



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:51 PM UTC

PDB ID : 5T1P / pdb_00005t1p
Title : Crystal structure of the putative periplasmic solute-binding protein from *Campylobacter jejuni*
Authors : Filippova, E.V.; Wawrzak, Z.; Sandoval, J.; Skarina, T.; Grimshaw, S.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-08-19
Resolution : 2.00 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:

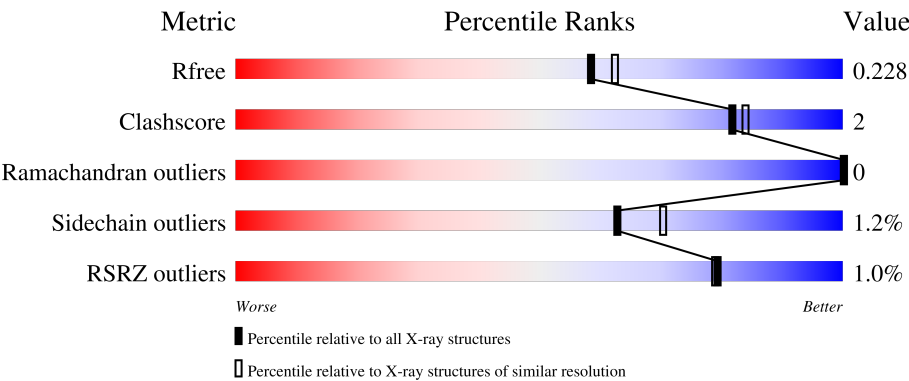
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	348	86%7% • 6%
1	B	348	86%7% • 6%
1	C	348	% 86%7% 6%
1	D	348	% 89%5% • 6%

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Mol	Chain	Length	Quality of chain
1	E	348	% 88% 6%6%
1	F	348	% 89% 5%6%
1	G	348	83% 10%6%
1	H	348	3% 86% 7%6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22353 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 ABC transporter, periplasmic substrate-binding protein.

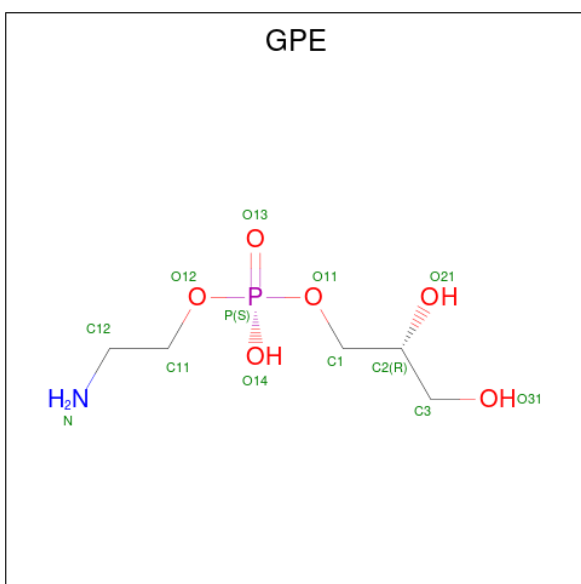
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	Se	0	6	0
			2607	1663	442	498	4			
1	B	326	Total	C	N	O	Se	0	3	0
			2573	1642	437	491	3			
1	C	326	Total	C	N	O	Se	0	1	0
			2557	1631	433	490	3			
1	D	328	Total	C	N	O	Se	0	0	0
			2562	1634	434	491	3			
1	E	326	Total	C	N	O	Se	0	3	0
			2576	1642	438	493	3			
1	F	327	Total	C	N	O	Se	0	2	0
			2568	1637	434	494	3			
1	G	326	Total	C	N	O	Se	0	3	0
			2577	1642	438	494	3			
1	H	326	Total	C	N	O	Se	0	6	0
			2595	1653	441	496	5			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



