



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 01:20 AM UTC

PDB ID : 6O38 / pdb_00006o38
Title : Structure of a chaperone-substrate complex
Authors : Urusova, D.V.; Tolia, N.H.
Deposited on : 2019-02-26
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

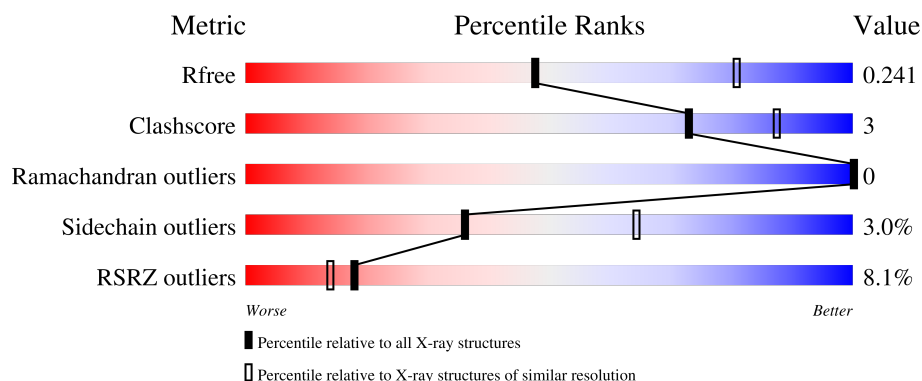
1 Overall quality at a glance

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	578	4% 91% 8%
1	B	578	3% 89% 10%
1	C	578	8% 79% 9% 11%
1	D	578	5% 91% 8%
1	E	578	2% 90% 9%

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Mol	Chain	Length	Quality of chain
1	F	578	11% 88% 9%
2	G	178	12% 61% 10% 28%
2	H	178	10% 53% 13% 34%
2	K	178	22% 53% 13% 34%
2	L	178	7% 62% 10% 27%
2	M	178	8% 60% 11% 28%
2	N	178	14% 58% 10% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32308 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 Acinetobacter secreted protease CpaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	B	573	Total	C	N	O	S	Se	0	0	0
			4398	2771	743	874	2	8			
1	C	514	Total	C	N	O	S	Se	0	0	0
			3949	2496	666	777	2	8			
1	D	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	E	573	Total	C	N	O	S	Se	0	0	0
			4399	2771	744	874	2	8			
1	F	561	Total	C	N	O	S	Se	0	0	0
			4308	2715	727	856	2	8			

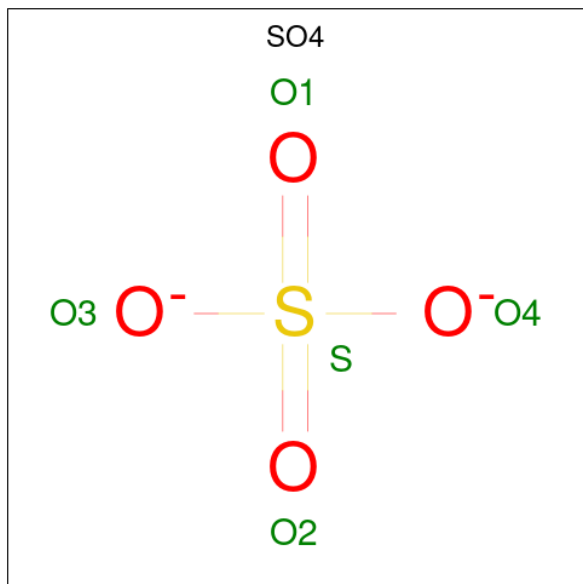
- Molecule 2 is a protein called Type II secretion chaperone CpaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	128	Total	C	N	O	Se	0	0	0
			1038	654	175	205	4			
2	H	118	Total	C	N	O	Se	0	0	0
			958	607	160	187	4			
2	K	117	Total	C	N	O	Se	0	0	0
			945	595	159	187	4			
2	L	130	Total	C	N	O	Se	0	0	0
			1054	664	178	208	4			
2	M	129	Total	C	N	O	Se	0	0	0
			1046	658	176	208	4			
2	N	124	Total	C	N	O	Se	0	0	0
			1006	635	170	197	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	54	Total	O	0	0
			54	54		
5	C	38	Total	O	0	0
			38	38		

