



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:57 am BST

PDB ID : 3V56
Title : Re-refinement of PDB entry 1OSG - Complex between BAFF and a BR3 derived peptide presented in a beta-hairpin scaffold - reveals an additional copy of the peptide.
Authors : Smart, O.S.; Womack, T.O.; Flensburg, C.; Keller, P.; Sharff, A.; Paciorek, W.; Vonnrhein, C.; Bricogne, G.
Deposited on : 2011-12-16
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

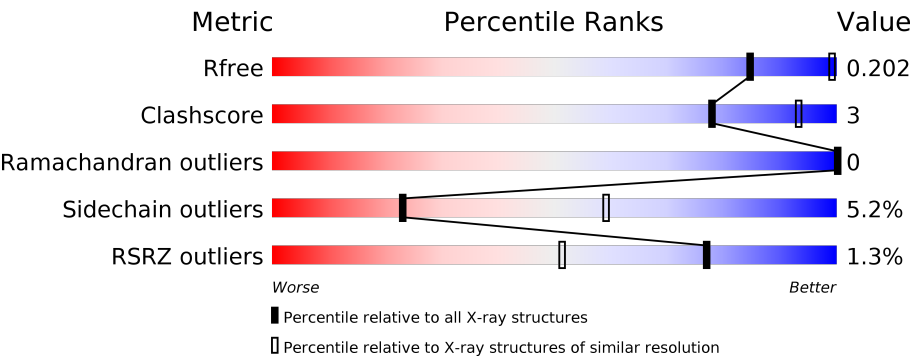
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	208	<div><div></div><div>63%5%31%</div></div>
1	B	208	<div><div>%</div><div>63%5%31%</div></div>
1	C	208	<div><div></div><div>63%6%31%</div></div>
1	D	208	<div><div></div><div>61%8%31%</div></div>
1	E	208	<div><div></div><div>61%8%31%</div></div>
1	F	208	<div><div></div><div>61%7%31%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	14	<div><div></div><div>93%7%</div></div>
2	H	14	<div><div></div><div>93%7%</div></div>
2	I	14	<div><div>14%</div><div>79%14%7%</div></div>
2	J	14	<div><div>21%</div><div>79%14%7%</div></div>
2	K	14	<div><div>14%</div><div>79%14%7%</div></div>
2	L	14	<div><div></div><div>93%7%</div></div>
2	Z	14	<div><div>14%</div><div>79%7%7%7%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7446 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 Tumor necrosis factor ligand superfamily member 13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	2	0
			1123	721	179	216	7			
1	B	144	Total	C	N	O	S	0	2	0
			1117	718	176	216	7			
1	C	144	Total	C	N	O	S	0	2	0
			1118	719	178	214	7			
1	D	144	Total	C	N	O	S	0	2	0
			1103	707	177	212	7			
1	E	144	Total	C	N	O	S	0	2	0
			1117	719	177	214	7			
1	F	144	Total	C	N	O	S	0	2	0
			1125	723	179	216	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLY	-	EXPRESSION TAG	UNP Q9Y275
A	79	SER	-	EXPRESSION TAG	UNP Q9Y275
A	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
A	81	MET	-	EXPRESSION TAG	UNP Q9Y275
B	78	GLY	-	EXPRESSION TAG	UNP Q9Y275
B	79	SER	-	EXPRESSION TAG	UNP Q9Y275
B	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
B	81	MET	-	EXPRESSION TAG	UNP Q9Y275
C	78	GLY	-	EXPRESSION TAG	UNP Q9Y275
C	79	SER	-	EXPRESSION TAG	UNP Q9Y275
C	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
C	81	MET	-	EXPRESSION TAG	UNP Q9Y275
D	78	GLY	-	EXPRESSION TAG	UNP Q9Y275
D	79	SER	-	EXPRESSION TAG	UNP Q9Y275
D	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
D	81	MET	-	EXPRESSION TAG	UNP Q9Y275
E	78	GLY	-	EXPRESSION TAG	UNP Q9Y275