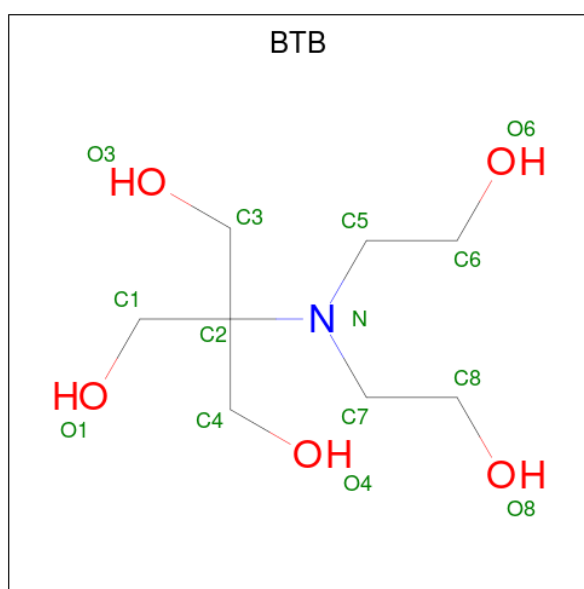
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is L-ALPHA-GLYCEROPHOSPHORYLETHANOLAMINE (CCD ID: GPE) (formula: $C_5H_{14}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			13	5	1	6	1		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			8	4	1	3		
5	H	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

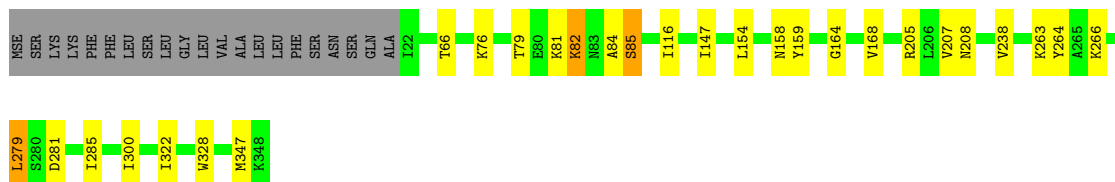
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	267	Total	O	0	2
			269	269		
6	B	208	Total	O	0	0
			208	208		
6	C	145	Total	O	0	0
			145	145		
6	D	219	Total	O	0	0
			219	219		
6	E	254	Total	O	0	2
			255	255		
6	F	192	Total	O	0	0
			192	192		
6	G	189	Total	O	0	0
			189	189		
6	H	145	Total	O	0	1
			146	146		

3 Residue-property plots

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.

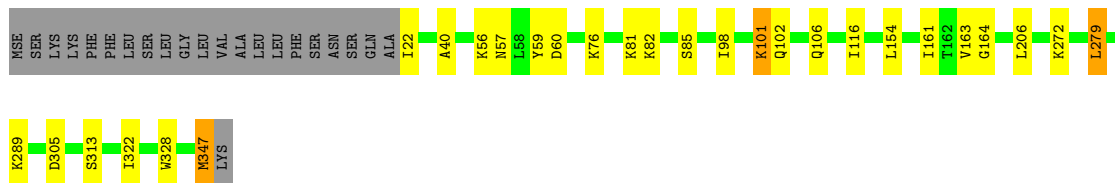
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain A: 



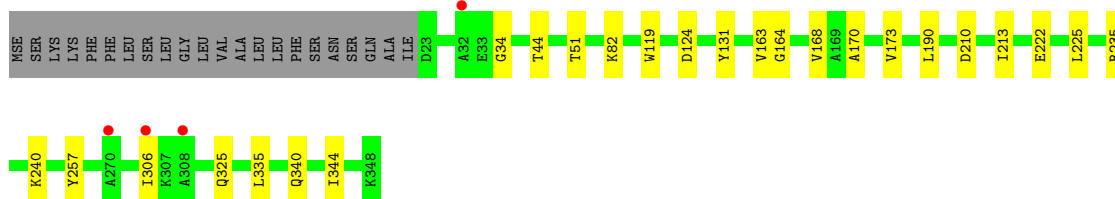
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain B: 



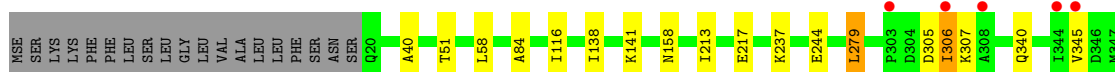
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain C: 



- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain D: 



LYS

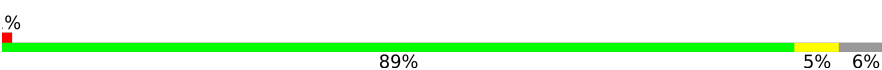
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain E: 

