wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2020 – 04:37 PM BST

PDB ID	:	5T1P
Title	:	Crystal structure of the putative periplasmic solute-binding protein from Campylobacter jejuni
Authors	:	Filippova, E.V.; Wawrzsak, 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

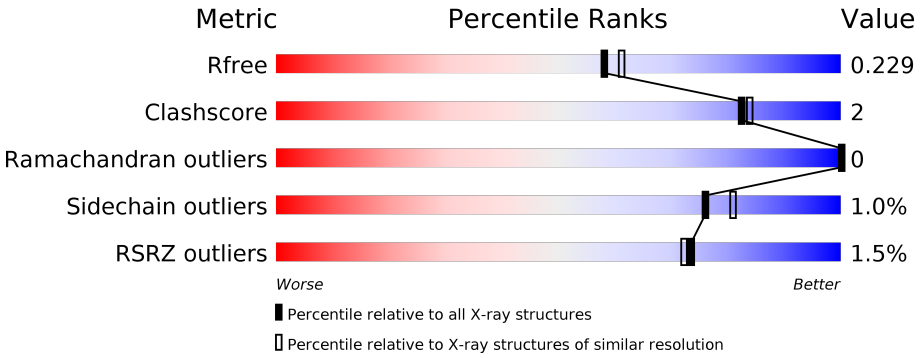
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 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.



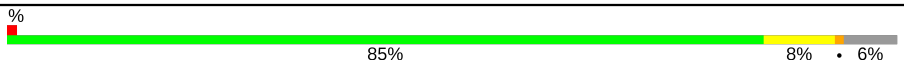
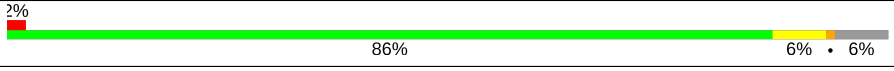
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	87% 6% 6%
1	C	348	4% 88% 5% 6%
1	D	348	3% 90% 6%
1	E	348	89% 5% 6%
1	F	348	89% 5% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	348	
1	H	348	

2 Entry composition (i)

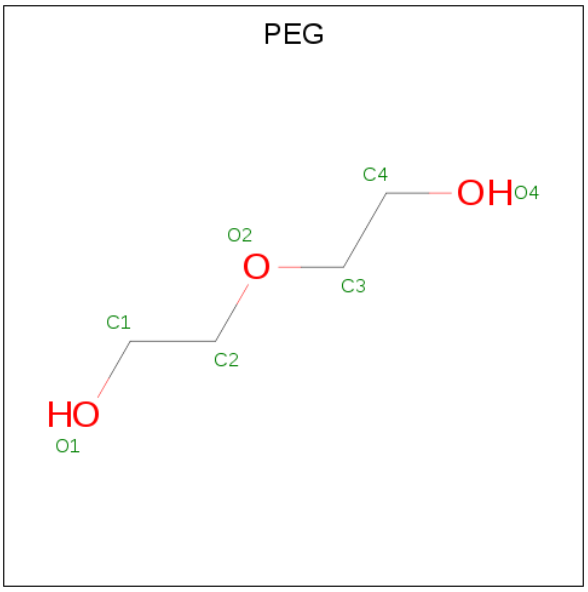
There are 6 unique types of molecules in this entry. The entry contains 22353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

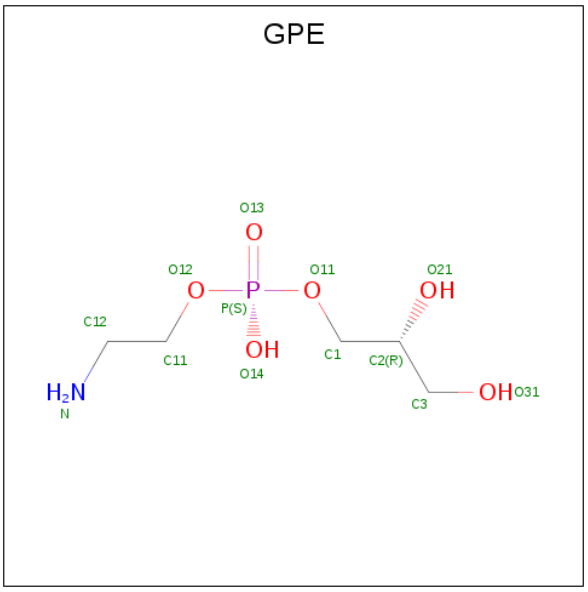
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	Se	0	6	0
			2607	1663	442	498	4			
1	B	326	Total	C	N	O	Se	0	3	0
			2573	1642	437	491	3			
1	C	326	Total	C	N	O	Se	0	1	0
			2557	1631	433	490	3			
1	D	328	Total	C	N	O	Se	0	0	0
			2562	1634	434	491	3			
1	E	326	Total	C	N	O	Se	0	3	0
			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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



