4670
All	All	0.28	0/21241	0.45	0/28707

There are no bond length outliers.

There are no bond angle outliers.

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	3513	0	3461	27	0
1	B	3504	0	3450	27	0
1	C	3518	0	3466	25	0
1	D	3513	0	3461	40	0
1	E	3370	0	3323	19	0
1	F	3382	0	3324	23	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	57	0	0	4	0
3	B	51	0	0	5	0
3	C	52	0	0	4	0
3	D	62	0	0	3	0
3	E	54	0	0	3	0
3	F	41	0	0	4	0
All	All	21147	0	20485	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (156) 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:D:218:GLU:OE1	3:D:601:HOH:O	1.88	0.91
1:B:173:GLU:HG2	1:B:197:LYS:HD2	1.60	0.82
1:B:337:LYS:HB2	1:B:399:LEU:HD12	1.65	0.77
1:C:263:ARG:O	3:C:601:HOH:O	2.03	0.76
1:E:358:VAL:HG11	1:E:408:LEU:HD21	1.69	0.74
1:F:411:PHE:O	1:F:415:ASN:ND2	2.21	0.73
1:D:349:GLU:H	1:D:381:PRO:HB3	1.55	0.71
1:B:297:ASP:HA	1:B:323:GLU:HG3	1.73	0.71
1:C:250:ASP:OD2	3:C:602:HOH:O	2.07	0.70
1:A:239:ILE:O	3:A:601:HOH:O	2.08	0.69
1:B:248:TYR:O	3:B:601:HOH:O	2.10	0.69
1:C:184:ILE:O	3:C:604:HOH:O	2.11	0.67
1:D:344:LYS:HB2	1:D:384:ASN:O	1.96	0.66
1:B:205:SER:OG	3:B:602:HOH:O	2.14	0.65
1:D:366:ILE:HG21	1:D:370:ILE:HG13	1.79	0.64
1:D:360:ILE:HG12	1:D:385:LEU:HD12	1.80	0.64
1:D:441:ILE:HG22	1:D:442:CYS:H	1.63	0.64
1:A:188:LEU:HD21	1:A:225:LEU:HD23	1.80	0.64
1:A:336:GLN:HG2	1:A:398:ASN:HB3	1.79	0.63
1:D:355:GLU:HG2	1:D:419:LYS:HB3	1.80	0.63
1:A:373:THR:HG22	1:A:454:TYR:HB2	1.80	0.62
1:B:387:SER:OG	1:B:388:SER:N	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:THR:OG1	1:E:386:GLU:O	2.14	0.61
1:B:341:PHE:HB2	1:B:399:LEU:HD22	1.82	0.61
1:F:397:LEU:HD21	1:F:433:VAL:HG21	1.81	0.61
1:D:344:LYS:HB2	1:D:385:LEU:HA	1.82	0.60
1:E:398:ASN:ND2	3:E:603:HOH:O	2.32	0.60
1:C:358:VAL:HG11	1:C:408:LEU:HD21	1.82	0.60
1:C:173:GLU:HG2	1:C:197:LYS:HD2	1.84	0.59
1:C:355:GLU:HG2	1:C:419:LYS:HB3	1.84	0.59
1:D:321:GLU:OE1	1:D:330:ARG:NH2	2.36	0.58
1:D:437:ARG:NE	3:D:602:HOH:O	2.29	0.58
1:C:373:THR:HG22	1:C:454:TYR:HB2	1.84	0.58
1:E:68:ALA:O	3:E:601:HOH:O	2.17	0.58
1:C:374:ILE:HG22	1:C:376:GLU:H	1.68	0.58
1:D:344:LYS:HG3	1:D:385:LEU:HD23	1.84	0.58
1:C:351:GLN:NE2	1:C:353:GLU:OE2	2.36	0.58
1:C:23:GLN:HB2	1:C:51:ILE:HD11	1.87	0.57
1:B:405:LYS:NZ	3:B:605:HOH:O	2.37	0.56
1:F:291:ARG:NH1	3:F:605:HOH:O	2.36	0.56
1:E:247:GLN:O	3:E:602:HOH:O	2.18	0.56