MSE SER LYS PHE PHE LEU SER LEU LEU VAL ALA LEU PHE SER ASN SER GLN ALA I22 Y59 D60 I61 P107 F108 K109 L128 K141 V144 K145 K156 A169 N208 N209 D210 D236 K237 E244 K289 R293 P303 I306 S313

K347
LYS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain F: 

MSE SER LYS PHE PHE LEU SER LEU LEU VAL ALA LEU PHE SER ASN SER GLN A21 E24 V36 F77 G89 Q102 G103 V104 L128 V143 G164 V168 I213 T259 A270 R293 P312 S313 E314 K326 K347 LYS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain G: 

MSE SER LYS PHE PHE LEU SER LEU LEU VAL ALA LEU PHE SER ASN SER GLN A22 A32 V36 I74 F95 K101 Q102 D124 L128 L129 V139 V143 V144 L155 Y159 V166 S167 V168 A169 E187 R205 N208 I213

A214 N215 K218 K240 Q256 A270 Y291 A292 R293 I297 L302 P303 I306 K309 S313 E314 W339 V343 K347 LYS

- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain H: 

MSE SER LYS PHE PHE LEU SER LEU LEU VAL ALA LEU PHE SER ASN SER GLN A21 L26 A30 L39 A40 N41 T66 D67 P68 Q72 E73 I74 A75 K76 F77 K78 I79 K82 A84 S85 I88 G89 D90 V91 F95 G96 V104 T110

A120 D124 L128 L129 V168 V211 Y257 N262 A265 L279 S280 D281 I285 R293 L302 K347 LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.19Å 89.28Å 100.39Å 68.88° 82.52° 70.66°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.00) 96.3 (30.00-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.176 , 0.224 0.184 , 0.228	Depositor DCC
R_{free} test set	8289 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22353	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.30 % 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 8.7704e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, GPE, TRS, PEG

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	0.88	0/2656	1.09	7/3591 (0.2%)
1	B	0.85	1/2622 (0.0%)	1.08	6/3550 (0.2%)
1	C	0.82	0/2606	1.08	5/3526 (0.1%)
1	D	0.84	0/2611	1.05	5/3535 (0.1%)
1	E	0.88	0/2625	1.11	9/3553 (0.3%)
1	F	0.80	0/2617	1.06	3/3543 (0.1%)
1	G	0.85	0/2626	1.07	6/3555 (0.2%)
1	H	0.79	0/2643	1.06	8/3575 (0.2%)
All	All	0.84	1/21006 (0.0%)	1.08	49/28428 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	LYS	C-O	-5.38	1.17	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	208	ASN	CB-CA-C	-11.65	88.80	110.36
1	E	208	ASN	N-CA-C	8.62	123.41	113.15
1	E	209	ASN	N-CA-C	7.89	120.12	110.41
1	B	164	GLY	N-CA-C	-6.85	105.44	111.95
1	G	169	ALA	N-CA-C	6.81	119.79	108.96
1	B	347	MSE	CG-SE-CE	-6.49	84.64	98.92
1	G	208	ASN	N-CA-C	6.43	121.95	113.20
1	D	306	ILE	N-CA-C	6.39	119.04	111.05
1	F	164	GLY	N-CA-C	-6.27	105.64	112.04
1	C	34	GLY	N-CA-C	6.24	122.51	115.08
1	B	57	ASN	N-CA-C	6.14	118.06	111.36
1	E	156	LYS	N-CA-C	6.11	120.91	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	139	VAL	N-CA-C	6.01	116.53	107.75
1	A	82	LYS	N-CA-C	5.93	118.53	111.71
1	H	91	VAL	N-CA-CB	-5.91	101.43	112.36
1	D	305	ASP	N-CA-C	5.80	119.46	112.38
1	D	84	ALA	N-CA-C	5.72	118.85	109.76
1	A	85	SER	N-CA-C	-5.71	106.15	113.23
1	H	168	VAL	N-CA-C	5.59	120.96	109.34
1	E	347	MSE	N-CA-CB	5.55	119.93	110.50
1	G	187	GLU	N-CA-C	5.50	119.48	112.87
1	G	124	ASP	N-CA-C	5.47	120.10	113.38
1	A	164	GLY	N-CA-C	-5.44	105.74	112.33
1	C	222	GLU	N-CA-C	-5.44	102.75	111.02
1	B	305	ASP	N-CA-C	5.43	119.53	113.01
1	E	109	LYS	N-CA-C	5.37	118.05	111.82
1	G	155	LEU	N-CA-C	5.35	117.86	111.71
1	F	168	VAL	N-CA-C	5.34	120.44	109.34
1	H	68[A]	MSE	CG-SE-CE	-5.34	87.18	98.92
1	H	68[B]	MSE	CG-SE-CE	-5.34	87.18	98.92
1	D	138	ILE	N-CA-C	-5.33	100.65	108.11
1	C	306	ILE	N-CA-C	5.31	120.39	109.34
1	B	313	SER	N-CA-C	5.29	117.05	111.28
1	B	101	LYS	CA-CB-CG	5.19	124.48	114.10
1	F	104	VAL	N-CA-CB	-5.18	104.19	112.07
1	H	211	VAL	N-CA-C	-5.17	102.92	109.58
1	C	124	ASP	N-CA-C	5.16	119.72	113.38
1	A	147	ILE	CA-C-N	-5.14	114.61	119.76
1	A	147	ILE	C-N-CA	-5.14	114.61	119.76
1	D	58	LEU	N-CA-C	5.13	118.00	111.69
1	E	237	LYS	N-CA-C	5.12	117.99	111.69
1	A	238	VAL	N-CA-C	5.12	117.00	111.58
1	H	124	ASP	N-CA-C	5.11	119.61	113.17
1	C	168	VAL	N-CA-C	5.11	119.97	109.34
1	E	169	ALA	N-CA-C	5.08	117.04	108.96
1	E	107	PRO	N-CA-C	5.07	119.98	111.32
1	A	168	VAL	N-CA-C	5.06	119.86	109.34
1	H	96	GLY	N-CA-C	-5.04	106.39	112.49
1	H	168	VAL	CB-CA-C	-5.03	103.05	111.29

