



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:41 AM UTC

PDB ID : 4NF0 / pdb_00004nf0
Title : CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM PSEUDOMONAS AERUGINOSA PAO1 (PA4616), TARGET EFI-510182, WITH BOUND L-Malate
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Deposited on : 2013-10-30
Resolution : 1.85 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)

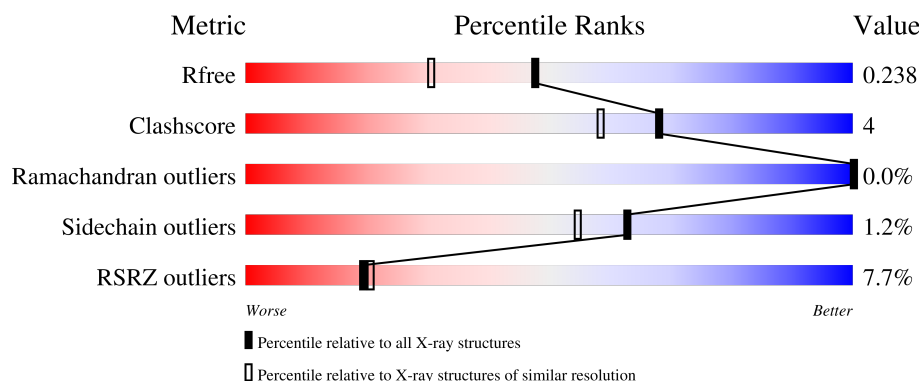
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	339	
1	B	339	
1	C	339	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	339	81% 5% 15%
1	E	339	34% 56% 12% 31%
1	F	339	2% 79% 5% 15%
1	G	339	2% 77% 7% 15%
1	H	339	8% 64% 12% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19172 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 Probable c4-dicarboxylate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2299	1462	395	435	7			
1	B	273	Total	C	N	O	S	0	0	0
			2156	1369	370	410	7			
1	C	291	Total	C	N	O	S	0	1	0
			2297	1464	393	433	7			
1	D	289	Total	C	N	O	S	0	1	0
			2280	1448	391	434	7			
1	E	233	Total	C	N	O	S	0	0	0
			1780	1127	301	346	6			
1	F	288	Total	C	N	O	S	0	0	0
			2281	1451	392	431	7			
1	G	287	Total	C	N	O	S	0	0	0
			2276	1449	392	428	7			
1	H	261	Total	C	N	O	S	0	0	0
			2056	1308	348	393	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	-	expression tag	UNP Q9HVVH5
A	335	GLU	-	expression tag	UNP Q9HVVH5
A	336	ASN	-	expression tag	UNP Q9HVVH5
A	337	LEU	-	expression tag	UNP Q9HVVH5
A	338	TYR	-	expression tag	UNP Q9HVVH5
A	339	PHE	-	expression tag	UNP Q9HVVH5
A	340	GLN	-	expression tag	UNP Q9HVVH5
B	334	ALA	-	expression tag	UNP Q9HVVH5
B	335	GLU	-	expression tag	UNP Q9HVVH5
B	336	ASN	-	expression tag	UNP Q9HVVH5
B	337	LEU	-	expression tag	UNP Q9HVVH5
B	338	TYR	-	expression tag	UNP Q9HVVH5
B	339	PHE	-	expression tag	UNP Q9HVVH5

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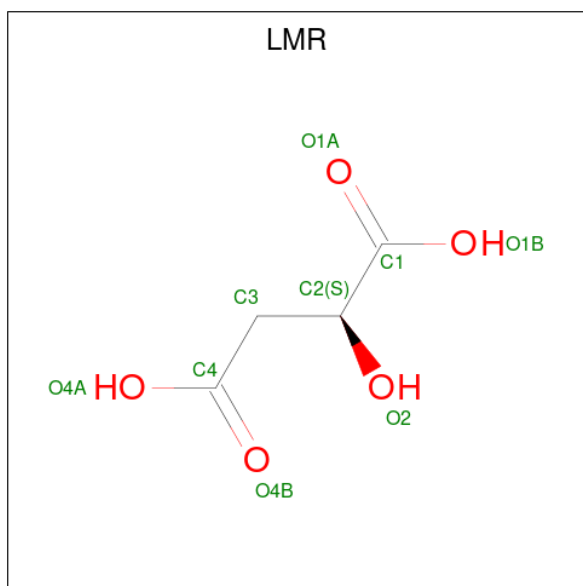
Chain	Residue	Modelled	Actual	Comment	Reference
B	340	GLN	-	expression tag	UNP Q9HVVH5
C	334	ALA	-	expression tag	UNP Q9HVVH5
C	335	GLU	-	expression tag	UNP Q9HVVH5
C	336	ASN	-	expression tag	UNP Q9HVVH5
C	337	LEU	-	expression tag	UNP Q9HVVH5
C	338	TYR	-	expression tag	UNP Q9HVVH5
C	339	PHE	-	expression tag	UNP Q9HVVH5
C	340	GLN	-	expression tag	UNP Q9HVVH5
D	334	ALA	-	expression tag	UNP Q9HVVH5
D	335	GLU	-	expression tag	UNP Q9HVVH5
D	336	ASN	-	expression tag	UNP Q9HVVH5
D	337	LEU	-	expression tag	UNP Q9HVVH5
D	338	TYR	-	expression tag	UNP Q9HVVH5
D	339	PHE	-	expression tag	UNP Q9HVVH5
D	340	GLN	-	expression tag	UNP Q9HVVH5
E	334	ALA	-	expression tag	UNP Q9HVVH5
E	335	GLU	-	expression tag	UNP Q9HVVH5
E	336	ASN	-	expression tag	UNP Q9HVVH5
E	337	LEU	-	expression tag	UNP Q9HVVH5
E	338	TYR	-	expression tag	UNP Q9HVVH5
E	339	PHE	-	expression tag	UNP Q9HVVH5
E	340	GLN	-	expression tag	UNP Q9HVVH5
F	334	ALA	-	expression tag	UNP Q9HVVH5
F	335	GLU	-	expression tag	UNP Q9HVVH5
F	336	ASN	-	expression tag	UNP Q9HVVH5
F	337	LEU	-	expression tag	UNP Q9HVVH5
F	338	TYR	-	expression tag	UNP Q9HVVH5
F	339	PHE	-	expression tag	UNP Q9HVVH5
F	340	GLN	-	expression tag	UNP Q9HVVH5
G	334	ALA	-	expression tag	UNP Q9HVVH5
G	335	GLU	-	expression tag	UNP Q9HVVH5
G	336	ASN	-	expression tag	UNP Q9HVVH5
G	337	LEU	-	expression tag	UNP Q9HVVH5
G	338	TYR	-	expression tag	UNP Q9HVVH5
G	339	PHE	-	expression tag	UNP Q9HVVH5
G	340	GLN	-	expression tag	UNP Q9HVVH5
H	334	ALA	-	expression tag	UNP Q9HVVH5
H	335	GLU	-	expression tag	UNP Q9HVVH5
H	336	ASN	-	expression tag	UNP Q9HVVH5
H	337	LEU	-	expression tag	UNP Q9HVVH5
H	338	TYR	-	expression tag	UNP Q9HVVH5
H	339	PHE	-	expression tag	UNP Q9HVVH5

