



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2018 – 10:10 PM EST

PDB ID : 6F45
Title : Crystal structure of the gp37-gp38 adhesin tip complex of the bacteriophage S16 long tail fiber
Authors : Dunne, M.; Leiman, P.; Klumpp, J.; Loessner, M.J.
Deposited on : 2017-11-29
Resolution : 1.70 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

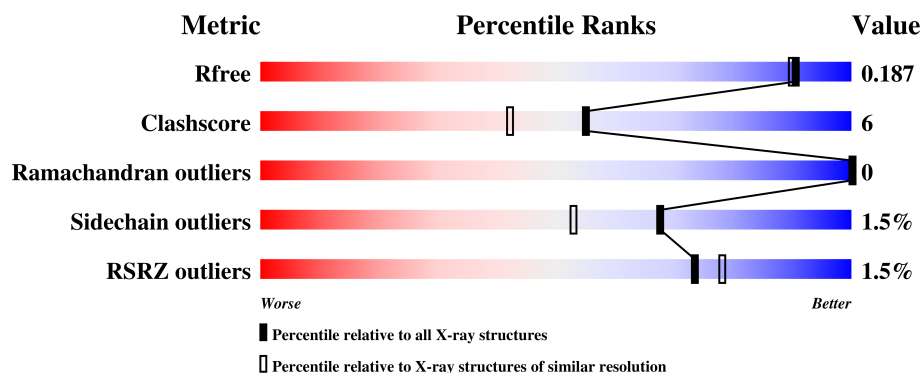
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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. 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	D	249	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
2	A	204	<div> <div>28%</div> <div>67%</div> </div>
2	B	204	<div> <div>32%</div> <div>65%</div> </div>
2	C	204	<div> <div>29%</div> <div>5%</div> <div>66%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4057 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 Receptor recognition protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	248	Total	C	N	O	S	0	7	0
			1850	1151	340	356	3			

- Molecule 2 is a protein called Long tail fiber distal subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	68	Total	C	N	O	S	0	3	0
			509	312	92	104	1			
2	B	72	Total	C	N	O	S	0	1	0
			520	321	94	104	1			
2	C	69	Total	C	N	O	S	0	1	0
			504	309	92	102	1			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	MET	-	initiating methionine	UNP M1EAS5
A	547	GLY	-	expression tag	UNP M1EAS5
A	548	SER	-	expression tag	UNP M1EAS5
A	549	SER	-	expression tag	UNP M1EAS5
A	550	HIS	-	expression tag	UNP M1EAS5
A	551	HIS	-	expression tag	UNP M1EAS5
A	552	HIS	-	expression tag	UNP M1EAS5
A	553	HIS	-	expression tag	UNP M1EAS5
A	554	HIS	-	expression tag	UNP M1EAS5
A	555	HIS	-	expression tag	UNP M1EAS5
A	556	SER	-	expression tag	UNP M1EAS5
A	557	GLN	-	expression tag	UNP M1EAS5
A	558	ASP	-	expression tag	UNP M1EAS5
A	559	PRO	-	expression tag	UNP M1EAS5
A	560	GLU	-	expression tag	UNP M1EAS5
A	561	ASN	-	expression tag	UNP M1EAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	562	LEU	-	expression tag	UNP M1EAS5
A	563	TYR	-	expression tag	UNP M1EAS5
A	564	PHE	-	expression tag	UNP M1EAS5
A	565	GLN	-	expression tag	UNP M1EAS5
A	566	GLY	-	expression tag	UNP M1EAS5
B	546	MET	-	initiating methionine	UNP M1EAS5
B	547	GLY	-	expression tag	UNP M1EAS5
B	548	SER	-	expression tag	UNP M1EAS5
B	549	SER	-	expression tag	UNP M1EAS5
B	550	HIS	-	expression tag	UNP M1EAS5
B	551	HIS	-	expression tag	UNP M1EAS5
B	552	HIS	-	expression tag	UNP M1EAS5
B	553	HIS	-	expression tag	UNP M1EAS5
B	554	HIS	-	expression tag	UNP M1EAS5
B	555	HIS	-	expression tag	UNP M1EAS5
B	556	SER	-	expression tag	UNP M1EAS5
B	557	GLN	-	expression tag	UNP M1EAS5
B	558	ASP	-	expression tag	UNP M1EAS5
B	559	PRO	-	expression tag	UNP M1EAS5
B	560	GLU	-	expression tag	UNP M1EAS5
B	561	ASN	-	expression tag	UNP M1EAS5
B	562	LEU	-	expression tag	UNP M1EAS5
B	563	TYR	-	expression tag	UNP M1EAS5
B	564	PHE	-	expression tag	UNP M1EAS5
B	565	GLN	-	expression tag	UNP M1EAS5
B	566	GLY	-	expression tag	UNP M1EAS5
C	546	MET	-	initiating methionine	UNP M1EAS5
C	547	GLY	-	expression tag	UNP M1EAS5
C	548	SER	-	expression tag	UNP M1EAS5
C	549	SER	-	expression tag	UNP M1EAS5
C	550	HIS	-	expression tag	UNP M1EAS5
C	551	HIS	-	expression tag	UNP M1EAS5
C	552	HIS	-	expression tag	UNP M1EAS5
C	553	HIS	-	expression tag	UNP M1EAS5
C	554	HIS	-	expression tag	UNP M1EAS5
C	555	HIS	-	expression tag	UNP M1EAS5
C	556	SER	-	expression tag	UNP M1EAS5
C	557	GLN	-	expression tag	UNP M1EAS5
C	558	ASP	-	expression tag	UNP M1EAS5
C	559	PRO	-	expression tag	UNP M1EAS5
C	560	GLU	-	expression tag	UNP M1EAS5
C	561	ASN	-	expression tag	UNP M1EAS5