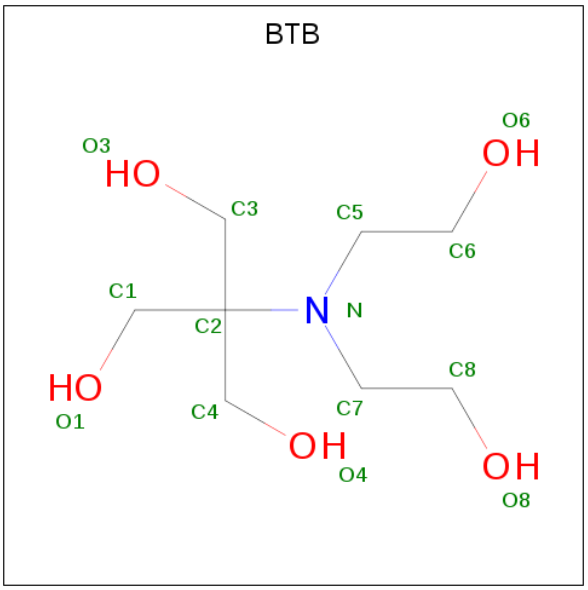
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is L-ALPHA-GLYCEROPHOSPHORYLETHANOLAMINE (three-letter code: GPE) (formula: $C_5H_{14}NO_6P$).



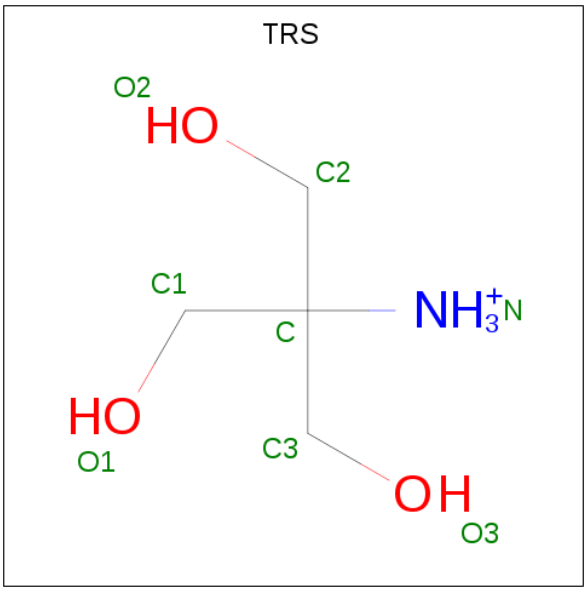
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			13	5	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			13	5	1	6	1		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: 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 (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 6 is water.

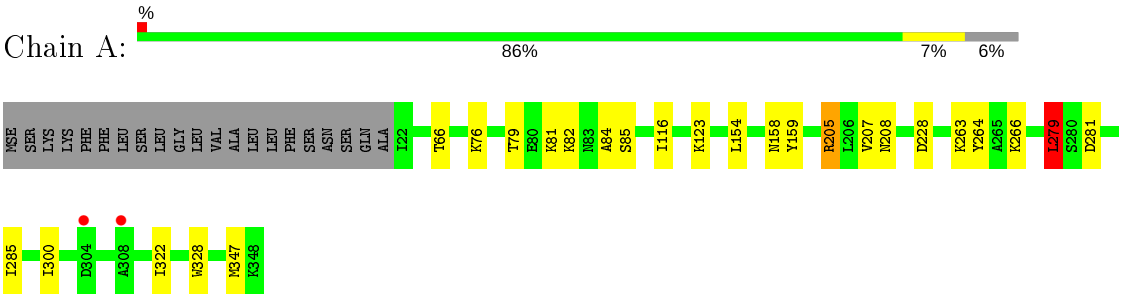
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	267	Total O 269 269	0	2
6	B	208	Total O 208 208	0	0
6	C	145	Total O 145 145	0	0
6	D	219	Total O 219 219	0	0
6	E	254	Total O 255 255	0	2
6	F	192	Total O 192 192	0	0
6	G	189	Total O 189 189	0	0
6	H	145	Total O 146 146	0	1