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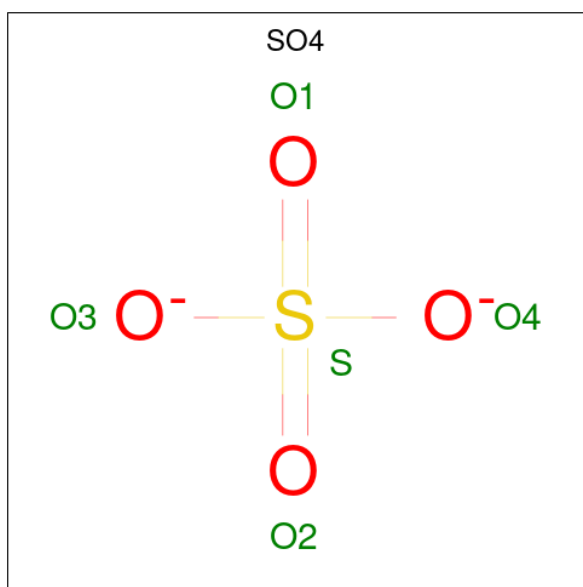
Chain	Residue	Modelled	Actual	Comment	Reference
H	340	GLN	-	expression tag	UNP Q9HVVH5

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		
2	G	1	Total	C	O	0	0
			9	4	5		
2	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		
4	B	221	Total	O	0	0
			221	221		
4	C	270	Total	O	0	0
			270	270		
4	D	263	Total	O	0	0
			263	263		
4	E	100	Total	O	0	0
			100	100		
4	F	201	Total	O	0	0
			201	201		

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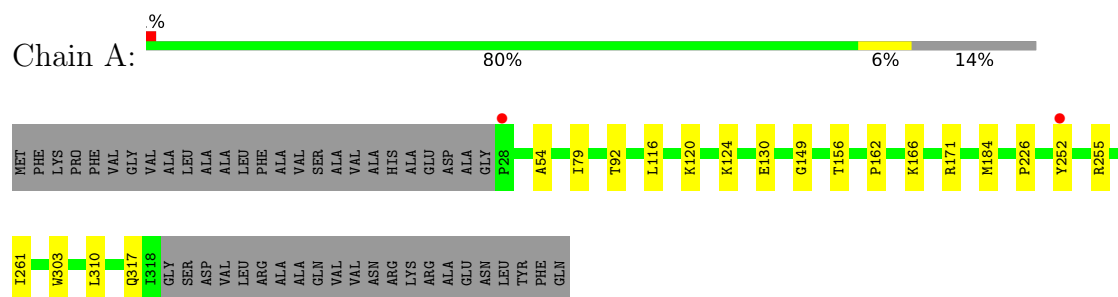
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	261	Total 261	O 261	0	0
4	H	117	Total 117	O 117	0	0

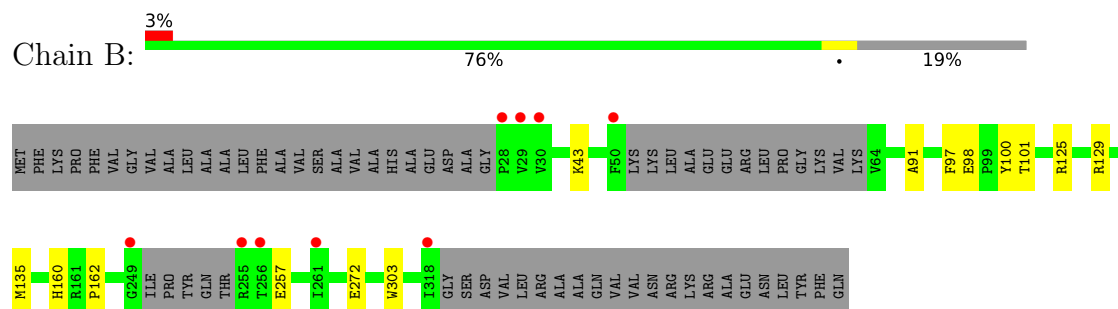
3 Residue-property plots [i](#)

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.