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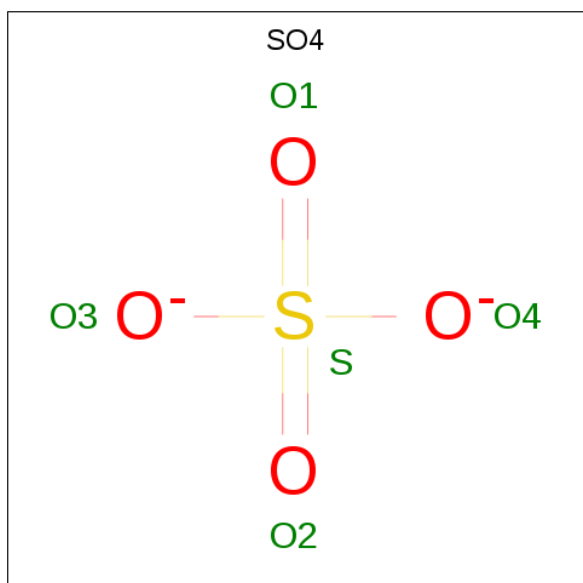
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Chain	Residue	Modelled	Actual	Comment	Reference
E	79	SER	-	EXPRESSION TAG	UNP Q9Y275
E	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
E	81	MET	-	EXPRESSION TAG	UNP Q9Y275
F	78	GLY	-	EXPRESSION TAG	UNP Q9Y275
F	79	SER	-	EXPRESSION TAG	UNP Q9Y275
F	80	HIS	-	EXPRESSION TAG	UNP Q9Y275
F	81	MET	-	EXPRESSION TAG	UNP Q9Y275

- Molecule 2 is a protein called BR3 derived peptive.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	14	Total	C	N	O	S	0	0	1
			111	72	22	15	2			
2	H	13	Total	C	N	O	S	0	0	1
			99	66	17	14	2			
2	I	13	Total	C	N	O	S	0	0	1
			99	66	17	14	2			
2	J	13	Total	C	N	O	S	0	0	1
			99	66	17	14	2			
2	K	13	Total	C	N	O	S	0	0	1
			108	70	22	14	2			
2	L	13	Total	C	N	O	S	0	0	1
			108	70	22	14	2			
2	Z	13	Total	C	N	O	S	0	0	1
			91	58	17	14	2			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

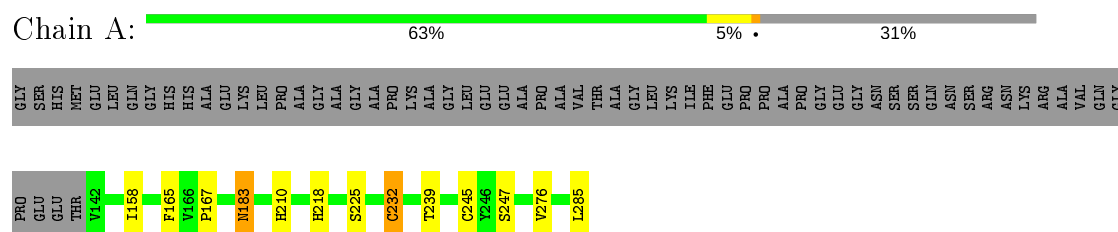
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	4	Total O 4 4	0	0
4	C	2	Total O 2 2	0	0
4	D	3	Total O 3 3	0	0
4	E	2	Total O 2 2	0	0
4	F	4	Total O 4 4	0	0

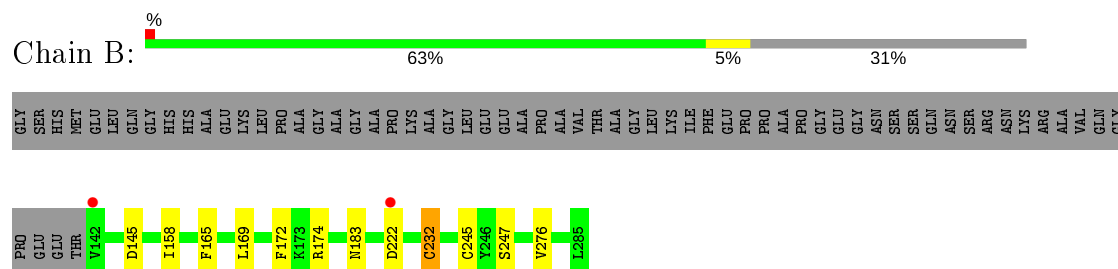
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