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	2607	0	2613	17	0
1	B	2573	0	2575	15	0
1	C	2557	0	2557	14	0
1	D	2562	0	2560	8	0
1	E	2576	0	2575	8	0
1	F	2568	0	2561	9	0
1	G	2577	0	2572	15	0
1	H	2595	0	2588	19	0
2	A	7	0	10	0	0
2	E	4	0	5	0	0
2	F	4	0	5	0	0
2	H	4	0	5	0	0
3	A	13	0	13	0	0
3	B	13	0	13	1	0
3	C	13	0	13	0	0
3	D	13	0	13	1	0
4	E	14	0	19	0	0
4	G	14	0	19	0	0
5	F	8	0	12	0	0
5	H	8	0	12	0	0
6	A	269	0	0	2	0
6	B	208	0	0	1	0
6	C	145	0	0	2	0
6	D	219	0	0	0	0
6	E	255	0	0	0	0
6	F	192	0	0	1	0
6	G	189	0	0	1	0
6	H	146	0	0	0	0
All	All	22353	0	20740	103	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 2.

All (103) 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:H:293[A]:ARG:HH11	1:H:293[A]:ARG:HG3	1.16	1.02
1:H:91:VAL:CG1	1:H:95:PHE:HB2	2.04	0.88
1:H:293[A]:ARG:HG3	1:H:293[A]:ARG:NH1	1.84	0.81
1:H:281:ASP:O	1:H:285:ILE:HG12	1.83	0.78
1:H:91:VAL:HG13	1:H:95:PHE:HB2	1.69	0.74
1:B:154:LEU:HD21	1:B:161:ILE:HD13	1.69	0.74
1:H:293[A]:ARG:NH1	1:H:293[A]:ARG:CG	2.58	0.67
1:H:41[A]:MSE:HE1	1:H:88:ILE:HG12	1.78	0.64
1:A:263:LYS:HE2	1:A:264:TYR:CZ	2.33	0.64
1:B:154:LEU:C	1:B:154:LEU:HD23	2.22	0.63
1:D:306:ILE:HD12	1:D:307:LYS:N	2.15	0.61
1:C:163[B]:VAL:HG13	1:C:225:LEU:HD12	1.83	0.60
1:C:119:TRP:O	1:C:325:GLN:NE2	2.35	0.59
1:G:293[B]:ARG:NH1	6:G:505:HOH:O	2.35	0.59
1:A:84:ALA:O	1:A:266:LYS:HD3	2.01	0.58
1:E:293[A]:ARG:NH2	1:E:313:SER:OG	2.37	0.58
1:H:41[A]:MSE:HE3	1:H:89:GLY:C	2.31	0.56
1:B:116:ILE:HD11	1:B:279:LEU:HD22	1.88	0.56
1:G:159:TYR:O	1:G:205:ARG:HD2	2.06	0.55
1:F:24:GLU:CD	1:F:24:GLU:H	2.14	0.55
1:C:340:GLN:NE2	6:C:503:HOH:O	2.36	0.55
1:B:98:ILE:CG2	1:B:102:GLN:HE21	2.20	0.54
1:F:213:ILE:H	1:F:213:ILE:HD12	1.73	0.54
1:G:291:TYR:CE1	1:G:309:LYS:HG3	2.42	0.54
1:A:208:ASN:ND2	1:A:347[B]:MSE:SE	2.91	0.53
1:A:281:ASP:O	1:A:285:ILE:HG12	2.09	0.53
1:G:36:VAL:HB	1:G:270:ALA:HB1	1.90	0.53
1:F:293:ARG:NH2	1:F:313:SER:OG	2.42	0.53
1:A:159:TYR:O	1:A:205:ARG:HD2	2.09	0.52
1:A:76[A]:LYS:HE2	1:A:85:SER:OG	2.10	0.52
1:A:116:ILE:HD11	1:A:279:LEU:HD22	1.92	0.52