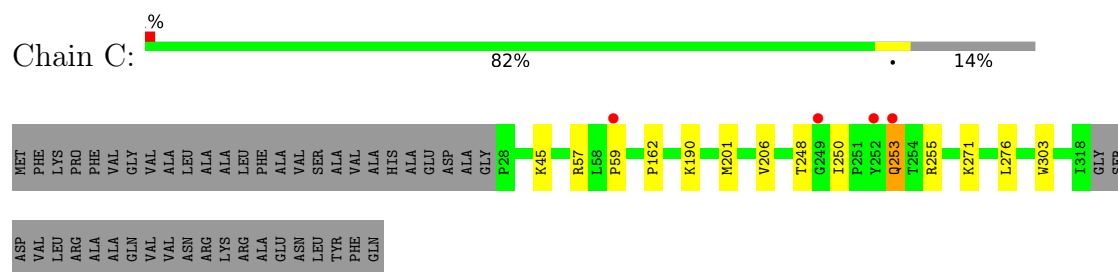
- Molecule 1: Probable c4-dicarboxylate-binding protein



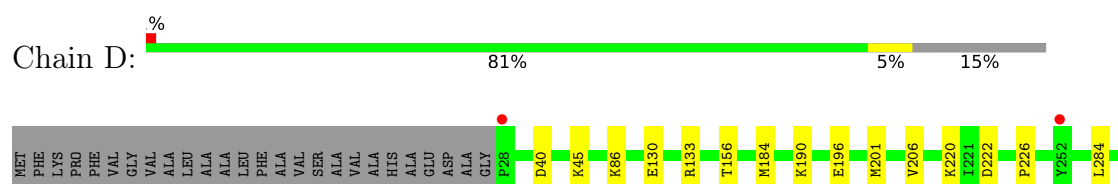
- Molecule 1: Probable c4-dicarboxylate-binding protein



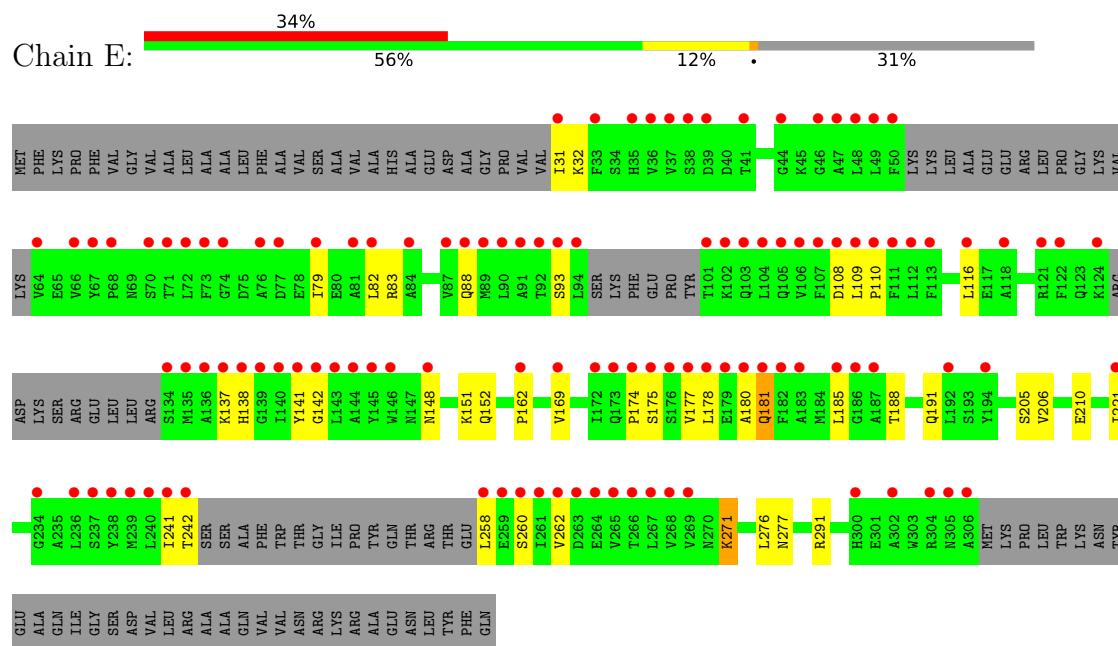
- Molecule 1: Probable c4-dicarboxylate-binding protein



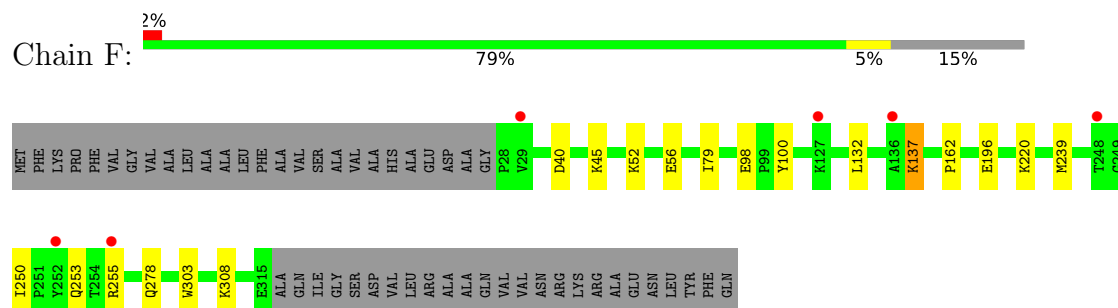
- Molecule 1: Probable c4-dicarboxylate-binding protein