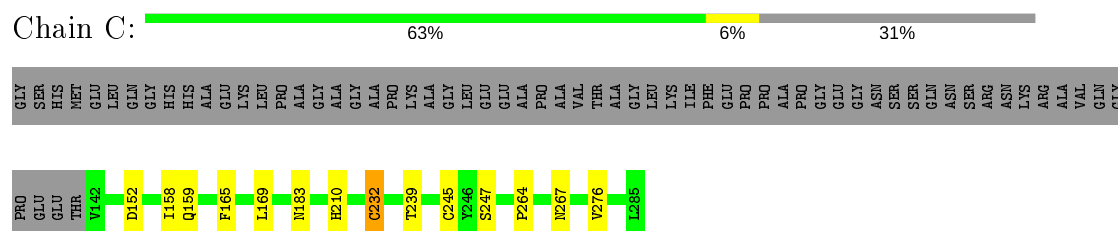
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



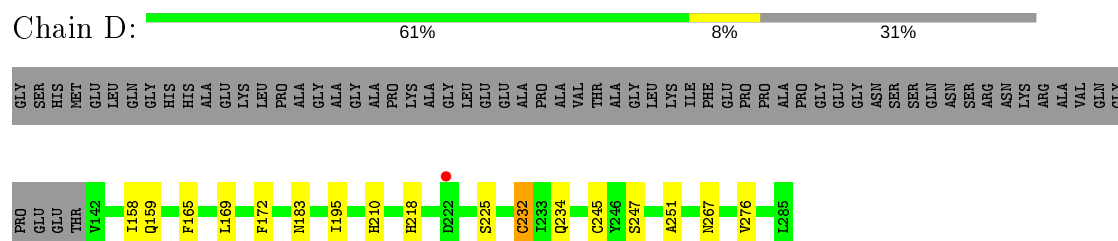
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain E: 

GLY SER HIS MET LEU GLN GLY HIS HIS ALA GLU LYS LEU PRO ALA GLY ALA GLY PRO LYS ALA GLY LEU GLU GLU ALA PRO VAL THR ALA GLY LEU LYS ILE PHE GLU PRO ALA PRO GLY GLY GLY ASN SER SER GLN ASN SER ARG ASN LYS ARG ALA VAL GLN GLY

PRO GLU GLU THR V142 I158 S162 F165 L169 M183 F193 H210 L211 T228 C232 T233 Q234 C245 S247 P264 V276 K283 L284 L285

- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain F: 

GLY SER HIS MET LEU GLN GLY HIS HIS ALA GLU LYS LEU PRO ALA GLY ALA GLY PRO LYS ALA GLU GLU ALA PRO VAL THR ALA GLY LEU LYS ILE PHE GLU PRO ALA PRO GLY GLY GLY ASN SER SER GLN ASN SER ARG ASN LYS ARG ALA VAL GLN GLY

PRO GLU GLU THR V142 I158 F165 V167 W168 L169 M183 L200 H210 L211 H218 S225 T228 C232 T239 S244 C245 S247 V276 L285

- Molecule 2: BR3 derived peptide

Chain G: 


T22 H31 T35

- Molecule 2: BR3 derived peptide

Chain H: 


ACE C23 T35

- Molecule 2: BR3 derived peptide

Chain I: 

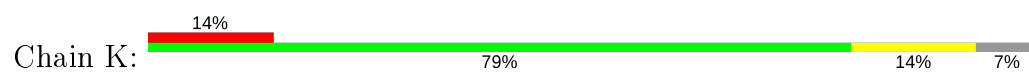
ACE C23 D26 V29 C34 T35

- Molecule 2: BR3 derived peptide

Chain J: 