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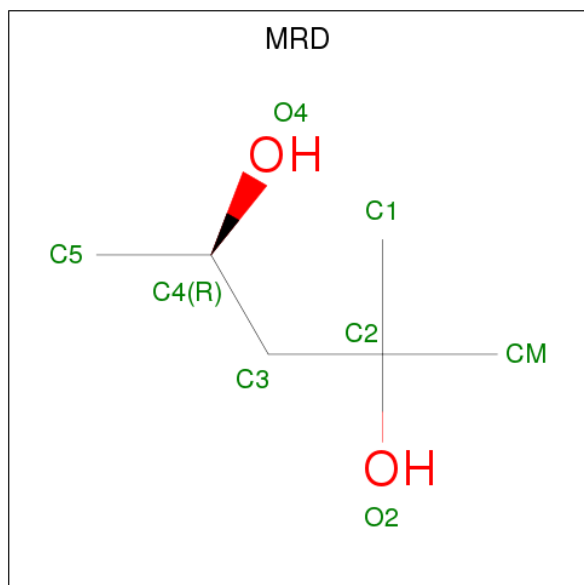
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Chain	Residue	Modelled	Actual	Comment	Reference
C	562	LEU	-	expression tag	UNP M1EAS5
C	563	TYR	-	expression tag	UNP M1EAS5
C	564	PHE	-	expression tag	UNP M1EAS5
C	565	GLN	-	expression tag	UNP M1EAS5
C	566	GLY	-	expression tag	UNP M1EAS5

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	3	Total	Mg	0	0
			3	3		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



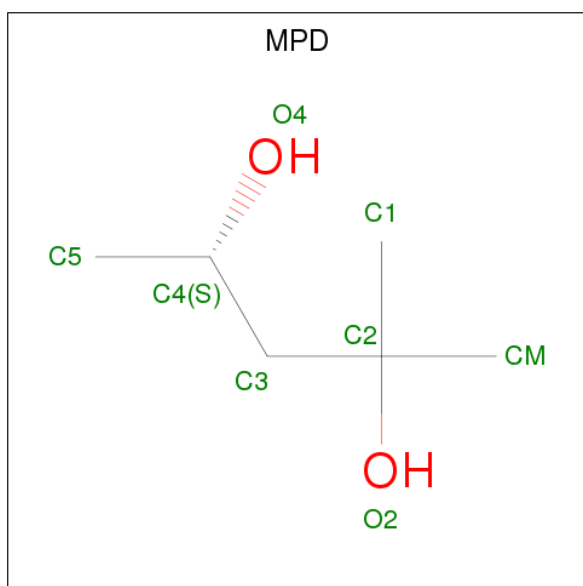
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		