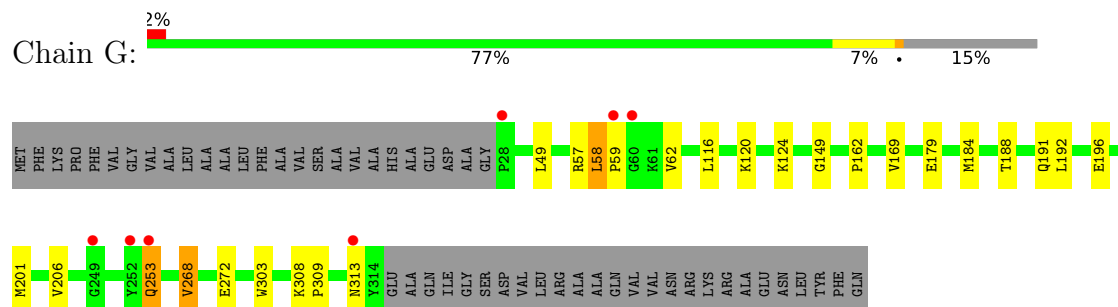
- Molecule 1: Probable c4-dicarboxylate-binding protein



- Molecule 1: Probable c4-dicarboxylate-binding protein

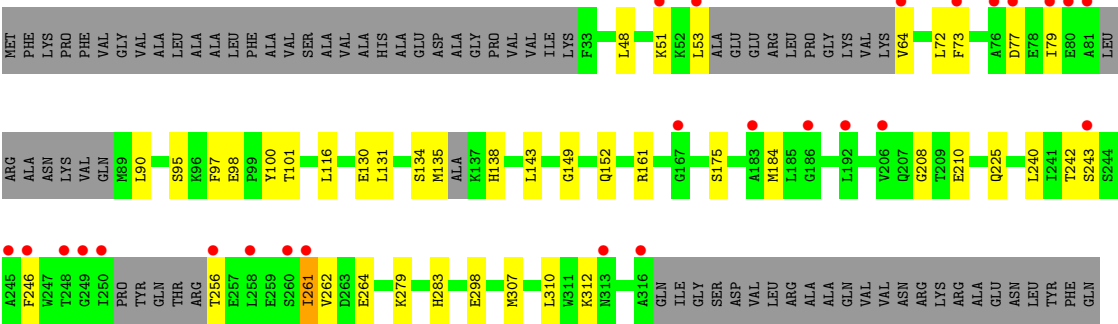


- Molecule 1: Probable c4-dicarboxylate-binding protein



- Molecule 1: Probable c4-dicarboxylate-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.96Å 73.91Å 122.14Å 99.01° 91.59° 95.09°	Depositor
Resolution (Å)	33.56 – 1.85 33.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (33.56-1.85) 96.6 (33.56-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.84Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.195 , 0.239 0.196 , 0.238	Depositor DCC
R_{free} test set	10268 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19172	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1104e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LMR, 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	0.43	0/2345	0.73	0/3170
1	B	0.46	0/2197	0.73	2/2967 (0.1%)
1	C	0.49	0/2343	0.75	1/3168 (0.0%)
1	D	0.47	0/2326	0.75	0/3147
1	E	0.48	0/1808	0.82	2/2446 (0.1%)
1	F	0.44	0/2327	0.79	4/3144 (0.1%)
1	G	0.48	0/2322	0.76	2/3136 (0.1%)
1	H	0.43	0/2094	0.77	2/2826 (0.1%)
All	All	0.46	0/17762	0.76	13/24004 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	308	LYS	CA-C-N	-8.21	111.27	119.56
1	F	308	LYS	C-N-CA	-8.21	111.27	119.56
1	F	98	GLU	CA-C-N	-6.82	112.77	119.87
1	F	98	GLU	C-N-CA	-6.82	112.77	119.87
1	G	58	LEU	CA-C-N	6.47	127.93	119.84
1	G	58	LEU	C-N-CA	6.47	127.93	119.84
1	C	253	GLN	N-CA-C	5.98	118.29	111.11
1	E	180	ALA	CA-C-N	5.71	128.25	120.54
1	E	180	ALA	C-N-CA	5.71	128.25	120.54
1	B	98	GLU	CA-C-N	-5.39	114.27	119.87
1	B	98	GLU	C-N-CA	-5.39	114.27	119.87
1	H	98	GLU	CA-C-N	-5.21	114.45	119.87
1	H	98	GLU	C-N-CA	-5.21	114.45	119.87

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	2299	0	2302	11	0
1	B	2156	0	2146	13	0
1	C	2297	0	2302	9	0
1	D	2280	0	2265	12	0
1	E	1780	0	1732	24	0
1	F	2281	0	2289	10	0
1	G	2276	0	2294	19	0
1	H	2056	0	2023	26	1
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0
2	D	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	H	9	0	4	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	F	5	0	0	0	0
4	A	221	0	0	2	0
4	B	221	0	0	2	0
4	C	270	0	0	1	0
4	D	263	0	0	3	1
4	E	100	0	0	2	0
4	F	201	0	0	1	0
4	G	261	0	0	7	0
4	H	117	0	0	1	0
All	All	19172	0	17381	124	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 4.