ACE C23 V32 V33 C34 T35

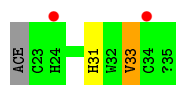
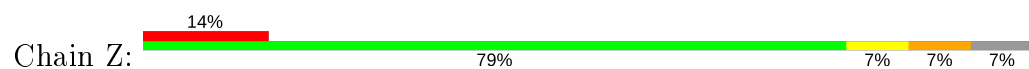
- Molecule 2: BR3 derived peptide



- Molecule 2: BR3 derived peptive



- Molecule 2: BR3 derived peptive



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	121.63Å 121.63Å 157.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 3.00 29.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.85-3.00) 99.7 (29.22-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.00Å)	Xtriage
Refinement program	BUSTER 2.13.0	Depositor
R, R_{free}	0.162 , 0.200 0.165 , 0.202	Depositor DCC
R_{free} test set	2536 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7446	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACE, NH2

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	0.52	0/1155	0.71	0/1566
1	B	0.54	0/1149	0.72	0/1561
1	C	0.52	0/1150	0.71	0/1561
1	D	0.52	0/1134	0.74	0/1541
1	E	0.50	0/1149	0.71	0/1560
1	F	0.53	0/1157	0.72	0/1569
2	G	0.38	0/113	0.79	1/155 (0.6%)
2	H	0.53	0/102	0.66	0/140
2	I	0.42	0/102	0.83	0/140
2	J	0.41	0/102	0.75	0/140
2	K	0.49	0/112	0.73	0/153
2	L	0.44	0/112	0.70	0/153
2	Z	0.39	0/94	0.74	0/130
All	All	0.51	0/7631	0.72	1/10369 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	G	31	HIS	N-CA-CB	5.02	119.63	110.60

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	1123	0	1089	7	0
1	B	1117	0	1071	6	0
1	C	1118	0	1083	7	0
1	D	1103	0	1056	8	0
1	E	1117	0	1078	7	0
1	F	1125	0	1096	8	0
2	G	111	0	95	0	0
2	H	99	0	79	0	0
2	I	99	0	79	1	0
2	J	99	0	79	0	0
2	K	108	0	91	2	0
2	L	108	0	91	0	0
2	Z	91	0	57	2	0
3	A	5	0	0	0	0
3	D	5	0	0	1	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
4	E	2	0	0	0	0
4	F	4	0	0	0	0
All	All	7446	0	7044	42	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.