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.

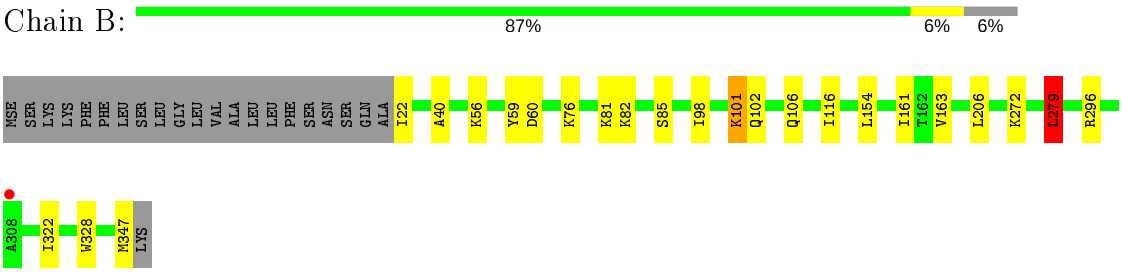
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain A:



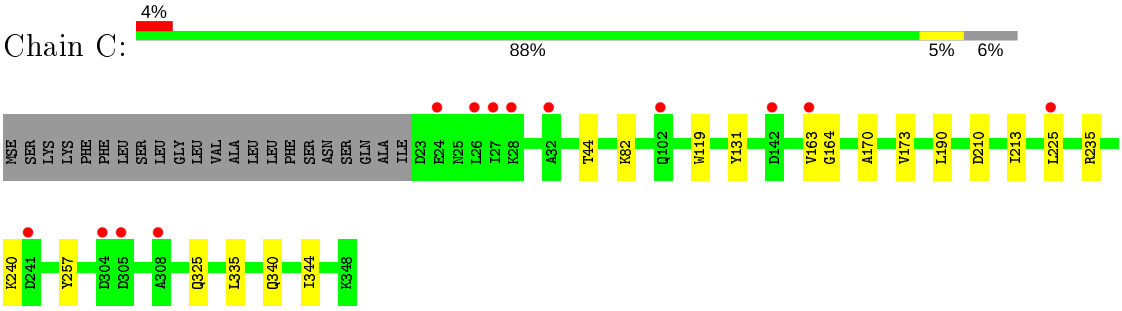
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain B:



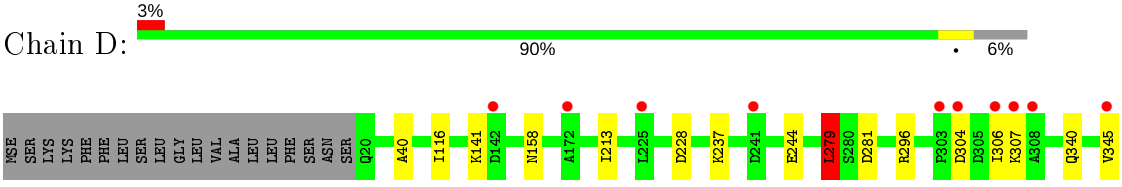
- Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain C:



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

Chain D:

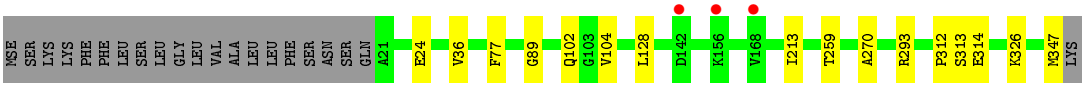


• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain E:

