



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:27 PM EDT

PDB ID : 6WAM / pdb_00006wam
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 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

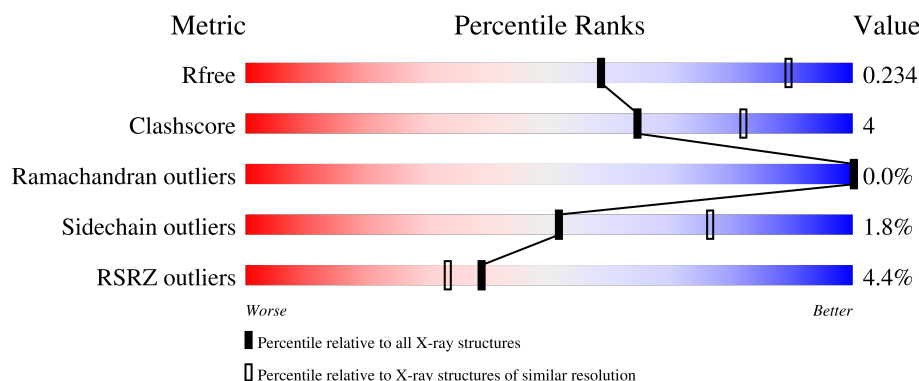
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

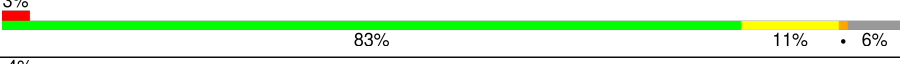
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	462	
1	B	462	
1	C	462	
1	D	462	

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Mol	Chain	Length	Quality of chain
1	E	462	7% 82% 9% 9%
1	F	462	5% 84% 7% 9%

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 (CCD ID: 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		

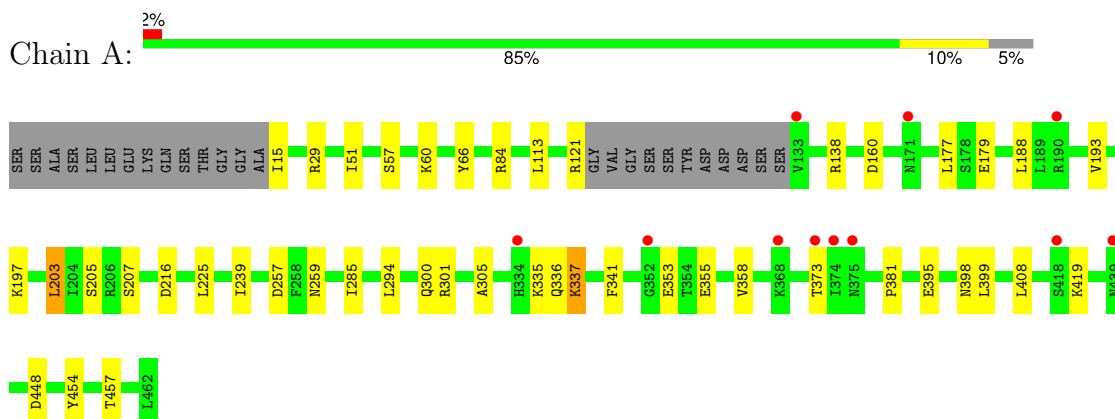
- Molecule 3 is water.