All (42) 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:232[B]:CYS:HB3	1:B:245[B]:CYS:SG	2.15	0.87
1:A:232[B]:CYS:HB3	1:A:245[B]:CYS:SG	2.15	0.86
1:C:232[B]:CYS:HB3	1:C:245[B]:CYS:SG	2.16	0.86
1:D:232[B]:CYS:HB3	1:D:245[B]:CYS:SG	2.16	0.84
1:F:232[B]:CYS:HB3	1:F:245[B]:CYS:SG	2.18	0.84
1:E:232[B]:CYS:HB3	1:E:245[B]:CYS:SG	2.17	0.84
2:K:27:LEU:HD11	2:Z:33:VAL:HG13	1.80	0.63
1:A:218:HIS:CD2	1:D:172:PHE:HA	2.43	0.53
1:F:210:HIS:CE1	1:F:232[B]:CYS:HG	2.27	0.52
1:B:172:PHE:HA	1:F:218:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:32:TRP:HH2	2:Z:31:HIS:CG	2.31	0.49
1:D:232[B]:CYS:SG	1:D:247:SER:HB2	2.53	0.48
1:D:210:HIS:CE1	1:D:232[B]:CYS:HG	2.33	0.47
1:B:232[B]:CYS:SG	1:B:247:SER:HB2	2.55	0.47
1:E:232[B]:CYS:SG	1:E:247:SER:HB2	2.55	0.47
1:E:158:ILE:HB	1:E:165:PHE:HB2	1.97	0.47
1:F:232[B]:CYS:SG	1:F:247:SER:HB2	2.55	0.47
1:C:152:ASP:HB2	1:C:169:LEU:HD13	1.97	0.46
1:B:158:ILE:HB	1:B:165:PHE:HB2	1.98	0.46
1:B:232[B]:CYS:HB3	1:B:245[B]:CYS:HG	1.76	0.46
1:A:158:ILE:HB	1:A:165:PHE:HB2	1.97	0.45
1:D:158:ILE:HB	1:D:165:PHE:HB2	1.99	0.45
1:C:158:ILE:HB	1:C:165:PHE:HB2	1.99	0.45
1:C:210:HIS:CE1	1:C:232[B]:CYS:HG	2.34	0.45
1:C:232[B]:CYS:SG	1:C:247:SER:HB2	2.57	0.45
1:A:167:PRO:HA	1:A:183:ASN:HD21	1.82	0.44
1:D:195:ILE:CD1	1:D:251:ALA:HB3	2.48	0.44
1:F:167:PRO:HA	1:F:183:ASN:HD21	1.83	0.43
1:A:232[B]:CYS:SG	1:A:247:SER:HB2	2.59	0.43
1:C:169:LEU:HA	1:C:169:LEU:HD12	1.87	0.43
1:C:159:GLN:HE22	1:C:267:ASN:HB2	1.84	0.43
1:A:210:HIS:CE1	1:A:232[B]:CYS:HG	2.37	0.43
1:D:234:GLN:NE2	3:D:499:SO4:O2	2.52	0.42
1:D:234:GLN:HE22	1:E:234:GLN:HE22	1.67	0.42
1:F:158:ILE:HB	1:F:165:PHE:HB2	2.00	0.42
1:E:211:LEU:HB3	1:E:228:THR:HG23	2.02	0.42
1:E:210:HIS:CE1	1:E:232[B]:CYS:HG	2.37	0.41
1:F:211:LEU:HB3	1:F:228:THR:HG23	2.02	0.41
1:F:200:LEU:HA	1:F:244:SER:HA	2.03	0.41
1:E:193:PHE:CZ	1:E:283:LYS:HD2	2.56	0.41
2:I:26:ASP:HB3	2:I:29:VAL:HG22	2.03	0.41
1:A:285:LEU:C	1:B:174:ARG:HH22	2.25	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/208 (69%)	139 (96%)	5 (4%)	0	100	100
1	B	144/208 (69%)	141 (98%)	3 (2%)	0	100	100
1	C	144/208 (69%)	141 (98%)	3 (2%)	0	100	100
1	D	144/208 (69%)	140 (97%)	4 (3%)	0	100	100
1	E	144/208 (69%)	140 (97%)	4 (3%)	0	100	100
1	F	144/208 (69%)	141 (98%)	3 (2%)	0	100	100
2	G	12/14 (86%)	12 (100%)	0	0	100	100
2	H	11/14 (79%)	11 (100%)	0	0	100	100
2	I	11/14 (79%)	11 (100%)	0	0	100	100
2	J	11/14 (79%)	11 (100%)	0	0	100	100
2	K	11/14 (79%)	11 (100%)	0	0	100	100
2	L	11/14 (79%)	11 (100%)	0	0	100	100
2	Z	11/14 (79%)	11 (100%)	0	0	100	100
All	All	942/1346 (70%)	920 (98%)	22 (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	121/171 (71%)	115 (95%)	6 (5%)	24	60
1	B	119/171 (70%)	112 (94%)	7 (6%)	19	54
1	C	120/171 (70%)	114 (95%)	6 (5%)	24	60
1	D	116/171 (68%)	107 (92%)	9 (8%)	12	42
1	E	119/171 (70%)	111 (93%)	8 (7%)	16	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	122/171 (71%)	115 (94%)	7 (6%)	20	56
2	G	11/12 (92%)	11 (100%)	0	100	100
2	H	9/12 (75%)	9 (100%)	0	100	100
2	I	9/12 (75%)	9 (100%)	0	100	100
2	J	9/12 (75%)	7 (78%)	2 (22%)	1	4
2	K	11/12 (92%)	11 (100%)	0	100	100
2	L	11/12 (92%)	11 (100%)	0	100	100
2	Z	7/12 (58%)	6 (86%)	1 (14%)	3	15
All	All	784/1110 (71%)	738 (94%)	46 (6%)	23	54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	225	SER
1	A	232[A]	CYS
1	A	232[B]	CYS
1	A	239	THR
1	A	276	VAL
1	B	145	ASP
1	B	169	LEU
1	B	183	ASN
1	B	222	ASP
1	B	232[A]	CYS
1	B	232[B]	CYS
1	B	276	VAL
1	C	183	ASN
1	C	232[A]	CYS
1	C	232[B]	CYS
1	C	239	THR
1	C	264	PRO
1	C	276	VAL
1	D	159	GLN
1	D	169	LEU
1	D	183	ASN
1	D	218	HIS
1	D	225	SER
1	D	232[A]	CYS
1	D	232[B]	CYS