1:G:129:LEU:HD13	1:G:256:GLY:HA3	1.91	0.51
1:E:289:LYS:HG3	1:E:306:ILE:HD13	1.91	0.51
1:C:164:GLY:HA2	1:C:210:ASP:HA	1.93	0.51
1:G:293[A]:ARG:NH2	1:G:313:SER:OG	2.43	0.51
1:E:303:PRO:HG2	1:E:306:ILE:HD12	1.93	0.50
1:H:110:THR:HG21	1:H:279:LEU:HD12	1.94	0.50
1:H:285:ILE:HD12	1:H:302:LEU:HD23	1.93	0.50
1:D:213:ILE:HD13	1:D:237:LYS:HD3	1.94	0.50
1:G:339:TRP:O	1:G:343:VAL:HG22	2.12	0.50
1:H:128:LEU:HD12	1:H:128:LEU:O	2.11	0.49
1:A:79:THR:HG23	1:C:344:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:HD13	1:B:328:TRP:CD1	2.47	0.49
1:H:285:ILE:CD1	1:H:302:LEU:HD23	2.43	0.49
1:C:190:LEU:HD12	1:C:335:LEU:HD13	1.94	0.48
1:A:84:ALA:O	1:A:266:LYS:CD	2.61	0.48
1:D:141:LYS:HD3	1:D:244:GLU:HB2	1.95	0.48
1:H:91:VAL:CG1	1:H:95:PHE:CB	2.85	0.47
1:B:163[A]:VAL:HG21	1:B:206:LEU:CD1	2.43	0.47
1:F:89:GLY:O	1:F:259:THR:HA	2.15	0.47
1:E:59:TYR:HB2	1:E:61:ILE:HD13	1.97	0.47
1:E:141:LYS:HD3	1:E:244:GLU:HB2	1.97	0.47
1:H:120:ALA:HB1	1:H:129:LEU:HB2	1.97	0.47
1:F:77:PHE:HB2	1:F:104:VAL:HG13	1.96	0.47
1:C:235:ARG:NH2	6:C:501:HOH:O	2.30	0.47
1:A:207:VAL:HG22	1:C:82:LYS:HG3	1.96	0.47
1:C:163[B]:VAL:HG12	1:C:163[B]:VAL:O	2.13	0.47
1:D:40:ALA:HB1	3:D:401:GPE:H121	1.97	0.47
1:B:98:ILE:HG23	1:B:102:GLN:HE21	1.81	0.46
1:A:285:ILE:HD13	1:A:300:ILE:HD12	1.97	0.46
1:A:322:ILE:HD13	1:A:328:TRP:CD1	2.50	0.45
1:A:66[B]:THR:HG22	6:A:717:HOH:O	2.15	0.45
1:B:56:LYS:O	1:B:60:ASP:HA	2.16	0.45
1:C:131:TYR:CZ	1:C:257:TYR:HB2	2.52	0.45
1:C:190:LEU:CD1	1:C:335:LEU:HD13	2.47	0.45
1:C:235:ARG:HG2	1:C:240:LYS:HA	1.98	0.45
1:G:166:VAL:HG21	1:G:339:TRP:CG	2.51	0.45
1:F:77:PHE:CB	1:F:104:VAL:HG13	2.47	0.44
1:H:76:LYS:HE2	1:H:85:SER:OG	2.17	0.44
1:F:312:PRO:HB2	1:F:314[B]:GLU:HG3	1.99	0.44
1:F:102:GLN:NE2	6:F:508:HOH:O	2.50	0.44
1:B:76:LYS:HE3	1:B:85:SER:OG	2.18	0.44
1:E:303:PRO:CG	1:E:306:ILE:HD12	2.48	0.44
1:B:106:GLN:OE1	1:B:272:LYS:NZ	2.51	0.43
1:H:262:ASN:HB3	1:H:265:ALA:HB2	2.00	0.43
1:H:68[B]:MSE:CE	1:H:73:GLU:HA	2.48	0.43
1:A:154:LEU:O	1:A:205:ARG:NH2	2.49	0.43
1:H:68[A]:MSE:SE	1:H:72:GLN:HB3	2.69	0.42