1:D:346:GLU:HG3	1:D:383:LEU:HD13	1.87	0.55
1:A:51:ILE:HB	1:A:66:TYR:HB2	1.89	0.55
1:D:240:ASN:ND2	3:D:606:HOH:O	2.34	0.55
1:A:29:ARG:NH1	1:A:179:GLU:OE1	2.40	0.55
1:A:355:GLU:HG2	1:A:419:LYS:HB3	1.89	0.55
1:A:203:LEU:HD11	1:A:216:ASP:HB3	1.89	0.54
1:D:337:LYS:HG3	1:D:395:GLU:HB3	1.88	0.54
1:E:297:ASP:HA	1:E:323:GLU:HG3	1.88	0.54
1:D:448:ASP:HB2	1:D:457:THR:HG21	1.90	0.54
1:D:353:GLU:OE1	1:D:381:PRO:HD3	2.08	0.54
1:C:271:TRP:CE3	1:C:458:ALA:HB2	2.43	0.54
1:D:349:GLU:O	1:D:351:GLN:N	2.38	0.53
1:E:355:GLU:HG2	1:E:419:LYS:HB3	1.89	0.53
1:A:177:LEU:HD22	1:A:193:VAL:HG12	1.89	0.53
1:A:341:PHE:HB2	1:A:399:LEU:HD22	1.90	0.53
1:B:348:VAL:HB	1:B:381:PRO:HA	1.90	0.53
1:D:51:ILE:HB	1:D:66:TYR:HB2	1.91	0.52
1:A:177:LEU:HD21	1:A:197:LYS:HD3	1.92	0.52
1:C:321:GLU:HG2	1:C:330:ARG:HG2	1.91	0.52
1:A:57:SER:HB3	1:A:60:LYS:O	2.09	0.52
1:F:355:GLU:HG2	1:F:419:LYS:HB3	1.92	0.51
1:F:412:LYS:HA	1:F:417:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ARG:HH11	1:E:384:ASN:HD21	1.59	0.51
1:E:57:SER:HB3	1:E:60:LYS:O	2.10	0.51
1:F:73:LEU:O	3:F:601:HOH:O	2.20	0.50
1:E:188:LEU:HD21	1:E:225:LEU:HD23	1.93	0.50
1:A:257:ASP:OD2	1:D:107:ASN:ND2	2.44	0.50
1:D:188:LEU:HD21	1:D:225:LEU:HD23	1.93	0.50
1:D:338:GLU:N	1:D:338:GLU:OE2	2.44	0.49
3:B:621:HOH:O	1:D:276:LYS:HE3	2.11	0.49
1:D:57:SER:HB3	1:D:60:LYS:O	2.11	0.49
1:E:359:ALA:HB1	1:E:366:ILE:HD12	1.94	0.49
1:F:188:LEU:HD21	1:F:225:LEU:HD23	1.94	0.48
1:C:19:GLY:N	2:C:501:SO4:O3	2.36	0.48
1:B:342:PHE:HA	1:B:387:SER:HB2	1.96	0.47
1:C:366:ILE:HG21	1:C:370:ILE:HG13	1.96	0.47
1:B:370:ILE:HG13	1:B:382:ARG:CZ	2.44	0.47
1:F:350:PRO:HG2	1:F:415:ASN:OD1	2.14	0.47
1:A:335:LYS:O	1:A:395:GLU:HA	2.14	0.47
1:F:379:SER:N	3:F:609:HOH:O	2.48	0.47
1:A:337:LYS:O	1:A:399:LEU:HD12	2.15	0.47
1:C:348:VAL:HB	1:C:382:ARG:H	1.80	0.47
1:D:441:ILE:O	1:D:462:LEU:HD13	2.14	0.47
1:B:360:ILE:HG12	1:B:385:LEU:HD12	1.95	0.47
1:B:448:ASP:HB2	1:B:457:THR:HG21	1.96	0.47
1:C:275:ILE:HD11	1:C:458:ALA:HB1	1.97	0.47
1:B:51:ILE:HB	1:B:66:TYR:HB2	1.96	0.47
1:D:412:LYS:HA	1:D:417:LEU:HD12	1.96	0.47
1:E:23:GLN:HB2	1:E:51:ILE:HD11	1.97	0.47
1:A:205:SER:HA	3:A:627:HOH:O	2.15	0.46
1:D:374:ILE:HG22	1:D:376:GLU:H	1.80	0.46
1:A:15:ILE:HG23	1:F:201:LYS:HE2	1.97	0.46
1:B:171:ASN:O	1:B:175:ILE:HG12	2.16	0.46
1:A:138:ARG:NH2	1:A:160:ASP:OD1	2.50	0.45
1:D:344:LYS:CB	1:D:385:LEU:HA	2.47	0.45
1:E:344:LYS:HE3	1:E:383:LEU:HD11	1.98	0.45