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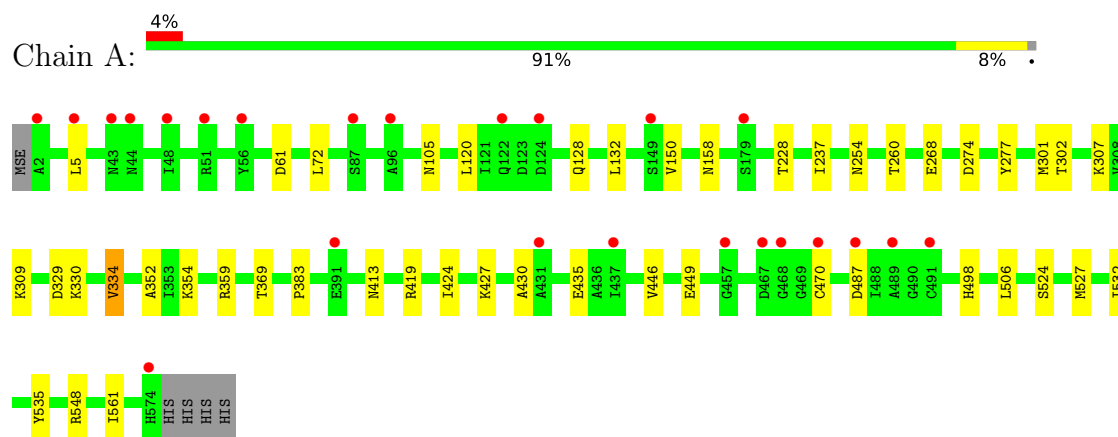
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	49	Total 49	O 49	0	0
5	E	56	Total 56	O 56	0	0
5	F	46	Total 46	O 46	0	0
5	H	3	Total 3	O 3	0	0
5	L	5	Total 5	O 5	0	0
5	M	3	Total 3	O 3	0	0
5	N	3	Total 3	O 3	0	0

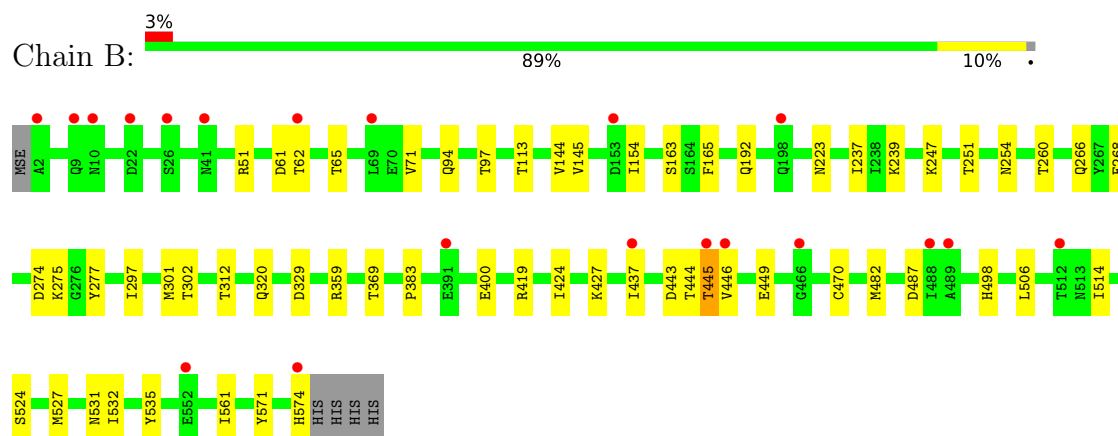
3 Residue-property plots [i](#)

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.