All (124) 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:B:100:TYR:HB2	1:B:135:MET:HE2	1.31	1.10
1:B:101:THR:HG22	1:B:135:MET:HE3	1.52	0.91
1:B:97:PHE:HB3	1:B:135:MET:HE1	1.64	0.78
1:B:135:MET:SD	4:B:608:HOH:O	2.41	0.78
1:C:250:ILE:O	1:C:255:ARG:NH2	2.20	0.73
1:F:40:ASP:OD1	1:F:45:LYS:NZ	2.21	0.73
1:G:179:GLU:OE1	1:G:191:GLN:NE2	2.21	0.72
1:G:120:LYS:NZ	4:G:709:HOH:O	2.27	0.67
1:E:142:GLY:HA2	1:E:241:ILE:HD12	1.78	0.65
1:E:88:GLN:OE1	1:E:88:GLN:N	2.29	0.64
1:B:97:PHE:CB	1:B:135:MET:HE1	2.29	0.63
1:B:160:HIS:ND1	4:B:549:HOH:O	2.30	0.63
1:E:108:ASP:OD1	4:E:411:HOH:O	2.15	0.62
1:H:243:SER:OG	1:H:246:PHE:HB3	1.98	0.62
1:B:97:PHE:HB3	1:B:135:MET:CE	2.29	0.62
1:D:184:MET:HE1	1:D:307:MET:HA	1.80	0.61
1:G:253:GLN:H	1:G:253:GLN:CD	2.08	0.61
1:H:79:ILE:HA	1:H:90:LEU:HD11	1.82	0.61
1:A:184:MET:HE1	1:A:310:LEU:HB2	1.83	0.60
1:A:116:LEU:HD11	1:A:149:GLY:HA2	1.83	0.59
1:D:190:LYS:NZ	4:D:661:HOH:O	2.32	0.59
1:D:86:LYS:NZ	4:D:666:HOH:O	2.35	0.58
1:E:174:PRO:HA	1:E:191:GLN:HB3	1.86	0.58
1:H:184:MET:HE1	1:H:310:LEU:HB2	1.85	0.58
1:E:110:PRO:HG3	1:E:181:GLN:HG2	1.85	0.57
1:E:169:VAL:HG23	1:E:206:VAL:HA	1.86	0.57
1:C:162:PRO:HG3	1:C:303:TRP:HA	1.86	0.55
1:G:57:ARG:NH2	4:G:692:HOH:O	2.27	0.55
1:G:58:LEU:HB2	1:G:62:VAL:HG22	1.88	0.55
1:D:40:ASP:OD1	1:D:45:LYS:NZ	2.39	0.54
1:E:32:LYS:NZ	1:E:88:GLN:HE22	2.06	0.53
1:G:162:PRO:HG3	1:G:303:TRP:HA	1.89	0.53
1:C:201:MET:HG2	1:C:206:VAL:HG23	1.90	0.53
1:C:201:MET:HG2	1:C:206:VAL:CG2	2.39	0.53
1:D:130:GLU:OE1	1:D:133:ARG:NH1	2.41	0.52
1:E:83:ARG:HE	1:E:138:HIS:HB3	1.73	0.52
1:F:196:GLU:OE2	4:F:699:HOH:O	2.19	0.52
1:H:184:MET:HE3	1:H:307:MET:HA	1.92	0.52
1:H:53:LEU:HB3	1:H:261:ILE:HD13	1.92	0.52
1:H:143:LEU:HD11	1:H:242:THR:HG22	1.92	0.52
1:A:162:PRO:HG3	1:A:303:TRP:HA	1.90	0.52
1:H:161:ARG:NH1	1:H:298:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:GLU:OE1	4:G:643:HOH:O	2.19	0.51
1:H:100:TYR:HB2	1:H:135:MET:HE2	1.92	0.51
1:F:162:PRO:HG3	1:F:303:TRP:HA	1.93	0.51
1:G:201:MET:HG3	1:G:206:VAL:HG23	1.92	0.51
1:E:32:LYS:HB2	1:E:88:GLN:OE1	2.11	0.50
1:B:162:PRO:HG3	1:B:303:TRP:HA	1.93	0.50
1:C:248:THR:O	1:C:255:ARG:NH2	2.45	0.49
1:E:151:LYS:NZ	1:E:210:GLU:OE2	2.34	0.49
1:A:166:LYS:NZ	4:A:623:HOH:O	2.45	0.49
1:C:45:LYS:HZ2	1:C:276:LEU:HD21	1.77	0.49
1:G:313:ASN:ND2	4:G:617:HOH:O	2.42	0.49
1:H:261:ILE:HA	1:H:264:GLU:H	1.78	0.49
1:E:169:VAL:HG21	1:E:205:SER:O	2.14	0.48
1:G:116:LEU:HD11	1:G:149:GLY:HA2	1.93	0.48
1:D:196:GLU:OE1	4:D:621:HOH:O	2.19	0.48
1:H:48:LEU:O	1:H:51:LYS:HB3	2.14	0.47
1:H:131:LEU:O	1:H:134:SER:HB2	2.14	0.47
1:G:192:LEU:HB3	1:G:196:GLU:HG3	1.96	0.47
1:H:242:THR:OG1	1:H:243:SER:N	2.47	0.47
1:H:312:LYS:HA	1:H:312:LYS:HD3	1.66	0.47
1:G:57:ARG:C	1:G:59:PRO:HD3	2.40	0.47
1:E:32:LYS:HZ3	1:E:88:GLN:HE22	1.62	0.46
1:H:279:LYS:HE2	1:H:283:HIS:HE1	1.80	0.46
1:E:178:LEU:HD13	4:E:408:HOH:O	2.14	0.46
1:G:49:LEU:CD2	1:G:268:VAL:HG11	2.46	0.46
1:G:169:VAL:HG22	1:G:188:THR:CG2	2.45	0.46
1:C:57:ARG:C	1:C:59:PRO:HD3	2.40	0.46
1:B:43:LYS:HD3	1:B:91:ALA:HB3	1.97	0.46
1:E:148:ASN:O	1:E:277:ASN:ND2	2.49	0.45
1:E:109:LEU:HA	1:E:110:PRO:HD2	1.83	0.45
1:B:101:THR:CG2	1:B:135:MET:HE3	2.36	0.45
1:A:156:THR:HA	1:A:226:PRO:HD2	1.98	0.45
1:D:220:LYS:HB2	1:D:220:LYS:HE2	1.76	0.45
1:B:97:PHE:CD1	1:B:135:MET:HE1	2.52	0.45
1:B:125:ARG:O	1:B:129:ARG:HG2	2.16	0.44
1:E:162:PRO:HB3	1:E:185:LEU:HD21	1.98	0.44
1:E:169:VAL:CG2	1:E:206:VAL:HA	2.46	0.44
1:H:152:GLN:O	1:H:210:GLU:HA	2.17	0.44
1:H:51:LYS:HE3	1:H:64:VAL:HG13	1.98	0.44
1:H:101:THR:HG22	1:H:135:MET:HE3	1.99	0.44
1:C:271:LYS:NZ	4:C:637:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:LEU:O	1:H:240:LEU:HD12	2.18	0.44
1:E:82:LEU:HD22	1:E:241:ILE:HG23	2.00	0.44
1:F:278:GLN:HG3	4:G:761:HOH:O	2.17	0.44
1:H:97:PHE:CD1	1:H:135:MET:HE1	2.53	0.43
1:A:252:TYR:HD1	1:A:255:ARG:NH2	2.16	0.43
1:D:156:THR:HA	1:D:226:PRO:HD2	2.01	0.43
1:G:184:MET:HE3	1:G:184:MET:HB2	1.87	0.43
1:B:100:TYR:HB2	1:B:135:MET:CE	2.22	0.43
1:H:116:LEU:HD11	1:H:149:GLY:HA2	1.99	0.43
1:E:116:LEU:HD12	1:E:116:LEU:HA	1.83	0.43
1:G:124:LYS:NZ	4:G:683:HOH:O	2.49	0.43
1:F:137:LYS:HB3	1:F:137:LYS:HE3	1.80	0.43
1:F:250:ILE:O	1:F:255:ARG:NH2	2.52	0.43
1:G:308:LYS:HG2	1:G:309:PRO:HD3	2.01	0.43
1:H:143:LEU:HB3	1:H:262:VAL:HG11	2.01	0.43
1:E:141:TYR:HB3	1:E:242:THR:HG23	2.01	0.42
1:A:54:ALA:HA	1:A:261:ILE:HD13	2.00	0.42
1:G:188:THR:HG22	4:G:760:HOH:O	2.20	0.42
1:E:152:GLN:O	1:E:210:GLU:HA	2.19	0.42
1:E:271:LYS:HB3	1:E:271:LYS:HE3	1.65	0.42
1:H:79:ILE:HD11	1:H:100:TYR:CZ	2.55	0.42
1:G:201:MET:CG	1:G:206:VAL:HG23	2.50	0.42
1:D:184:MET:CE	1:D:307:MET:HA	2.49	0.42
1:C:190:LYS:HE3	1:C:190:LYS:HB2	1.80	0.42
1:A:317:GLN:HG3	4:A:688:HOH:O	2.20	0.41
1:E:291:ARG:HH11	1:E:291:ARG:HG2	1.85	0.41
1:F:79:ILE:HG21	1:F:100:TYR:CZ	2.55	0.41
1:F:220:LYS:HB2	1:F:220:LYS:HE3	1.86	0.41
1:A:120:LYS:HG2	1:A:124:LYS:HE3	2.02	0.41
1:F:52:LYS:NZ	1:F:56:GLU:OE2	2.54	0.41
1:H:72:LEU:HG	1:H:73:PHE:CD1	2.54	0.41
1:F:132:LEU:HD23	1:F:239:MET:HE2	2.01	0.41
1:H:95:SER:O	1:H:175:SER:HB2	2.19	0.41
1:H:208:GLY:HA2	1:H:225:GLN:OE1	2.21	0.41
1:H:138:HIS:HA	4:H:567:HOH:O	2.20	0.41
1:A:79:ILE:HD11	1:A:92:THR:HG21	2.01	0.41
1:D:222:ASP:HB3	1:D:284:LEU:HD11	2.02	0.41
1:E:175:SER:HB3	1:E:178:LEU:HD12	2.03	0.41
1:D:201:MET:HG3	1:D:206:VAL:HG23	2.02	0.40
1:D:184:MET:HB3	1:D:184:MET:HE3	1.83	0.40
1:A:171:ARG:C	1:A:171:ARG:HD3	2.46	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:H:130:GLU:OE2	4:D:678:HOH:O[1_544]	2.02	0.18