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		

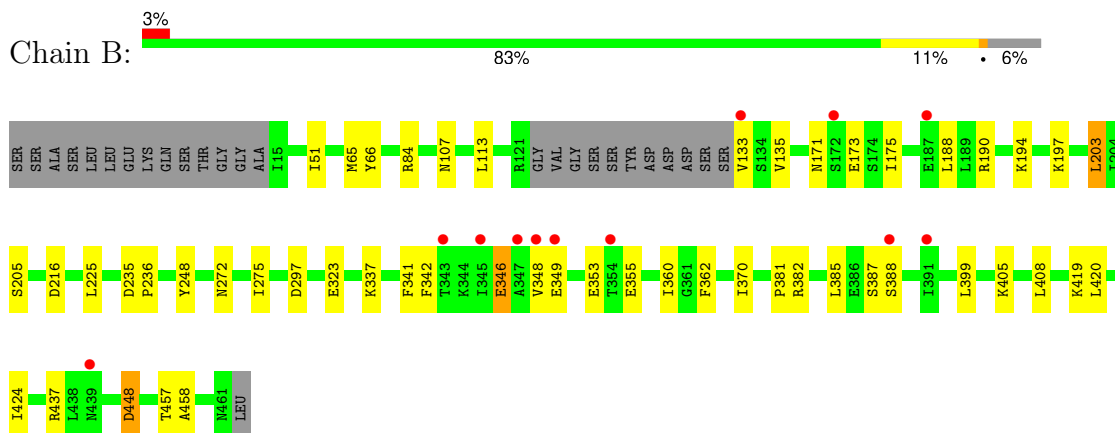
3 Residue-property plots [i](#)

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.

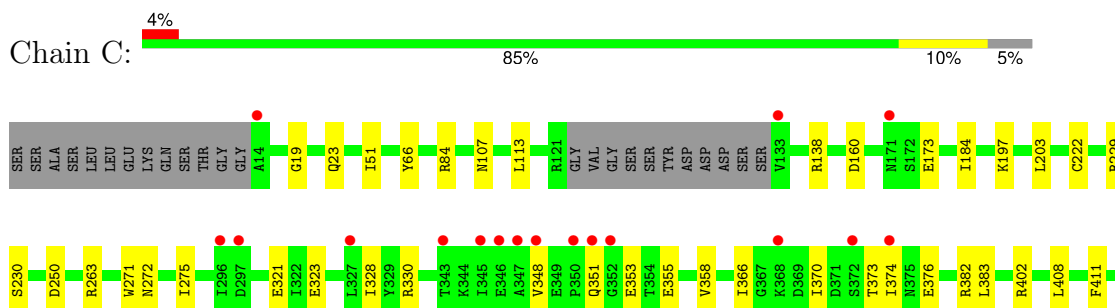
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein

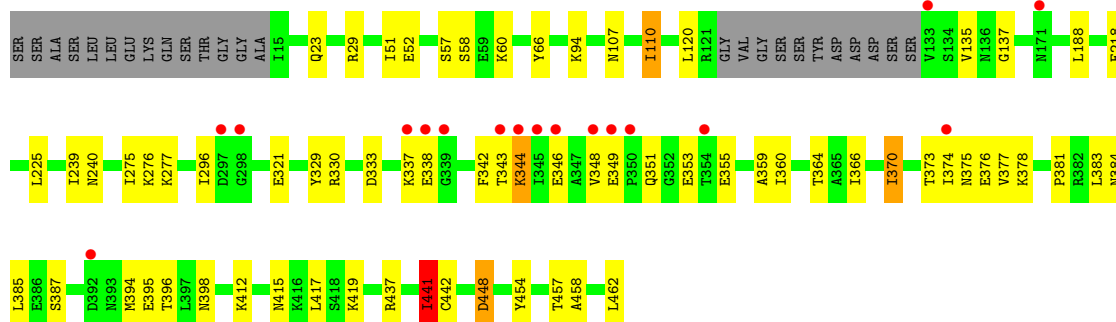
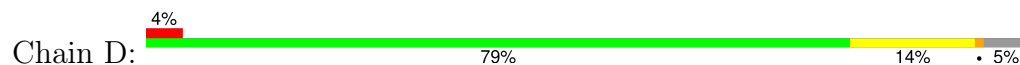