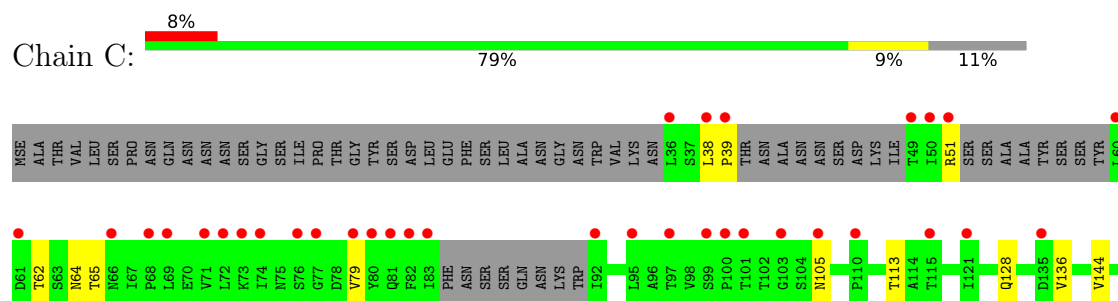
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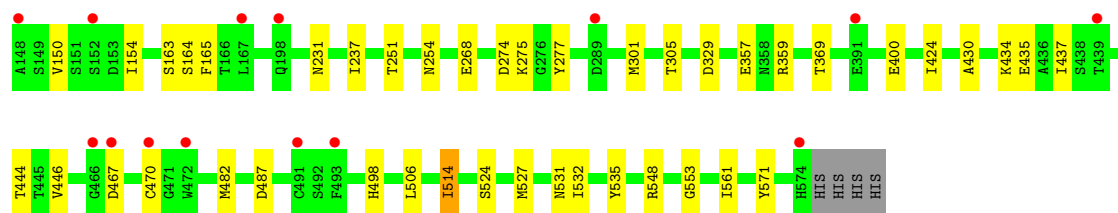


- Molecule 1: *Acinetobacter* secreted protease CpaA

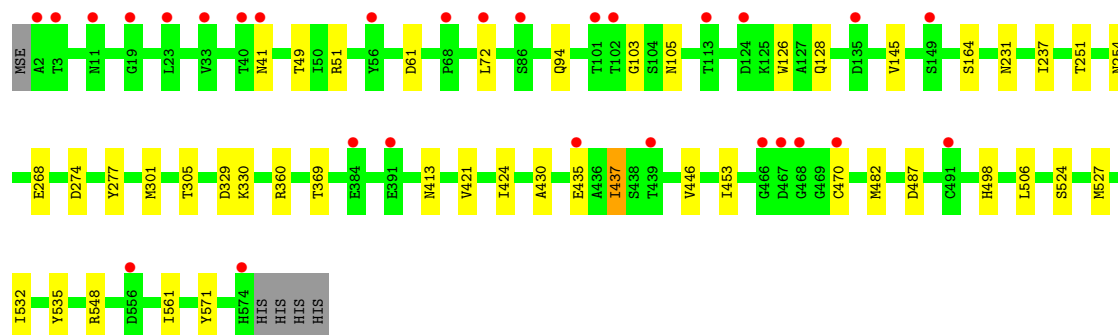
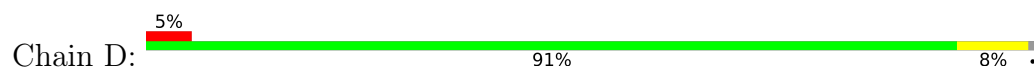