1:A:207:SER:HB2	1:F:17:ARG:CZ	2.47	0.45
1:B:355:GLU:HG2	1:B:419:LYS:HB3	1.97	0.45
1:E:271:TRP:CE3	1:E:458:ALA:HB2	2.52	0.45
1:B:353:GLU:OE1	1:B:381:PRO:HD3	2.16	0.44
1:C:229:ARG:NH2	3:C:610:HOH:O	2.50	0.44
1:D:275:ILE:HD11	1:D:458:ALA:HB1	1.98	0.44
1:B:188:LEU:HD21	1:B:225:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HD11	1:B:216:ASP:HB3	1.99	0.44
1:B:190:ARG:HG2	1:B:194:LYS:HE3	1.98	0.44
1:B:362:PHE:HB3	1:B:387:SER:HB3	2.00	0.44
1:F:177:LEU:HD21	1:F:197:LYS:HD3	2.00	0.44
1:A:259:ASN:HA	1:A:301:ARG:HG3	2.00	0.44
1:B:424:ILE:O	3:B:603:HOH:O	2.21	0.44
1:D:58:SER:HB3	1:D:277:LYS:HG2	1.98	0.44
1:A:448:ASP:HB2	1:A:457:THR:HG21	1.99	0.44
1:F:51:ILE:HB	1:F:66:TYR:HB2	2.00	0.43
1:B:408:LEU:HD22	1:B:420:LEU:HD13	2.00	0.43
1:B:235:ASP:HA	1:B:236:PRO:HD3	1.91	0.43
1:D:120:LEU:HD21	1:D:137:GLY:HA3	1.99	0.43
1:B:275:ILE:HD11	1:B:458:ALA:HB1	2.00	0.43
1:A:84:ARG:HD2	3:A:610:HOH:O	2.19	0.43
1:C:323:GLU:HB3	1:C:328:ILE:HD13	2.00	0.43
1:D:342:PHE:HA	1:D:387:SER:HB2	2.01	0.43
1:C:374:ILE:HD12	1:C:374:ILE:H	1.84	0.43
1:F:383:LEU:HB2	1:F:411:PHE:CE2	2.54	0.43
1:A:121:ARG:O	3:A:602:HOH:O	2.21	0.42
1:B:346:GLU:HG3	1:B:349:GLU:OE2	2.19	0.42
1:C:57:SER:OG	1:C:60:LYS:O	2.33	0.42
1:E:262:ASP:OD2	1:F:108:THR:OG1	2.31	0.42
1:F:346:GLU:O	1:F:346:GLU:HG2	2.19	0.42
1:A:285:ILE:HD13	1:A:294:LEU:HD21	2.01	0.42
1:F:235:ASP:HA	1:F:236:PRO:HD3	1.92	0.42
1:D:348:VAL:HG21	1:D:415:ASN:OD1	2.19	0.42
1:F:23:GLN:HB2	1:F:51:ILE:HD11	2.01	0.42
1:C:434:LEU:O	1:C:438:LEU:HG	2.20	0.42
1:E:263:ARG:NH2	1:E:450:VAL:HG22	2.35	0.42
1:A:358:VAL:HG11	1:A:408:LEU:HD21	2.02	0.42
1:D:329:TYR:HB3	1:D:394:MET:SD	2.60	0.42
1:F:321:GLU:HG2	1:F:330:ARG:HG2	2.01	0.42
1:C:222:CYS:HB3	1:C:229:ARG:HG3	2.02	0.41
1:D:374:ILE:HD12	1:D:374:ILE:H	1.84	0.41
1:F:291:ARG:HD2	3:F:605:HOH:O	2.19	0.41
1:A:353:GLU:OE1	1:A:381:PRO:HD3	2.20	0.41
1:D:375:ASN:HA	1:D:378:LYS:HG2	2.02	0.41
1:F:457:THR:OG1	1:F:458:ALA:N	2.53	0.41
1:D:52:GLU:OE1	1:D:94:LYS:NZ	2.44	0.41
1:D:107:ASN:HB3	1:D:110:ILE:HG13	2.02	0.41
1:D:359:ALA:HB1	1:D:366:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:THR:HG22	1:D:454:TYR:HB2	2.03	0.41
1:A:300:GLN:HB2	1:A:305:ALA:HB2	2.02	0.41
1:E:370:ILE:HG13	1:E:382:ARG:CZ	2.50	0.41
1:E:77:GLU:O	1:E:81:GLU:HG2	2.20	0.41
1:F:397:LEU:HD11	1:F:430:PHE:HA	2.02	0.41
1:D:23:GLN:HB2	1:D:51:ILE:HD11	2.01	0.41