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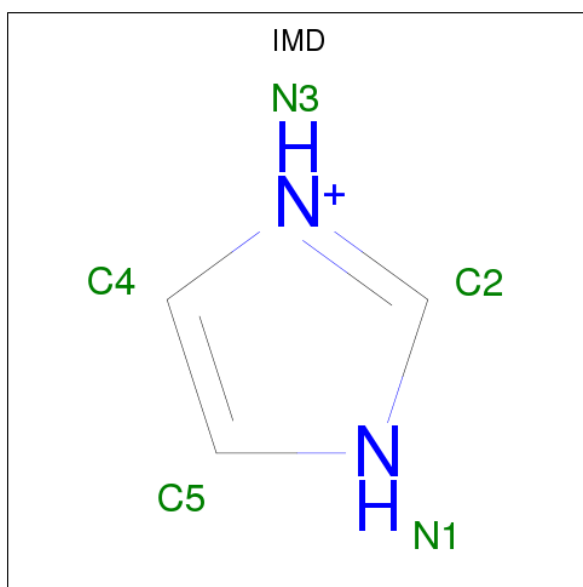
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

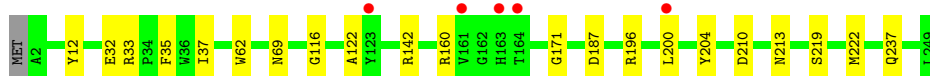


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	N	0	0
			5	3	2		
6	D	1	Total	C	N	0	0
			5	3	2		
6	A	1	Total	C	N	0	0
			5	3	2		

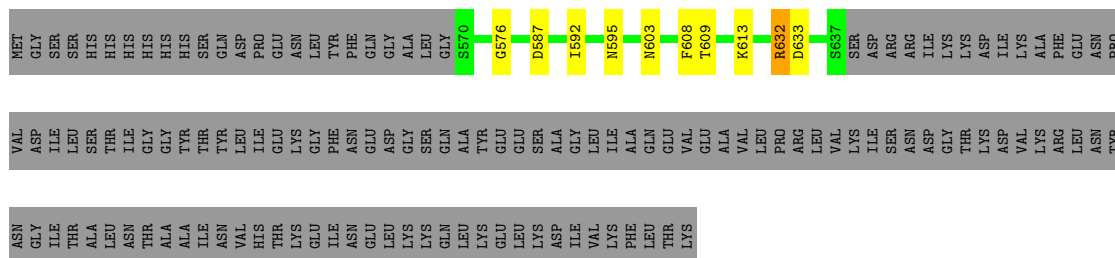
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	312	Total	O	0	0
			312	312		
7	A	87	Total	O	0	0
			87	87		
7	B	88	Total	O	0	0
			88	88		
7	C	86	Total	O	0	0
			86	86		

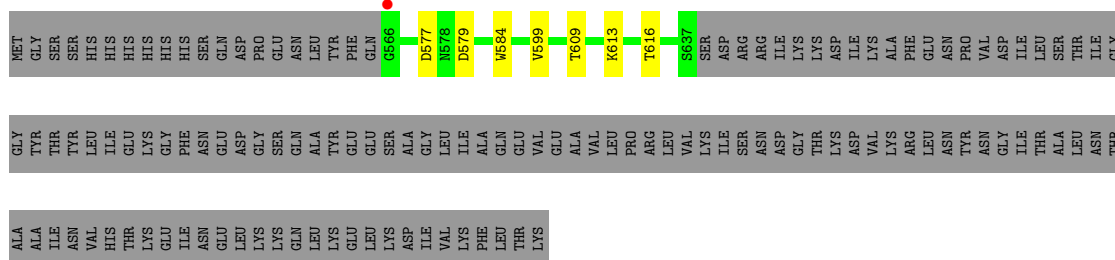
- Molecule 1: Receptor recognition protein