- Molecule 1: *Acinetobacter* secreted protease CpaA

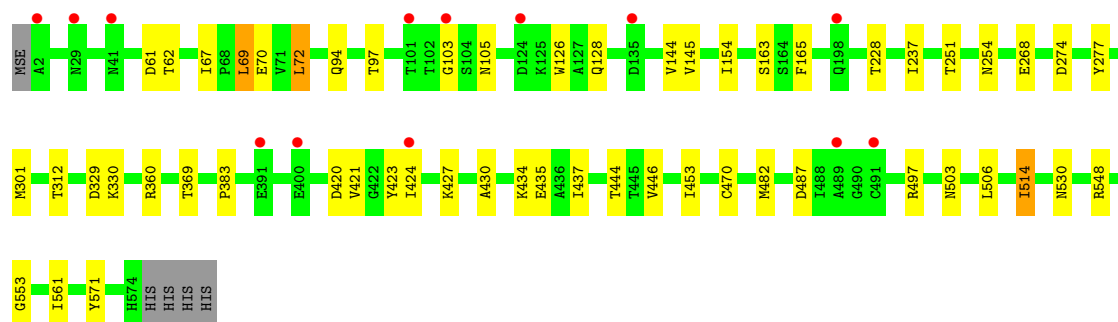
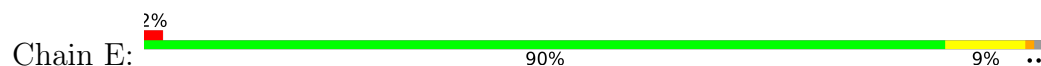




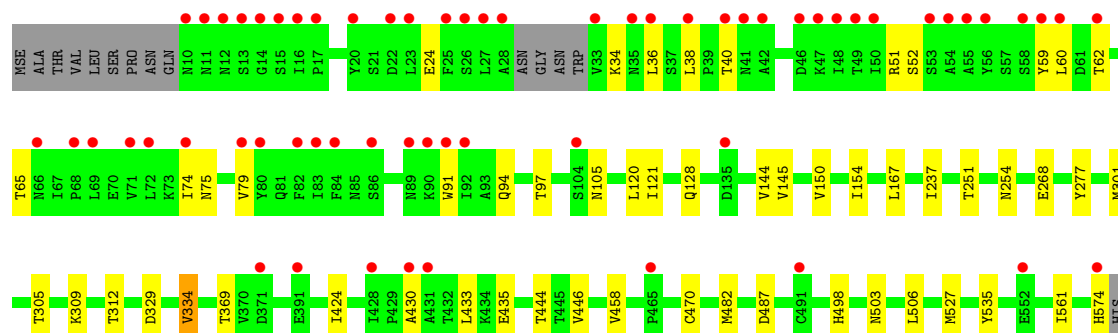
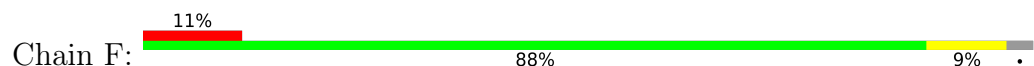
● Molecule 1: Acinetobacter secreted protease CpaA



● Molecule 1: Acinetobacter secreted protease CpaA



● Molecule 1: Acinetobacter secreted protease CpaA



HIS
HIS
HIS

• Molecule 2: Type II secretion chaperone CpaB

Chain G: 

MSE GLN SER SER SER LEU THR PHE SER PRO GLU SER ARG GLN GLN SER GLY ALA LYS MSE P33 S34 E35 K36 E37 R38 L39 S40 F46 V49 GLU LYS ASP GLN LEU HIS SER LYS ALA ASN PHE PRO LEU LYS ASN ALA

K66 G67 M68 K75 T85 V86 F88 Q89 M90 N96 E105 P106 V107 D108 I111 D119 Q120 G121 D122 D136 H137 Y138 M141 A152 E153 I154 G159 L160 V161 T163 V168 H174 H175 ASP HIS PRO

• Molecule 2: Type II secretion chaperone CpaB

Chain H: 