1:B:107:ASN:ND2	1:F:257:ASP:OD2	2.54	0.40
1:C:51:ILE:HB	1:C:66:TYR:HB2	2.04	0.40
1:E:51:ILE:HB	1:E:66:TYR:HB2	2.02	0.40
1:C:383:LEU:HD22	1:C:411:PHE:CG	2.56	0.40
1:C:138:ARG:NH2	1:C:160:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

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	433/462 (94%)	420 (97%)	13 (3%)	0	100	100
1	B	432/462 (94%)	422 (98%)	10 (2%)	0	100	100
1	C	434/462 (94%)	423 (98%)	11 (2%)	0	100	100
1	D	433/462 (94%)	417 (96%)	15 (4%)	1 (0%)	47	71
1	E	410/462 (89%)	404 (98%)	6 (2%)	0	100	100
1	F	413/462 (89%)	404 (98%)	9 (2%)	0	100	100
All	All	2555/2772 (92%)	2490 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	441	ILE

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	392/411 (95%)	389 (99%)	3 (1%)	81	92
1	B	391/411 (95%)	384 (98%)	7 (2%)	59	80
1	C	392/411 (95%)	388 (99%)	4 (1%)	76	90
1	D	392/411 (95%)	382 (97%)	10 (3%)	46	72
1	E	377/411 (92%)	369 (98%)	8 (2%)	53	77
1	F	376/411 (92%)	373 (99%)	3 (1%)	81	92
All	All	2320/2466 (94%)	2285 (98%)	35 (2%)	65	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	203	LEU
1	A	337	LYS
1	B	113	LEU
1	B	133	VAL
1	B	135	VAL
1	B	203	LEU
1	B	228	ASP
1	B	272	ASN
1	B	448	ASP
1	C	113	LEU
1	C	230	SER
1	C	272	ASN
1	C	402	ARG
1	D	29	ARG
1	D	84	ARG
1	D	138	ARG
1	D	296	ILE
1	D	343	THR
1	D	344	LYS
1	D	364	THR
1	D	396	THR

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Mol	Chain	Res	Type
1	D	412	LYS
1	D	448	ASP
1	E	29	ARG
1	E	108	THR
1	E	113	LEU
1	E	203	LEU
1	E	346	GLU
1	E	398	ASN
1	E	410	SER
1	E	413	SER
1	F	29	ARG
1	F	113	LEU
1	F	364	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	501	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	C	501	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	F	501	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	E	501	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	A	501	-	4,4,4	0.22	0	6,6,6	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/462 (94%)	-0.29	12 (2%) 54 48	28, 44, 84, 99	0
1	B	436/462 (94%)	-0.27	8 (1%) 68 64	26, 45, 83, 111	0
1	C	438/462 (94%)	-0.21	18 (4%) 37 30	21, 46, 105, 135	0
1	D	437/462 (94%)	-0.27	12 (2%) 54 48	21, 42, 79, 110	0
1	E	420/462 (90%)	-0.02	33 (7%) 12 9	24, 48, 110, 133	0
1	F	421/462 (91%)	-0.07	29 (6%) 16 12	28, 50, 100, 127	0