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	289/339 (85%)	283 (98%)	6 (2%)	0	100	100
1	B	267/339 (79%)	262 (98%)	5 (2%)	0	100	100
1	C	290/339 (86%)	284 (98%)	6 (2%)	0	100	100
1	D	288/339 (85%)	284 (99%)	4 (1%)	0	100	100
1	E	223/339 (66%)	216 (97%)	7 (3%)	0	100	100
1	F	286/339 (84%)	281 (98%)	5 (2%)	0	100	100
1	G	285/339 (84%)	277 (97%)	8 (3%)	0	100	100
1	H	251/339 (74%)	241 (96%)	9 (4%)	1 (0%)	30	17
All	All	2179/2712 (80%)	2128 (98%)	50 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	77	ASP

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	245/281 (87%)	244 (100%)	1 (0%)	84	82
1	B	230/281 (82%)	228 (99%)	2 (1%)	70	64
1	C	244/281 (87%)	243 (100%)	1 (0%)	84	82
1	D	242/281 (86%)	242 (100%)	0	100	100
1	E	185/281 (66%)	172 (93%)	13 (7%)	14	3
1	F	244/281 (87%)	242 (99%)	2 (1%)	73	67
1	G	244/281 (87%)	242 (99%)	2 (1%)	73	67
1	H	217/281 (77%)	215 (99%)	2 (1%)	70	64
All	All	1851/2248 (82%)	1828 (99%)	23 (1%)	63	55