MSE GLN SER SER SER LEU THR PHE SER PRO GLU SER ARG GLN GLN SER GLY ALA LYS MSE Q42 Q43 I44 V45 V49 LYS ASP GLN LEU HIS SER LYS ALA ASN PHE PRO LEU

LYS ASN K66 G67 M68 Y72 L79 K81 T85 V86 M90 G94 I95 N96 E103 I104 E105 P106 V107 D110 R113 F118 D119 Q120 Q125 T129 I130 S133 M141 I143 E146 K147 A152 E153 I154 V161 Q162 T163 M164 D165

E166 T169 L173 H174 H175 ASP HIS PRO

• Molecule 2: Type II secretion chaperone CpaB

Chain K: 

MSE GLN SER SER SER LEU THR PHE SER PRO GLU SER ARG GLN GLN SER GLY ALA LYS MSE Q41 Q42 Q43 I44 V45 F46 H47 E48 VAL GLU LYS ASP GLN LEU HIS SER LYS ALA ASN PHE PRO

LEU LEU LYS ASN ALA LYS G67 G68 V69 I70 K75 E78 L79 R80 K81 V86 K87 F88 Q89 M90 L91 F92 T94 G94 I95 N96 R97 E103 I104 E105 P106 D110 I111 V112 R113 W114 T115 F118 D119 Q120 G121 Q125 H126 K135 D136 H137 M141 E146 S151

A152 E153 I154 L160 M164 D166 E166 G167 V168 T169 L173 H174 H175 ASP HIS PRO

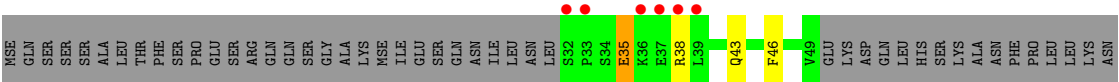
• Molecule 2: Type II secretion chaperone CpaB

Chain L: 

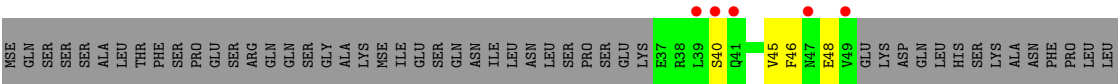
MSE GLN SER SER SER LEU THR PHE SER PRO GLU SER ARG GLN GLN SER GLY ALA LYS MSE N30 L31 S32 P33 S34 E35 K36 E37 R38 L39 S40 V45 E48 V49 GLU LYS ASP GLN LEU HIS SER LYS ALA ASN PHE PRO LEU LYS ASN



• Molecule 2: Type II secretion chaperone CpaB



• Molecule 2: Type II secretion chaperone CpaB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.75Å 118.49Å 129.58Å 108.94° 103.97° 100.10°	Depositor
Resolution (Å)	35.79 – 2.60 35.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.5 (35.79-2.60) 89.4 (35.79-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.225 , 0.240 0.225 , 0.241	Depositor DCC
R_{free} test set	7917 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	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	0.92	EDS
Total number of atoms	32308	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.09	0/4485	0.28	0/6109
1	B	0.09	0/4484	0.27	0/6107
1	C	0.09	0/4021	0.28	0/5470
1	D	0.09	0/4485	0.27	0/6109
1	E	0.09	0/4485	0.28	0/6109
1	F	0.10	0/4390	0.29	0/5975
2	G	0.12	0/1051	0.35	0/1407
2	H	0.12	0/970	0.31	0/1299
2	K	0.10	0/955	0.32	0/1277
2	L	0.09	0/1067	0.31	0/1429
2	M	0.10	0/1059	0.31	0/1418
2	N	0.13	0/1018	0.32	0/1363
All	All	0.09	0/32470	0.29	0/44072