All	All	2589/2772 (93%)	-0.19	112 (4%) 35 28	21, 46, 97, 135	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	347	ALA	8.2
1	C	372	SER	5.5
1	E	348	VAL	5.3
1	E	372	SER	5.3
1	C	368	LYS	5.1
1	B	347	ALA	5.1
1	A	372	SER	5.1
1	E	452	GLY	5.0
1	C	348	VAL	4.8
1	F	352	GLY	4.7
1	F	348	VAL	4.5
1	A	171	ASN	4.5
1	E	413	SER	4.4
1	E	346	GLU	4.4
1	F	350	PRO	4.3
1	F	351	GLN	4.3
1	E	325	ASN	4.2
1	F	347	ALA	4.0
1	E	379	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	371	ASP	3.9
1	F	133	VAL	3.9
1	E	380	LEU	3.8
1	A	374	ILE	3.8
1	F	171	ASN	3.8
1	C	371	ASP	3.8
1	B	338	GLU	3.6
1	E	375	ASN	3.6
1	D	171	ASN	3.5
1	E	171	ASN	3.5
1	D	351	GLN	3.4
1	C	347	ALA	3.4
1	D	298	GLY	3.3
1	C	370	ILE	3.3
1	C	367	GLY	3.3
1	A	334	HIS	3.2
1	E	327	LEU	3.2
1	D	349	GLU	3.1
1	F	353	GLU	3.1
1	F	392	ASP	3.1
1	E	415	ASN	3.1
1	F	462	LEU	3.1
1	F	416	LYS	3.0
1	E	374	ILE	3.0
1	C	366	ILE	3.0
1	A	375	ASN	3.0
1	F	345	ILE	2.9
1	C	389	HIS	2.9
1	E	411	PHE	2.9
1	D	350	PRO	2.9
1	C	345	ILE	2.9
1	E	326	GLY	2.8
1	C	376	GLU	2.8
1	E	377	VAL	2.8
1	F	349	GLU	2.8
1	F	324	HIS	2.7
1	F	346	GLU	2.7
1	F	414	GLU	2.7
1	E	439	ASN	2.7
1	C	462	LEU	2.7
1	D	338	GLU	2.7
1	E	368	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	133	VAL	2.6
1	D	379	SER	2.6
1	E	418	SER	2.6
1	F	334	HIS	2.6
1	C	340	GLN	2.6
1	B	376	GLU	2.6
1	C	375	ASN	2.5
1	E	299	LYS	2.5
1	D	352	GLY	2.5
1	C	119	ARG	2.5
1	E	417	LEU	2.5
1	A	170	GLU	2.5
1	F	344	LYS	2.5
1	D	462	LEU	2.4
1	C	134	SER	2.4
1	F	411	PHE	2.4
1	F	418	SER	2.4
1	E	376	GLU	2.4
1	A	352	GLY	2.4
1	A	373	THR	2.4
1	A	190	ARG	2.4
1	E	395	GLU	2.4
1	A	133	VAL	2.4
1	F	393	ASN	2.3
1	D	371	ASP	2.3
1	E	345	ILE	2.3
1	B	171	ASN	2.3
1	B	335	LYS	2.3
1	B	416	LYS	2.2
1	B	375	ASN	2.2
1	E	392	ASP	2.2
1	F	342	PHE	2.2
1	A	172	SER	2.2
1	E	383	LEU	2.2
1	F	119	ARG	2.2
1	F	327	LEU	2.2
1	F	389	HIS	2.2
1	C	373	THR	2.1
1	E	370	ILE	2.1
1	D	343	THR	2.1
1	E	416	LYS	2.1
1	D	416	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	373	THR	2.1
1	F	394	MET	2.1
1	A	335	LYS	2.1
1	F	412	LYS	2.1
1	E	133	VAL	2.1
1	B	334	HIS	2.0
1	F	390	ALA	2.0
1	F	391	ILE	2.0
1	E	386	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	501	5/5	0.98	0.12	45,46,50,58	0
2	SO4	C	501	5/5	0.98	0.14	54,55,59,65	0
2	SO4	F	501	5/5	0.98	0.12	45,45,49,56	0
2	SO4	E	501	5/5	0.98	0.16	48,54,57,59	0
2	SO4	B	501	5/5	0.98	0.18	67,70,74,76	0
2	SO4	A	501	5/5	0.98	0.17	62,62,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.