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	B	257	GLU
1	B	272	GLU
1	C	253	GLN
1	E	31	ILE
1	E	79	ILE
1	E	93	SER
1	E	137	LYS
1	E	177	VAL
1	E	181	GLN
1	E	188	THR
1	E	221	ILE
1	E	258	LEU
1	E	260	SER
1	E	262	VAL
1	E	271	LYS
1	E	276	LEU
1	F	137	LYS
1	F	253	GLN
1	G	253	GLN
1	G	268	VAL
1	H	256	THR
1	H	261	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	317	GLN
1	C	219	GLN
1	C	300	HIS
1	D	138	HIS
1	E	173	GLN
1	E	283	HIS
1	E	300	HIS
1	F	300	HIS
1	H	105	GLN
1	H	300	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](#)

13 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	LMR	C	401	-	8,8,8	1.14	0	10,10,10	1.35	2 (20%)
2	LMR	D	401	-	8,8,8	1.25	0	10,10,10	1.51	1 (10%)
3	SO4	D	402	-	4,4,4	0.27	0	6,6,6	0.25	0
3	SO4	F	402	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	403	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	D	403	-	4,4,4	0.22	0	6,6,6	0.16	0
2	LMR	B	401	-	8,8,8	1.33	1 (12%)	10,10,10	1.54	3 (30%)
2	LMR	A	401	-	8,8,8	1.12	0	10,10,10	1.36	1 (10%)
3	SO4	B	402	-	4,4,4	0.26	0	6,6,6	0.09	0
2	LMR	F	401	-	8,8,8	1.16	0	10,10,10	1.55	3 (30%)
3	SO4	C	402	-	4,4,4	0.26	0	6,6,6	0.22	0
2	LMR	G	401	-	8,8,8	1.17	0	10,10,10	1.32	1 (10%)
2	LMR	H	401	-	8,8,8	1.20	0	10,10,10	1.43	2 (20%)