- Molecule 1: SAVED domain-containing protein

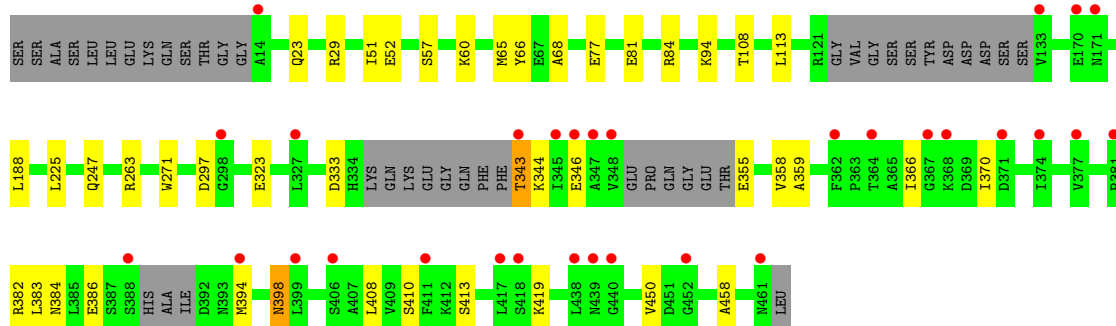
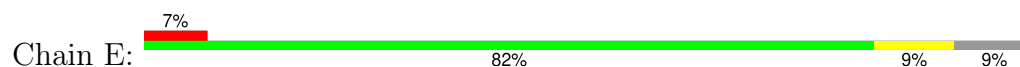




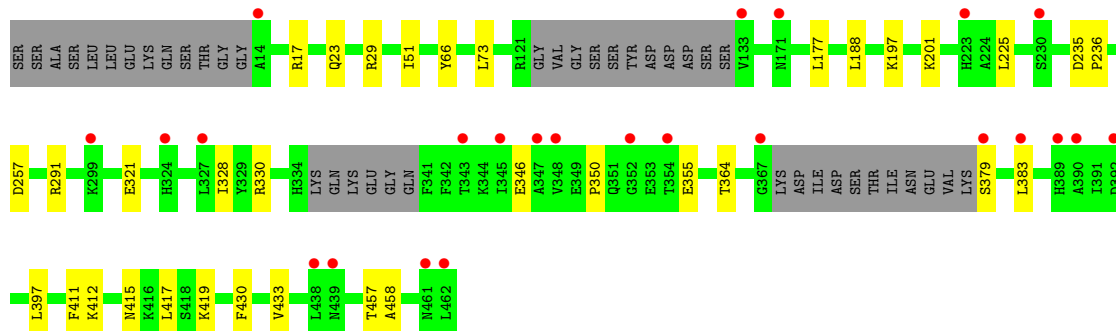
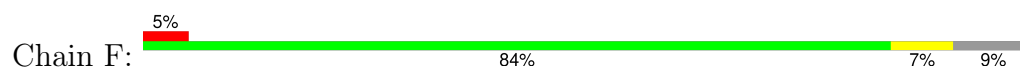
- Molecule 1: SAVED domain-containing protein