- Chain A:  28% . 67%



- Chain B: 32% 2% 65%



- Chain C:  29% 5% 66%



PRO	VAL	ASP	ILE	LEU	SER	THR	ILE	GLY	TYR	THR	TYR	LEU	ILE	GLU	LYS	GLY	PHE	ASN	ASP	GLY	SER	GLN	ALA	TYR	GLU	GLU	SER	ALA	GLY	LEU	ILE	GLN	VAL	LEU	PRO	ARG	LEU	VAL	VAL	LYS	ILE	SER	ASN	ASP	GLY	THR	LYS	ASP	VAL	LYS	ARG	LEU	LEU
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TYR	ASN	GLY	ILE	THR	ALA	LEU	ASN	THR	ALA	ALA	ILE	ASN	VAL	HIS	THR	LYS	GLU	ILE	ASN	GLU	LEU	LYS	LYS	GLN	LEU	LEU	GLU	LEU	LYS	ASP	ILE	VAL	LYS	PHE	LEU	THR	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.34Å 98.90Å 140.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 1.70 46.76 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.76-1.70) 99.4 (46.76-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.152 , 0.185 0.154 , 0.187	Depositor DCC
R_{free} test set	3075 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4057	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD, MG, IMD

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	D	0.78	0/1914	0.79	1/2604 (0.0%)
2	A	0.71	0/523	0.85	2/711 (0.3%)
2	B	0.79	0/531	0.86	0/722
2	C	0.74	0/515	0.81	0/700
All	All	0.77	0/3483	0.82	3/4737 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	A	633	ASP	CB-CG-OD1	5.31	123.08	118.30
2	A	632	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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	D	1850	0	1731	12	0
2	A	509	0	474	9	0
2	B	520	0	495	6	0
2	C	504	0	473	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	14	0	0
4	C	8	0	14	0	0
4	D	24	0	42	1	0
5	A	16	0	28	5	0
5	B	8	0	14	1	0
5	C	8	0	14	3	0
5	D	8	0	14	0	0
6	A	5	0	5	1	0
6	D	10	0	10	0	0
7	A	87	0	0	5	1
7	B	88	0	0	3	1
7	C	86	0	0	4	3
7	D	312	0	0	5	6
All	All	4057	0	3328	38	6