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

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	4399	0	4306	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4398	0	4302	29	0
1	C	3949	0	3895	26	0
1	D	4399	0	4306	20	0
1	E	4399	0	4306	25	0
1	F	4308	0	4222	22	0
2	G	1038	0	1017	8	0
2	H	958	0	938	14	0
2	K	945	0	919	12	0
2	L	1054	0	1034	10	0
2	M	1046	0	1021	13	0
2	N	1006	0	986	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	15	0	0	1	0
4	B	15	0	0	2	0
4	C	15	0	0	1	0
4	D	5	0	0	1	0
4	E	10	0	0	0	0
4	F	15	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	L	10	0	0	0	0
4	M	10	0	0	1	0
4	N	5	0	0	0	0
5	A	36	0	0	2	0
5	B	54	0	0	2	0
5	C	38	0	0	0	0
5	D	49	0	0	0	0
5	E	56	0	0	1	0
5	F	46	0	0	0	0
5	H	3	0	0	0	0
5	L	5	0	0	0	0
5	M	3	0	0	0	0
5	N	3	0	0	0	0
All	All	32308	0	31252	204	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 3.

The worst 5 of 204 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)
2:N:68:MSE:HE1	2:N:90:MSE:HG2	1.63	0.80
2:G:68:MSE:HE1	2:G:90:MSE:HG2	1.64	0.80
2:M:68:MSE:HE1	2:M:90:MSE:HG2	1.66	0.77
2:H:68:MSE:HE1	2:H:90:MSE:HG2	1.69	0.74
2:H:94:GLY:O	2:H:147:LYS:NZ	2.24	0.71

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	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	B	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	C	506/578 (88%)	498 (98%)	8 (2%)	0	100	100
1	D	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	E	571/578 (99%)	563 (99%)	8 (1%)	0	100	100
1	F	557/578 (96%)	549 (99%)	8 (1%)	0	100	100
2	G	124/178 (70%)	121 (98%)	3 (2%)	0	100	100
2	H	114/178 (64%)	113 (99%)	1 (1%)	0	100	100
2	K	111/178 (62%)	110 (99%)	1 (1%)	0	100	100
2	L	126/178 (71%)	117 (93%)	9 (7%)	0	100	100
2	M	125/178 (70%)	123 (98%)	2 (2%)	0	100	100
2	N	120/178 (67%)	118 (98%)	2 (2%)	0	100	100
All	All	4067/4536 (90%)	4001 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	485/481 (101%)	477 (98%)	8 (2%)	55	79
1	B	485/481 (101%)	471 (97%)	14 (3%)	37	65
1	C	434/481 (90%)	423 (98%)	11 (2%)	42	69
1	D	485/481 (101%)	473 (98%)	12 (2%)	42	69
1	E	485/481 (101%)	471 (97%)	14 (3%)	37	65
1	F	475/481 (99%)	458 (96%)	17 (4%)	31	58
2	G	117/156 (75%)	109 (93%)	8 (7%)	14	32
2	H	107/156 (69%)	103 (96%)	4 (4%)	30	57
2	K	106/156 (68%)	102 (96%)	4 (4%)	29	56
2	L	119/156 (76%)	115 (97%)	4 (3%)	32	60
2	M	118/156 (76%)	112 (95%)	6 (5%)	21	45
2	N	112/156 (72%)	107 (96%)	5 (4%)	24	50
All	All	3528/3822 (92%)	3421 (97%)	107 (3%)	36	64

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	446	VAL
1	F	424	ILE
2	M	129	THR
1	F	34	LYS
1	F	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	88	GLN
1	E	355	ASN
2	K	142	GLN
1	E	223	ASN