- 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) 86.2 (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 0.195 , 0.234	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)	0.32 , 39.6	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	0.18	0/3588	0.35	0/4849
1	B	0.19	0/3579	0.36	0/4838
1	C	0.18	0/3593	0.35	0/4856
1	D	0.19	0/3588	0.38	0/4849
1	E	0.17	0/3438	0.35	0/4645
1	F	0.17	0/3455	0.35	0/4670
All	All	0.18	0/21241	0.36	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	28	0
1	C	3518	0	3466	24	0
1	D	3513	0	3461	42	0
1	E	3370	0	3323	21	0
1	F	3382	0	3324	22	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	160	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 (160) 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:E:343:THR:OG1	1:E:386:GLU:O	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:333:ASP:HB2	1:D:394:MET:HE2	1.82	0.60
1:C:173:GLU:HG2	1:C:197:LYS:HD2	1.84	0.59
1:B:65:MET:HE2	1:B:84:ARG:HH12	1.68	0.59
1:E:333:ASP:HB3	1:E:394:MET:HE2	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:B:387:SER:OG	1:B:388:SER:N	2.28	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:F:291:ARG:NH1	3:F:605:HOH:O	2.36	0.56
1:D:394:MET:HE3	1:D:398:ASN:HD21	1.70	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:B:405:LYS:NZ	3:B:605:HOH:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:57:SER:HB3	1:E:60:LYS:O	2.10	0.51
1:E:382:ARG:HH11	1:E:384:ASN:HD21	1.59	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
1:E:52:GLU:OE1	1:E:94:LYS:NZ	2.42	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:346:GLU:HG2	1:F:346:GLU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:MET:HE2	1:E:84:ARG:HH22	1.86	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
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:D:23:GLN:HB2	1:D:51:ILE:HD11	2.01	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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	43	66
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%)	73	88
1	B	391/411 (95%)	383 (98%)	8 (2%)	48	74
1	C	392/411 (95%)	385 (98%)	7 (2%)	51	76
1	D	392/411 (95%)	379 (97%)	13 (3%)	33	61
1	E	377/411 (92%)	369 (98%)	8 (2%)	47	73
1	F	376/411 (92%)	373 (99%)	3 (1%)	73	88
All	All	2320/2466 (94%)	2278 (98%)	42 (2%)	51	76

All (42) 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	272	ASN
1	B	346	GLU
1	B	437	ARG
1	B	448	ASP
1	C	84	ARG
1	C	107	ASN
1	C	113	LEU
1	C	203	LEU
1	C	230	SER
1	C	272	ASN
1	C	402	ARG