1:A:81:LYS:HB3	1:A:82:LYS:H	1.74	0.42
1:E:145:LYS:N	1:E:145:LYS:HD2	2.34	0.42
1:F:36:VAL:HB	1:F:270:ALA:HB1	1.99	0.42
1:G:213:ILE:HD12	1:G:214:ALA:H	1.85	0.42
1:B:22:ILE:HD12	1:B:59:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:HA	1:A:205:ARG:HD3	2.02	0.42
1:G:101:LYS:HE3	1:G:102:GLN:HE21	1.85	0.42
1:B:40:ALA:HB1	3:B:401:GPE:H121	2.01	0.41
1:C:170:ALA:HA	1:C:173:VAL:HG22	2.02	0.41
1:A:66[B]:THR:HG23	6:A:537:HOH:O	2.20	0.41
1:C:44:THR:HG21	1:C:213:ILE:HD12	2.02	0.41
1:D:306:ILE:HD12	1:D:306:ILE:C	2.45	0.41
1:G:215:ASN:OD1	1:G:218:LYS:NZ	2.50	0.41
1:B:163[A]:VAL:HG21	1:B:206:LEU:HD11	2.02	0.41
1:G:74:ILE:HD11	1:G:95:PHE:HB3	2.03	0.41
1:B:22:ILE:HG12	6:B:510:HOH:O	2.21	0.41
1:D:116:ILE:HD11	1:D:279:LEU:HD22	2.02	0.41
1:D:158:ASN:OD1	1:D:158:ASN:N	2.54	0.41
1:G:303:PRO:HD2	1:G:306:ILE:HD12	2.02	0.41
1:H:257:TYR:CD1	1:H:257:TYR:N	2.89	0.40
1:B:81:LYS:HB3	1:B:82:LYS:H	1.69	0.40
1:D:340:GLN:O	1:D:345:VAL:HG13	2.22	0.40
1:G:297:ILE:CD1	1:G:302:LEU:HD11	2.52	0.40
1:E:59:TYR:HB2	1:E:61:ILE:CD1	2.52	0.40
1:G:143:VAL:HG23	1:G:144:VAL:HG23	2.03	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	331/348 (95%)	321 (97%)	10 (3%)	0	100	100
1	B	327/348 (94%)	319 (98%)	8 (2%)	0	100	100
1	C	325/348 (93%)	313 (96%)	12 (4%)	0	100	100
1	D	326/348 (94%)	317 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	327/348 (94%)	317 (97%)	10 (3%)	0	100	100
1	F	327/348 (94%)	319 (98%)	8 (2%)	0	100	100
1	G	327/348 (94%)	317 (97%)	10 (3%)	0	100	100
1	H	328/348 (94%)	318 (97%)	10 (3%)	0	100	100
All	All	2618/2784 (94%)	2541 (97%)	77 (3%)	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	273/281 (97%)	272 (100%)	1 (0%)	84	89
1	B	269/281 (96%)	266 (99%)	3 (1%)	65	73
1	C	267/281 (95%)	266 (100%)	1 (0%)	84	89
1	D	267/281 (95%)	264 (99%)	3 (1%)	65	73
1	E	269/281 (96%)	265 (98%)	4 (2%)	57	64
1	F	268/281 (95%)	264 (98%)	4 (2%)	57	64
1	G	269/281 (96%)	263 (98%)	6 (2%)	45	50
1	H	270/281 (96%)	265 (98%)	5 (2%)	50	56
All	All	2152/2248 (96%)	2125 (99%)	27 (1%)	63	68