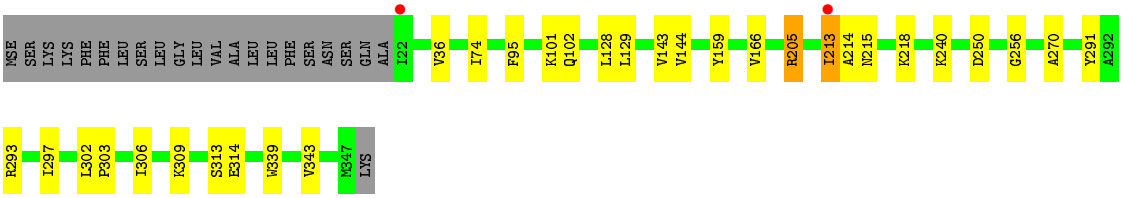
• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain F:



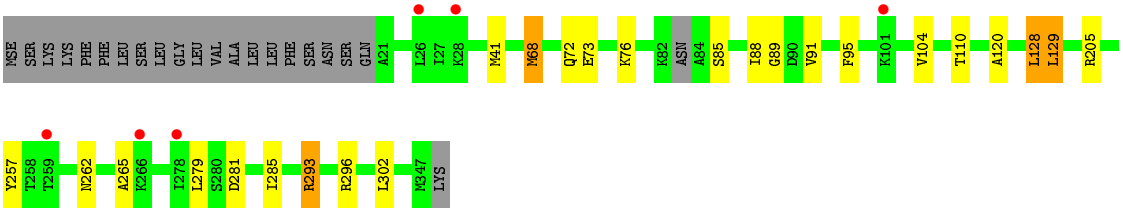
• Molecule 1: ABC transporter, periplasmic substrate-binding protein

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

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 29.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.00) 95.9 (29.67-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.176 , 0.224 0.184 , 0.229	Depositor DCC
R_{free} test set	8289 reflections (5.06%)	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)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GPE, TRS, PEG, BTB

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	0.67	0/2656	0.87	4/3591 (0.1%)
1	B	0.62	0/2622	0.85	4/3550 (0.1%)
1	C	0.60	0/2606	0.81	0/3526
1	D	0.60	0/2611	0.86	5/3535 (0.1%)
1	E	0.67	1/2625 (0.0%)	0.88	3/3553 (0.1%)
1	F	0.58	0/2617	0.81	0/3543
1	G	0.61	0/2626	0.82	2/3555 (0.1%)
1	H	0.57	0/2643	0.83	5/3575 (0.1%)
All	All	0.62	1/21006 (0.0%)	0.84	23/28428 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	334	GLU	CD-OE1	5.47	1.31	1.25

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	296	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	E	208	ASN	CB-CA-C	-10.80	88.80	110.40
1	D	296	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A	205	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	205	ARG	NE-CZ-NH2	-7.57	116.52	120.30

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	2607	0	2613	17	0
1	B	2573	0	2575	15	0
1	C	2557	0	2557	14	0
1	D	2562	0	2560	7	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	102	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.

The worst 5 of 102 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:NH1	1:H:293[A]:ARG:HG3	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

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
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 (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	273/281 (97%)	271 (99%)	2 (1%)	84 88
1	B	269/281 (96%)	267 (99%)	2 (1%)	84 88
1	C	267/281 (95%)	267 (100%)	0	100 100
1	D	267/281 (95%)	265 (99%)	2 (1%)	84 88
1	E	269/281 (96%)	265 (98%)	4 (2%)	65 69
1	F	268/281 (95%)	265 (99%)	3 (1%)	73 78
1	G	269/281 (96%)	265 (98%)	4 (2%)	65 69
1	H	270/281 (96%)	265 (98%)	5 (2%)	57 61
All	All	2152/2248 (96%)	2130 (99%)	22 (1%)	76 81