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Mol	Chain	Res	Type
1	D	29	ARG
1	D	110	ILE
1	D	135	VAL
1	D	239	ILE
1	D	296	ILE
1	D	343	THR
1	D	344	LYS
1	D	364	THR
1	D	370	ILE
1	D	377	VAL
1	D	396	THR
1	D	441	ILE
1	D	448	ASP
1	E	29	ARG
1	E	108	THR
1	E	113	LEU
1	E	343	THR
1	E	346	GLU
1	E	398	ASN
1	E	410	SER
1	E	413	SER
1	F	29	ARG
1	F	328	ILE
1	F	364	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	ASN
1	C	168	ASN
1	C	171	ASN
1	C	181	GLN
1	C	324	HIS
1	D	71	HIS
1	D	171	ASN
1	D	181	GLN
1	D	324	HIS
1	D	375	ASN
1	D	398	ASN
1	D	439	ASN
1	E	181	GLN
1	E	286	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	501	-	4,4,4	0.23	0	6,6,6	0.19	0
2	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	C	501	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	E	501	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	F	501	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.12	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%)	-0.08	11 (2%) 58 52	28, 44, 84, 99	0
1	B	436/462 (94%)	-0.10	12 (2%) 55 49	26, 45, 83, 111	0
1	C	438/462 (94%)	0.02	19 (4%) 40 34	21, 46, 105, 135	0
1	D	437/462 (94%)	-0.15	17 (3%) 43 38	21, 42, 79, 110	0
1	E	420/462 (90%)	0.16	31 (7%) 20 16	24, 48, 110, 133	0
1	F	421/462 (91%)	0.08	24 (5%) 29 24	28, 50, 100, 127	0
All	All	2589/2772 (93%)	-0.01	114 (4%) 39 33	21, 46, 97, 135	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	ALA	5.3
1	D	345	ILE	5.3
1	D	343	THR	5.2
1	C	345	ILE	5.0
1	E	347	ALA	4.9
1	C	348	VAL	4.8
1	E	348	VAL	4.8
1	F	367	GLY	4.7
1	D	298	GLY	4.3
1	E	388	SER	4.1
1	E	343	THR	3.9
1	E	374	ILE	3.9
1	D	346	GLU	3.8
1	D	344	LYS	3.7
1	D	350	PRO	3.7
1	F	348	VAL	3.6
1	C	343	THR	3.6
1	F	347	ALA	3.6
1	C	133	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	462	LEU	3.6
1	F	462	LEU	3.6
1	E	439	ASN	3.4
1	F	345	ILE	3.4
1	D	133	VAL	3.4
1	E	345	ILE	3.3
1	E	399	LEU	3.3
1	F	343	THR	3.2
1	F	133	VAL	3.2
1	C	14	ALA	3.1
1	F	14	ALA	3.1
1	B	343	THR	3.1
1	E	461	ASN	3.1
1	C	374	ILE	3.1
1	D	348	VAL	3.1
1	B	133	VAL	3.0
1	E	438	LEU	3.0
1	A	374	ILE	3.0
1	B	348	VAL	3.0
1	A	439	ASN	3.0
1	E	452	GLY	3.0
1	C	372	SER	3.0
1	F	324	HIS	2.9
1	C	350	PRO	2.9
1	A	171	ASN	2.9
1	D	297	ASP	2.9
1	E	327	LEU	2.8
1	D	339	GLY	2.8
1	F	438	LEU	2.8
1	D	338	GLU	2.8
1	E	133	VAL	2.8
1	B	172	SER	2.8
1	A	334	HIS	2.8
1	E	364	THR	2.7
1	E	440	GLY	2.6
1	F	379	SER	2.6
1	D	374	ILE	2.6
1	A	133	VAL	2.6
1	C	297	ASP	2.6
1	E	368	LYS	2.6
1	C	347	ALA	2.6
1	C	296	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	368	LYS	2.6
1	F	354	THR	2.5
1	E	298	GLY	2.5
1	E	417	LEU	2.5
1	F	439	ASN	2.5
1	E	371	ASP	2.5
1	F	390	ALA	2.4
1	F	171	ASN	2.4
1	F	461	ASN	2.4
1	E	170	GLU	2.4
1	C	327	LEU	2.3
1	C	352	GLY	2.3
1	C	171	ASN	2.3
1	D	171	ASN	2.3
1	F	299	LYS	2.3
1	A	352	GLY	2.3
1	F	352	GLY	2.3
1	B	439	ASN	2.3
1	C	346	GLU	2.3
1	E	346	GLU	2.3
1	A	418	SER	2.3
1	C	438	LEU	2.3
1	D	337	LYS	2.2
1	C	351	GLN	2.2
1	F	230	SER	2.2
1	E	418	SER	2.2
1	D	349	GLU	2.2
1	D	354	THR	2.2
1	F	389	HIS	2.2
1	A	190	ARG	2.1
1	E	381	PRO	2.1
1	E	367	GLY	2.1
1	E	377	VAL	2.1
1	E	411	PHE	2.1
1	B	349	GLU	2.1
1	A	373	THR	2.1
1	B	391	ILE	2.1
1	E	406	SER	2.1
1	E	14	ALA	2.1
1	E	362	PHE	2.1
1	F	392	ASP	2.1
1	B	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	171	ASN	2.1
1	F	223	HIS	2.1
1	E	394	MET	2.0
1	F	327	LEU	2.0
1	F	383	LEU	2.0
1	A	375	ASN	2.0
1	D	392	ASP	2.0
1	A	368	LYS	2.0
1	B	388	SER	2.0
1	B	354	THR	2.0
1	B	345	ILE	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
2	SO4	B	501	5/5	0.93	0.13	67,70,74,76	0
2	SO4	A	501	5/5	0.94	0.11	62,62,73,75	0
2	SO4	C	501	5/5	0.94	0.10	54,55,59,65	0
2	SO4	F	501	5/5	0.96	0.07	45,45,49,56	0
2	SO4	E	501	5/5	0.97	0.08	48,54,57,59	0
2	SO4	D	501	5/5	0.97	0.06	45,46,50,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.