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Mol	Chain	Res	Type
1	E	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	F	603	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	E	603	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	E	602	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	L	201	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	M	201	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	B	604	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	H	201	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	L	202	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	F	604	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	603	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	N	201	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	603	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	C	604	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	M	202	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	G	201	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	B	603	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	F	602	-	4,4,4	0.24	0	6,6,6	0.07	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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	SO4	1	0
4	C	603	SO4	1	0
4	A	603	SO4	1	0
4	D	602	SO4	1	0
4	M	202	SO4	1	0
4	B	603	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	565/578 (97%)	0.56	24 (4%)	40 35	31, 52, 78, 91	0
1	B	565/578 (97%)	0.44	20 (3%)	47 41	28, 43, 67, 80	0
1	C	506/578 (87%)	0.71	48 (9%)	14 10	31, 50, 102, 113	0
1	D	565/578 (97%)	0.56	29 (5%)	33 28	29, 45, 74, 82	0
1	E	565/578 (97%)	0.33	13 (2%)	61 55	28, 41, 64, 74	0
1	F	553/578 (95%)	0.76	62 (11%)	10 8	29, 51, 107, 124	0
2	G	124/178 (69%)	1.26	21 (16%)	4 3	56, 73, 101, 117	0
2	H	114/178 (64%)	1.22	17 (14%)	5 4	54, 68, 81, 94	0
2	K	113/178 (63%)	1.73	40 (35%)	1 1	63, 87, 107, 122	0
2	L	126/178 (70%)	1.02	13 (10%)	12 9	46, 57, 93, 104	0
2	M	125/178 (70%)	0.99	14 (11%)	10 8	45, 58, 96, 117	0
2	N	120/178 (67%)	1.43	25 (20%)	2 2	59, 77, 89, 103	0
All	All	4041/4536 (89%)	0.68	326 (8%)	18 14	28, 51, 89, 124	0

The worst 5 of 326 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	33	VAL	6.1
2	M	39	LEU	5.8
2	L	31	LEU	5.5
1	B	2	ALA	5.4
1	F	25	PHE	5.3

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	H	201	5/5	0.59	0.14	95,95,95,95	5
4	SO4	N	201	5/5	0.68	0.14	85,85,85,85	5
4	SO4	F	604	5/5	0.70	0.19	43,43,43,43	5
4	SO4	F	602	5/5	0.78	0.13	60,63,71,77	5
4	SO4	E	603	5/5	0.78	0.15	48,48,48,48	5
4	SO4	F	603	5/5	0.80	0.12	51,51,51,51	5
4	SO4	A	603	5/5	0.83	0.13	51,51,51,51	5
4	SO4	G	201	5/5	0.84	0.11	74,76,80,83	5
4	SO4	A	604	5/5	0.84	0.14	45,45,45,45	5
4	SO4	L	201	5/5	0.84	0.12	55,60,70,76	5
4	SO4	B	604	5/5	0.84	0.17	41,41,41,41	5
4	SO4	A	602	5/5	0.86	0.20	66,72,77,90	0
4	SO4	L	202	5/5	0.86	0.10	60,63,67,68	5
4	SO4	D	602	5/5	0.86	0.14	42,42,42,42	5
4	SO4	M	202	5/5	0.88	0.10	54,56,64,70	5
4	SO4	C	603	5/5	0.88	0.15	40,41,45,48	5
4	SO4	E	602	5/5	0.89	0.12	35,35,37,38	5
4	SO4	M	201	5/5	0.89	0.13	57,63,79,83	0
4	SO4	B	602	5/5	0.90	0.09	52,59,64,79	5
4	SO4	C	602	5/5	0.91	0.13	53,60,71,80	0
4	SO4	C	604	5/5	0.92	0.09	47,49,52,52	5
4	SO4	B	603	5/5	0.92	0.09	51,51,51,51	5
3	ZN	A	601	1/1	0.98	0.03	55,55,55,55	0
3	ZN	D	601	1/1	0.99	0.03	43,43,43,43	0
3	ZN	F	601	1/1	0.99	0.04	55,55,55,55	0
3	ZN	B	601	1/1	0.99	0.02	45,45,45,45	0
3	ZN	C	601	1/1	0.99	0.02	50,50,50,50	0
3	ZN	E	601	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.