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	347	MSE
1	F	347	MSE
1	H	293[A]	ARG
1	F	128	LEU
1	F	326	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	102	GLN
1	F	208	ASN
1	G	269	ASN
1	E	215	ASN
1	G	102	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	TRS	F	401	-	7,7,7	0.45	0	9,9,9	0.34	0
5	TRS	H	401	-	7,7,7	0.36	0	9,9,9	0.44	0
2	PEG	F	402	-	3,3,6	0.44	0	2,2,5	0.24	0
2	PEG	A	401	-	6,6,6	0.52	0	5,5,5	0.35	0
3	GPE	A	402	-	12,12,12	0.55	0	13,15,15	0.45	0
4	BTB	G	401	-	13,13,13	0.98	1 (7%)	7,16,16	1.53	1 (14%)
3	GPE	C	401	-	12,12,12	0.45	0	13,15,15	0.47	0
2	PEG	E	402	-	3,3,6	0.44	0	2,2,5	0.26	0
3	GPE	B	401	-	12,12,12	0.37	0	13,15,15	0.60	0
2	PEG	H	402	-	3,3,6	0.41	0	2,2,5	0.34	0
3	GPE	D	401	-	12,12,12	0.41	0	13,15,15	0.54	0
4	BTB	E	401	-	13,13,13	0.87	0	7,16,16	1.01	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
5	TRS	F	401	-	-	4/9/9/9	-
5	TRS	H	401	-	-	3/9/9/9	-
2	PEG	F	402	-	-	1/1/1/4	-
2	PEG	A	401	-	-	1/4/4/4	-
3	GPE	A	402	-	-	0/13/13/13	-
4	BTB	G	401	-	-	6/21/21/21	-
3	GPE	C	401	-	-	0/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	E	402	-	-	1/1/1/4	-
3	GPE	B	401	-	-	0/13/13/13	-
2	PEG	H	402	-	-	1/1/1/4	-
3	GPE	D	401	-	-	0/13/13/13	-
4	BTB	E	401	-	-	5/21/21/21	-

All (1) bond length outliers are listed below:

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

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O1-C1-C2-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	GPE	1	0
3	D	401	GPE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.33	2 (0%)	89 88	10, 20, 40, 58	0
1	B	323/348 (92%)	-0.22	1 (0%)	94 93	11, 25, 44, 58	0
1	C	323/348 (92%)	0.14	13 (4%)	38 37	17, 32, 55, 82	0
1	D	325/348 (93%)	-0.13	10 (3%)	49 48	13, 25, 55, 96	0
1	E	323/348 (92%)	-0.28	1 (0%)	94 93	11, 23, 45, 62	0
1	F	324/348 (93%)	-0.16	3 (0%)	84 83	16, 29, 50, 61	0
1	G	323/348 (92%)	-0.17	2 (0%)	89 88	14, 30, 56, 70	0
1	H	323/348 (92%)	0.10	6 (1%)	66 65	16, 35, 65, 102	0
All	All	2588/2784 (92%)	-0.13	38 (1%)	73 72	10, 27, 54, 102	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	308	ALA	5.9
1	D	307	LYS	5.6
1	D	304	ASP	4.4
1	E	208	ASN	4.1
1	C	308	ALA	3.8

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 monosaccharides 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, 95^{th} 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
5	TRS	H	401	8/8	0.74	0.20	53,58,61,62	0
5	TRS	F	401	8/8	0.77	0.19	42,49,54,54	0
2	PEG	H	402	4/7	0.82	0.19	56,56,59,59	0
4	BTB	G	401	14/14	0.84	0.15	27,30,32,34	0
2	PEG	A	401	7/7	0.84	0.21	49,54,60,66	0
4	BTB	E	401	14/14	0.87	0.15	33,36,46,55	0
2	PEG	F	402	4/7	0.90	0.14	45,46,46,46	0
2	PEG	E	402	4/7	0.92	0.13	44,46,48,52	0
3	GPE	D	401	13/13	0.97	0.16	15,19,30,35	0
3	GPE	C	401	13/13	0.97	0.14	20,22,30,32	0
3	GPE	B	401	13/13	0.98	0.13	13,14,26,28	0
3	GPE	A	402	13/13	0.99	0.10	11,12,23,27	0

6.5 Other polymers

There are no such residues in this entry.