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 6.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ASP:OD2	7:B:901:HOH:O	1.90	0.90
1:D:213[A]:ASN:OD1	7:D:401:HOH:O	1.98	0.80
5:A:805:MPD:H4	7:A:908:HOH:O	1.82	0.77
2:C:577:ASP:OD1	7:C:902:HOH:O	2.06	0.73
2:C:595[B]:ASN:OD1	7:C:901:HOH:O	2.06	0.73
5:A:805:MPD:H12	7:A:908:HOH:O	1.88	0.71
2:A:576[A]:GLY:HA3	2:B:584:TRP:CD1	2.28	0.68
1:D:237[B]:GLN:OE1	7:D:402:HOH:O	2.13	0.67
6:A:807:IMD:H4	7:B:949:HOH:O	1.95	0.66
2:C:624:TRP:CE3	5:C:803:MPD:H13	2.36	0.60
1:D:69:ASN:ND2	7:D:408:HOH:O	2.29	0.58
7:A:901:HOH:O	2:C:595[A]:ASN:OD1	2.16	0.58
1:D:187[B]:ASP:OD2	1:D:196:ARG:HB3	2.04	0.57
2:A:587:ASP:OD1	7:A:901:HOH:O	2.16	0.56
2:C:632:ARG:NH1	7:C:905:HOH:O	2.37	0.56
2:C:624:TRP:CE3	5:C:803:MPD:C1	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:802:MPD:H31	7:B:913:HOH:O	2.06	0.55
2:B:599[B]:VAL:HG11	2:C:603:ASN:O	2.08	0.54
1:D:32[B]:GLU:HG3	1:D:35:PHE:HB3	1.90	0.54
2:A:576[A]:GLY:HA3	2:B:584:TRP:CG	2.43	0.53
1:D:210:ASP:O	1:D:213[B]:ASN:HB2	2.09	0.52
5:C:803:MPD:O4	5:C:803:MPD:H12	2.09	0.52
2:C:579:ASP:OD2	7:C:903:HOH:O	2.19	0.47
5:A:806:MPD:H12	2:C:592:ILE:HD13	1.99	0.45
2:B:616:THR:O	2:C:608:PHE:HA	2.16	0.45
1:D:116:GLY:HA3	1:D:171:GLY:O	2.17	0.45
2:A:595[B]:ASN:ND2	7:A:906:HOH:O	2.50	0.44
2:A:609:THR:HB	2:A:613:LYS:HB2	2.00	0.44
2:A:592:ILE:HD13	5:A:806:MPD:HM2	2.00	0.43
1:D:200:LEU:HA	7:D:466:HOH:O	2.18	0.43
1:D:122:ALA:HA	1:D:160:ARG:HB2	2.01	0.43
1:D:204:TYR:CE2	1:D:219:SER:HB3	2.53	0.43
1:D:237[A]:GLN:NE2	7:D:403:HOH:O	2.15	0.42
2:A:603:ASN:O	2:C:599:VAL:HG21	2.20	0.42
1:D:62:TRP:HE1	4:D:302:MRD:H3C1	1.85	0.41
2:B:609:THR:HB	2:B:613:LYS:HB2	2.01	0.41
2:A:632:ARG:HH12	5:A:805:MPD:H12	1.85	0.41
2:A:608:PHE:HA	2:C:616:THR:O	2.21	0.41

All (6) 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)
7:D:411:HOH:O	7:C:968:HOH:O[4_565]	1.85	0.35
7:D:670:HOH:O	7:B:962:HOH:O[8_555]	1.85	0.35
7:D:672:HOH:O	7:C:968:HOH:O[4_565]	1.86	0.34
7:D:632:HOH:O	7:C:920:HOH:O[3_555]	1.93	0.27
7:D:634:HOH:O	7:A:966:HOH:O[8_555]	1.95	0.25
7:D:403:HOH:O	7:D:461:HOH:O[3_555]	2.18	0.02

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	D	253/249 (102%)	250 (99%)	3 (1%)	0	100	100
2	A	69/204 (34%)	65 (94%)	4 (6%)	0	100	100
2	B	71/204 (35%)	69 (97%)	2 (3%)	0	100	100
2	C	68/204 (33%)	63 (93%)	5 (7%)	0	100	100
All	All	461/861 (54%)	447 (97%)	14 (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	D	179/173 (104%)	175 (98%)	4 (2%)	55	36
2	A	52/167 (31%)	52 (100%)	0	100	100
2	B	52/167 (31%)	51 (98%)	1 (2%)	60	43
2	C	51/167 (30%)	51 (100%)	0	100	100
All	All	334/674 (50%)	329 (98%)	5 (2%)	67	53