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	LEU
1	B	101	LYS
1	B	279	LEU
1	B	347	MSE
1	C	51	THR
1	D	51	THR

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Mol	Chain	Res	Type
1	D	217	GLU
1	D	279	LEU
1	E	128	LEU
1	E	144	VAL
1	E	236	ASP
1	E	347	MSE
1	F	128	LEU
1	F	143	VAL
1	F	326	LYS
1	F	347	MSE
1	G	128	LEU
1	G	168	VAL
1	G	213	ILE
1	G	240	LYS
1	G	314	GLU
1	G	343	VAL
1	H	91	VAL
1	H	104	VAL
1	H	129	LEU
1	H	293[A]	ARG
1	H	293[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	B	102	GLN
1	B	126	ASN
1	C	209	ASN
1	D	106	GLN
1	E	106	GLN
1	E	215	ASN
1	E	340	GLN
1	F	102	GLN
1	F	106	GLN
1	F	208	ASN
1	F	209	ASN
1	G	102	GLN
1	G	269	ASN
1	G	340	GLN
1	H	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
4	BTB	G	401	-	13,13,13	1.03	2 (15%)	7,16,16	1.57	1 (14%)
3	GPE	D	401	-	12,12,12	0.42	0	13,15,15	0.55	0
5	TRS	H	401	-	7,7,7	0.38	0	9,9,9	0.52	0
2	PEG	F	402	-	3,3,6	0.40	0	2,2,5	0.29	0
3	GPE	C	401	-	12,12,12	0.46	0	13,15,15	0.47	0
3	GPE	B	401	-	12,12,12	0.38	0	13,15,15	0.62	0
2	PEG	E	402	-	3,3,6	0.41	0	2,2,5	0.30	0
2	PEG	A	401	-	6,6,6	0.52	0	5,5,5	0.35	0
3	GPE	A	402	-	12,12,12	0.56	0	13,15,15	0.46	0
5	TRS	F	401	-	7,7,7	0.47	0	9,9,9	0.38	0
2	PEG	H	402	-	3,3,6	0.37	0	2,2,5	0.38	0
4	BTB	E	401	-	13,13,13	0.93	1 (7%)	7,16,16	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	G	401	-	-	8/21/21/21	-
3	GPE	D	401	-	-	0/13/13/13	-
5	TRS	H	401	-	-	3/9/9/9	-
2	PEG	F	402	-	-	1/1/1/4	-
3	GPE	C	401	-	-	0/13/13/13	-
3	GPE	B	401	-	-	0/13/13/13	-
2	PEG	E	402	-	-	1/1/1/4	-
2	PEG	A	401	-	-	1/4/4/4	-
3	GPE	A	402	-	-	0/13/13/13	-
5	TRS	F	401	-	-	5/9/9/9	-
2	PEG	H	402	-	-	1/1/1/4	-
4	BTB	E	401	-	-	5/21/21/21	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	401	BTB	C7-N	2.08	1.50	1.48
4	G	401	BTB	C5-N	2.03	1.50	1.48
4	E	401	BTB	C5-N	2.02	1.50	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	BTB	C8-C7-N	3.17	123.97	111.59