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	LMR	C	401	-	-	2/8/8/8	-
2	LMR	D	401	-	-	2/8/8/8	-
2	LMR	B	401	-	-	1/8/8/8	-
2	LMR	A	401	-	-	0/8/8/8	-
2	LMR	F	401	-	-	1/8/8/8	-
2	LMR	G	401	-	-	4/8/8/8	-
2	LMR	H	401	-	-	2/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	LMR	C2-C1	2.54	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	LMR	O1A-C1-C2	-2.95	116.71	122.60
2	D	401	LMR	O1A-C1-C2	-2.89	116.82	122.60
2	A	401	LMR	O1A-C1-C2	-2.79	117.02	122.60
2	B	401	LMR	O1A-C1-C2	-2.79	117.03	122.60
2	F	401	LMR	O1A-C1-C2	-2.75	117.10	122.60
2	G	401	LMR	O1A-C1-C2	-2.59	117.42	122.60
2	C	401	LMR	O1B-C1-C2	2.52	118.06	112.74
2	H	401	LMR	O1B-C1-C2	2.47	117.95	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	LMR	O1B-C1-C2	2.43	117.89	112.74
2	C	401	LMR	O1A-C1-C2	-2.41	117.79	122.60
2	F	401	LMR	O4B-C4-C3	-2.19	116.13	122.84
2	B	401	LMR	O4B-C4-C3	-2.12	116.34	122.84
2	F	401	LMR	C2-C3-C4	-2.09	106.63	112.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	LMR	O1B-C1-C2-C3
2	F	401	LMR	O1B-C1-C2-C3
2	G	401	LMR	O1B-C1-C2-C3
2	B	401	LMR	O1B-C1-C2-C3
2	C	401	LMR	O1A-C1-C2-C3
2	C	401	LMR	O1B-C1-C2-C3
2	D	401	LMR	O1A-C1-C2-C3
2	G	401	LMR	O1A-C1-C2-C3
2	H	401	LMR	O1A-C1-C2-C3
2	H	401	LMR	C2-C3-C4-O4A
2	G	401	LMR	C2-C3-C4-O4A
2	G	401	LMR	O1B-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	291/339 (85%)	0.07	2 (0%) 84 87	16, 28, 48, 61	0
1	B	273/339 (80%)	0.04	9 (3%) 49 53	13, 26, 48, 60	0
1	C	291/339 (85%)	-0.17	4 (1%) 73 77	7, 24, 43, 71	1 (0%)
1	D	289/339 (85%)	-0.21	3 (1%) 79 83	9, 22, 41, 53	1 (0%)
1	E	233/339 (68%)	2.09	114 (48%) 0 0	23, 52, 75, 90	0
1	F	288/339 (84%)	0.08	6 (2%) 63 67	15, 28, 48, 61	0
1	G	287/339 (84%)	-0.09	7 (2%) 59 63	12, 24, 40, 52	0
1	H	261/339 (76%)	0.73	26 (9%) 12 12	18, 38, 60, 79	0
All	All	2213/2712 (81%)	0.27	171 (7%) 19 20	7, 28, 58, 90	2 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	64	VAL	7.3
1	E	82	LEU	6.2
1	E	93	SER	5.9
1	E	141	TYR	5.7
1	E	68	PRO	5.6
1	E	140	ILE	5.6
1	E	258	LEU	5.5
1	E	36	VAL	5.5
1	H	261	ILE	5.3
1	E	110	PRO	5.3
1	E	72	LEU	5.2
1	E	87	VAL	5.1
1	E	50	PHE	5.1
1	E	31	ILE	4.9
1	H	81	ALA	4.9
1	E	144	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	260	SER	4.8
1	E	241	ILE	4.8
1	E	262	VAL	4.6
1	E	79	ILE	4.6
1	E	71	THR	4.5
1	H	250	ILE	4.5
1	E	240	LEU	4.5
1	H	316	ALA	4.5
1	E	94	LEU	4.5
1	E	122	PHE	4.4
1	E	177	VAL	4.4
1	H	249	GLY	4.4
1	E	143	LEU	4.3
1	E	113	PHE	4.3
1	E	178	LEU	4.2
1	E	104	LEU	4.2
1	E	90	LEU	4.1
1	E	181	GLN	4.1
1	E	64	VAL	4.1
1	E	172	ILE	4.1
1	E	238	TYR	4.1
1	E	137	LYS	4.1
1	E	101	THR	4.0
1	H	243	SER	4.0
1	E	124	LYS	4.0
1	E	134	SER	4.0
1	E	107	PHE	4.0
1	E	179	GLU	3.9
1	B	28	PRO	3.9
1	E	267	LEU	3.8
1	E	66	VAL	3.8
1	E	37	VAL	3.8
1	E	118	ALA	3.7
1	E	88	GLN	3.7
1	E	92	THR	3.7
1	E	136	ALA	3.7
1	E	261	ILE	3.7
1	E	265	VAL	3.7
1	E	73	PHE	3.7
1	E	142	GLY	3.7
1	E	306	ALA	3.6
1	E	145	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	102	LYS	3.6
1	E	106	VAL	3.6
1	E	76	ALA	3.6
1	H	256	THR	3.6
1	E	105	GLN	3.5
1	B	261	ILE	3.5
1	E	242	THR	3.5
1	E	70	SER	3.5
1	E	33	PHE	3.5
1	E	91	ALA	3.5
1	E	176	SER	3.4
1	E	77	ASP	3.4
1	E	139	GLY	3.4
1	E	109	LEU	3.4
1	E	111	PHE	3.3
1	F	252	TYR	3.3
1	H	79	ILE	3.3
1	E	183	ALA	3.3
1	E	259	GLU	3.3
1	E	175	SER	3.3
1	E	67	TYR	3.2
1	E	185	LEU	3.2
1	E	239	MET	3.2
1	E	146	TRP	3.2
1	G	59	PRO	3.2
1	G	60	GLY	3.1
1	E	48	LEU	3.1
1	B	50	PHE	3.1
1	B	29	VAL	3.1
1	G	249	GLY	3.0
1	E	263	ASP	3.0
1	E	186	GLY	3.0
1	E	174	PRO	3.0
1	E	187	ALA	3.0
1	C	252	TYR	2.9
1	H	80	GLU	2.9
1	E	268	VAL	2.9
1	E	180	ALA	2.9
1	E	108	ASP	2.9
1	E	89	MET	2.9
1	E	38	SER	2.9
1	H	245	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	173	GLN	2.8
1	B	256	THR	2.8
1	H	206	VAL	2.8
1	H	260	SER	2.8
1	H	192	LEU	2.8
1	A	28	PRO	2.8
1	C	59	PRO	2.8
1	C	253	GLN	2.7
1	H	167	GLY	2.7
1	E	49	LEU	2.7
1	E	194	TYR	2.7
1	E	266	THR	2.7
1	E	81	ALA	2.6
1	E	234	GLY	2.6
1	H	76	ALA	2.6
1	H	73	PHE	2.6
1	E	221	ILE	2.6
1	E	74	GLY	2.6
1	D	316	ALA	2.6
1	G	253	GLN	2.6
1	A	252	TYR	2.6
1	E	138	HIS	2.6
1	E	302	ALA	2.5
1	F	136	ALA	2.5
1	E	269	VAL	2.5
1	F	255	ARG	2.5
1	E	264	GLU	2.5
1	E	121	ARG	2.4
1	E	112	LEU	2.4
1	E	47	ALA	2.4
1	H	246	PHE	2.4
1	E	46	GLY	2.4
1	H	53	LEU	2.4
1	H	258	LEU	2.4
1	E	169	VAL	2.4
1	E	192	LEU	2.3
1	E	182	PHE	2.3
1	E	84	ALA	2.3
1	B	255	ARG	2.3
1	H	313	ASN	2.3
1	E	44	GLY	2.3
1	G	313	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	135	MET	2.3
1	G	252	TYR	2.3
1	E	35	HIS	2.3
1	E	300	HIS	2.3
1	H	51	LYS	2.3
1	H	248	THR	2.3
1	B	249	GLY	2.2
1	E	41	THR	2.2
1	F	248	THR	2.2
1	D	252	TYR	2.2
1	E	305	ASN	2.2
1	E	304	ARG	2.2
1	E	237	SER	2.2
1	E	116	LEU	2.2
1	E	39	ASP	2.1
1	F	29	VAL	2.1
1	C	249	GLY	2.1
1	E	162	PRO	2.1
1	G	28	PRO	2.1
1	E	148	ASN	2.1
1	B	318	ILE	2.1
1	E	236	LEU	2.1
1	H	77	ASP	2.1
1	F	127	LYS	2.1
1	H	186	GLY	2.1
1	B	30	VAL	2.1
1	H	183	ALA	2.1
1	D	28	PRO	2.0
1	E	103	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [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	LMR	H	401	9/9	0.83	0.12	25,26,30,31	0
3	SO4	C	402	5/5	0.83	0.13	45,50,57,64	0
3	SO4	B	402	5/5	0.90	0.09	37,40,48,57	0
3	SO4	F	402	5/5	0.90	0.09	59,60,66,69	0
3	SO4	B	403	5/5	0.91	0.08	42,51,55,55	0
3	SO4	D	403	5/5	0.93	0.08	50,52,53,54	0
2	LMR	A	401	9/9	0.95	0.06	19,21,25,26	0
3	SO4	D	402	5/5	0.95	0.09	35,36,40,41	0
2	LMR	F	401	9/9	0.96	0.05	14,18,19,21	0
2	LMR	B	401	9/9	0.97	0.06	13,17,18,19	0
2	LMR	G	401	9/9	0.97	0.05	14,16,17,19	0
2	LMR	C	401	9/9	0.97	0.05	13,16,19,20	0
2	LMR	D	401	9/9	0.98	0.04	10,12,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.