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	12	TYR
1	D	37	ILE
1	D	142	ARG
1	D	222	MET
2	B	579	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MRD	A	804	-	7,7,7	0.61	0	9,10,10	0.86	0
5	MPD	A	805	-	7,7,7	0.39	0	9,10,10	1.17	1 (11%)
5	MPD	A	806	-	7,7,7	0.44	0	9,10,10	0.82	0
6	IMD	A	807	-	3,5,5	0.36	0	4,5,5	0.64	0
5	MPD	B	802	-	7,7,7	0.28	0	9,10,10	0.57	0
4	MRD	C	802	-	7,7,7	0.31	0	9,10,10	0.75	0
5	MPD	C	803	-	7,7,7	0.60	0	9,10,10	1.26	1 (11%)
4	MRD	D	302	-	7,7,7	0.54	0	9,10,10	0.83	0
4	MRD	D	303	-	7,7,7	0.36	0	9,10,10	0.48	0
4	MRD	D	304	-	7,7,7	0.58	0	9,10,10	0.84	0
5	MPD	D	305	-	7,7,7	0.40	0	9,10,10	0.40	0
6	IMD	D	306	-	3,5,5	0.37	0	4,5,5	0.66	0
6	IMD	D	307	-	3,5,5	0.40	0	4,5,5	0.55	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	MRD	A	804	-	-	0/5/5/5	0/0/0/0
5	MPD	A	805	-	-	0/5/5/5	0/0/0/0
5	MPD	A	806	-	-	0/5/5/5	0/0/0/0
6	IMD	A	807	-	-	0/0/0/0	0/1/1/1
5	MPD	B	802	-	-	0/5/5/5	0/0/0/0
4	MRD	C	802	-	-	0/5/5/5	0/0/0/0
5	MPD	C	803	-	-	0/5/5/5	0/0/0/0
4	MRD	D	302	-	-	0/5/5/5	0/0/0/0
4	MRD	D	303	-	-	0/5/5/5	0/0/0/0
4	MRD	D	304	-	-	0/5/5/5	0/0/0/0
5	MPD	D	305	-	-	0/5/5/5	0/0/0/0
6	IMD	D	306	-	-	0/0/0/0	0/1/1/1
6	IMD	D	307	-	-	0/0/0/0	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	MPD	CM-C2-C1	-2.64	104.88	110.51
5	C	803	MPD	O2-C2-C1	-2.12	101.03	108.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	MPD	3	0
5	A	806	MPD	2	0
6	A	807	IMD	1	0
5	B	802	MPD	1	0
5	C	803	MPD	3	0
4	D	302	MRD	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	248/249 (99%)	-0.44	5 (2%) 65 70	18, 25, 44, 69	0
2	A	68/204 (33%)	-0.35	0 100 100	18, 23, 34, 54	0
2	B	72/204 (35%)	-0.41	1 (1%) 75 79	18, 24, 43, 54	0
2	C	69/204 (33%)	-0.20	1 (1%) 75 79	18, 25, 46, 69	0
All	All	457/861 (53%)	-0.38	7 (1%) 73 78	18, 25, 45, 69	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	569	GLY	4.6
1	D	163	HIS	3.3
1	D	161	VAL	3.1
2	B	566	GLY	3.0
1	D	200	LEU	3.0
1	D	123	TYR	2.7
1	D	164	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 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	MG	B	801	1/1	0.69	0.09	71,71,71,71	0
5	MPD	D	305	8/8	0.81	0.20	53,60,71,72	0
6	IMD	D	307	5/5	0.84	0.25	72,75,82,88	0
5	MPD	A	805	8/8	0.85	0.15	31,42,49,56	8
5	MPD	B	802	8/8	0.86	0.16	43,55,63,64	8
5	MPD	A	806	8/8	0.88	0.26	21,32,44,53	8
3	MG	A	802	1/1	0.88	0.20	32,32,32,32	1
6	IMD	D	306	5/5	0.89	0.14	59,65,71,72	0
3	MG	C	801	1/1	0.90	0.17	62,62,62,62	0
4	MRD	C	802	8/8	0.90	0.11	31,41,52,53	8
3	MG	A	803	1/1	0.91	0.07	27,27,27,27	1
4	MRD	D	304	8/8	0.92	0.14	24,32,38,44	8
5	MPD	C	803	8/8	0.94	0.13	27,34,46,46	8
4	MRD	D	302	8/8	0.94	0.16	32,45,62,68	0
3	MG	A	801	1/1	0.95	0.08	35,35,35,35	0
4	MRD	A	804	8/8	0.96	0.08	27,33,35,45	0
6	IMD	A	807	5/5	0.96	0.15	40,46,50,51	5
4	MRD	D	303	8/8	0.97	0.07	26,32,36,37	0
3	MG	D	301	1/1	0.99	0.14	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.