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Mol	Chain	Res	Type
1	D	267	ASN
1	D	276	VAL
1	E	142	VAL
1	E	162	SER
1	E	169	LEU
1	E	183	ASN
1	E	232[A]	CYS
1	E	232[B]	CYS
1	E	264	PRO
1	E	276	VAL
1	F	169	LEU
1	F	183	ASN
1	F	225	SER
1	F	232[A]	CYS
1	F	232[B]	CYS
1	F	239	THR
1	F	276	VAL
2	J	23	CYS
2	J	34	CYS
2	Z	33	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	234	GLN
1	B	234	GLN
1	C	234	GLN
1	D	159	GLN
1	D	218	HIS
1	D	234	GLN
1	D	269	GLN
1	E	234	GLN
1	F	218	HIS
1	F	234	GLN
2	K	24	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	SO4	A	499	-	4,4,4	0.34	0	6,6,6	0.16	0
3	SO4	D	499	-	4,4,4	0.15	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	499	SO4	1	0

5.7 Other polymers [i](#)

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, 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	144/208 (69%)	-0.64	0 100 100	26, 42, 64, 73	0
1	B	144/208 (69%)	-0.58	2 (1%) 75 49	29, 43, 66, 89	0
1	C	144/208 (69%)	-0.62	0 100 100	33, 47, 63, 79	0
1	D	144/208 (69%)	-0.53	1 (0%) 87 69	32, 49, 83, 122	0
1	E	144/208 (69%)	-0.63	0 100 100	32, 49, 69, 84	0
1	F	144/208 (69%)	-0.66	0 100 100	28, 39, 59, 76	0
2	G	12/14 (85%)	0.21	0 100 100	46, 76, 102, 107	0
2	H	12/14 (85%)	0.34	0 100 100	50, 73, 95, 98	0
2	I	12/14 (85%)	0.71	2 (16%) 1 0	60, 83, 108, 110	0
2	J	12/14 (85%)	0.88	3 (25%) 0 0	67, 89, 121, 125	0
2	K	12/14 (85%)	0.55	2 (16%) 1 0	45, 82, 98, 102	0
2	L	12/14 (85%)	0.27	0 100 100	45, 76, 106, 106	0
2	Z	12/14 (85%)	1.17	2 (16%) 1 0	84, 91, 99, 100	0
All	All	948/1346 (70%)	-0.50	12 (1%) 77 51	26, 46, 88, 125	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	34	CYS	3.9
2	I	23	CYS	3.5
2	J	34	CYS	2.8
1	B	142	VAL	2.8
2	Z	24	HIS	2.8
2	J	23	CYS	2.7
2	I	34	CYS	2.6
1	D	222	ASP	2.5
1	B	222	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	24	HIS	2.4
2	Z	34	CYS	2.1
2	J	32	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
3	SO4	A	499	5/5	0.90	0.27	105,106,108,109	0
3	SO4	D	499	5/5	0.91	0.33	125,128,129,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.