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	401	BTB	O1-C1-C2-C4
4	E	401	BTB	C6-C5-N-C7
4	G	401	BTB	C1-C2-N-C7
4	G	401	BTB	C3-C2-N-C7
4	G	401	BTB	C4-C2-N-C7
4	G	401	BTB	C6-C5-N-C7
4	E	401	BTB	N-C7-C8-O8
2	A	401	PEG	O2-C3-C4-O4
5	F	401	TRS	C2-C-C3-O3
5	H	401	TRS	C2-C-C3-O3
2	F	402	PEG	O2-C3-C4-O4
2	H	402	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	E	402	PEG	O2-C3-C4-O4
5	F	401	TRS	N-C-C3-O3
5	H	401	TRS	C1-C-C3-O3
5	H	401	TRS	N-C-C3-O3
4	G	401	BTB	C8-C7-N-C2
4	E	401	BTB	O1-C1-C2-N
4	G	401	BTB	C4-C2-N-C5
5	F	401	TRS	C1-C-C3-O3
4	G	401	BTB	C3-C2-C4-O4
5	F	401	TRS	C3-C-C2-O2
4	E	401	BTB	N-C2-C4-O4
4	G	401	BTB	N-C2-C3-O3
5	F	401	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	GPE	1	0
3	B	401	GPE	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	324/348 (93%)	-0.49	0	100	100	7, 20, 40, 58	5 (1%)
1	B	323/348 (92%)	-0.31	0	100	100	7, 25, 44, 58	3 (0%)
1	C	323/348 (92%)	0.14	4 (1%)	76	76	12, 32, 55, 82	1 (0%)
1	D	325/348 (93%)	-0.23	5 (1%)	72	71	13, 25, 55, 96	0
1	E	323/348 (92%)	-0.33	3 (0%)	81	80	8, 22, 45, 62	3 (0%)
1	F	324/348 (93%)	-0.20	2 (0%)	85	85	9, 29, 50, 61	2 (0%)
1	G	323/348 (92%)	-0.12	1 (0%)	90	89	12, 30, 56, 70	3 (0%)
1	H	323/348 (92%)	0.13	11 (3%)	48	47	11, 35, 65, 102	4 (1%)
All	All	2588/2784 (92%)	-0.18	26 (1%)	79	79	7, 27, 54, 102	21 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	306	ILE	5.5
1	E	208	ASN	4.7
1	H	82	LYS	3.2
1	C	306	ILE	3.1
1	D	345	VAL	2.7
1	C	270	ALA	2.6
1	H	21	ALA	2.5
1	H	74	ILE	2.5
1	H	79	THR	2.4
1	D	308	ALA	2.4
1	H	30	ALA	2.4
1	E	210	ASP	2.3
1	D	303	PRO	2.3
1	D	344	ILE	2.3
1	G	32	ALA	2.3
1	H	26	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	84	ALA	2.2
1	C	32	ALA	2.1
1	F	21	ALA	2.1
1	H	39	LEU	2.1
1	H	77	PHE	2.1
1	F	168	VAL	2.1
1	C	308	ALA	2.1
1	H	265	ALA	2.1
1	E	209	ASN	2.1
1	H	66	THR	2.1

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	PEG	H	402	4/7	0.69	0.21	56,56,59,59	0
5	TRS	H	401	8/8	0.74	0.15	53,58,61,62	0
5	TRS	F	401	8/8	0.81	0.14	42,49,54,54	0
2	PEG	A	401	7/7	0.84	0.14	49,54,60,66	0
4	BTB	E	401	14/14	0.84	0.14	33,36,46,55	0
2	PEG	E	402	4/7	0.86	0.17	44,46,48,52	0
4	BTB	G	401	14/14	0.87	0.11	27,30,32,34	0
2	PEG	F	402	4/7	0.89	0.16	45,46,46,46	0
3	GPE	C	401	13/13	0.97	0.06	20,22,30,32	0
3	GPE	D	401	13/13	0.97	0.07	15,19,30,35	0
3	GPE	B	401	13/13	0.98	0.06	13,14,26,28	0
3	GPE	A	402	13/13	0.99	0.05	11,12,23,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.