WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 09:01 am BST

PDB ID	:	6SVL
Title	:	human Myeloid-derived growth factor (MYDGF) in complex with neutralizing Fab
Authors	:	Ebenhoch, R.; Nar, H.
Deposited on	:	2019-09-18
Resolution	:	1.58 Å(reported)

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

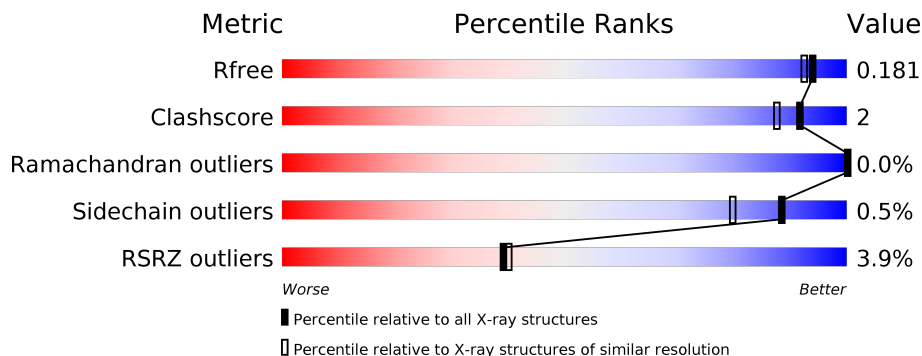|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.58 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	Percentile Ranks	Value
Rfree		0.181
Clashscore		2
Ramachandran outliers		0.0%
Sidechain outliers		0.5%
RSRZ outliers		3.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	244	2% / 81% / 6% / 13%
1	D	244	83% / • / 13%
1	G	244	% / 86% / • / 12%
1	H	244	6% / 84% / • / 13%
1	K	244	% / 84% / • / 13%
1	O	244	3% / 83% / 5% / 13%

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Mol	Chain	Length	Quality of chain
2	B	234	4% / 87% / • 10%
2	E	234	% / 86% / • 9%
2	I	234	88% / • 9%
2	L	234	2% / 86% / • 9%
2	M	234	88% / • 9%
2	P	234	5% / 77% / 5% / 18%
3	C	142	8% / 65% / • 33%
3	F	142	11% / 80% / • 18%
3	J	142	5% / 85% / • 11%
3	N	142	13% / 85% / • 13%
3	Q	142	6% / 84% / • 13%
3	R	142	4% / 85% / 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27628 atoms, of which 24 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 Fab_heavy_chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total 1645	C 1036	N 274	O 329	S 6	0	4	0
1	D	213	Total 1636	C 1031	N 273	O 324	S 8	0	2	0
1	G	215	Total 1640	C 1033	N 274	O 326	S 7	0	1	0
1	H	213	Total 1630	C 1028	N 272	O 323	S 7	0	1	0
1	K	213	Total 1622	C 1023	N 271	O 322	S 6	0	0	0
1	O	213	Total 1630	C 1028	N 272	O 323	S 7	0	1	0

- Molecule 2 is a protein called Fab_light_chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total 1628	C 1023	N 271	O 329	S 5	0	1	0
2	E	212	Total 1638	C 1028	N 275	O 330	S 5	0	0	0
2	I	212	Total 1638	C 1028	N 275	O 330	S 5	0	0	0
2	L	212	Total 1638	C 1028	N 275	O 330	S 5	0	0	0
2	M	212	Total 1638	C 1028	N 275	O 330	S 5	0	0	0
2	P	191	Total 1458	C 914	N 242	O 297	S 5	0	0	0

- Molecule 3 is a protein called Myeloid-derived growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total 747	C 484	N 124	O 134	S 5	0	0	0
3	F	116	Total 903	C 579	N 151	O 168	S 5	0	0	0
3	J	126	Total 995	C 633	N 169	O 188	S 5	0	0	0
3	N	123	Total 981	C 630	N 164	O 182	S 5	0	1	0
3	Q	123	Total 972	C 624	N 163	O 180	S 5	0	0	0
3	R	120	Total 943	C 606	N 158	O 174	S 5	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
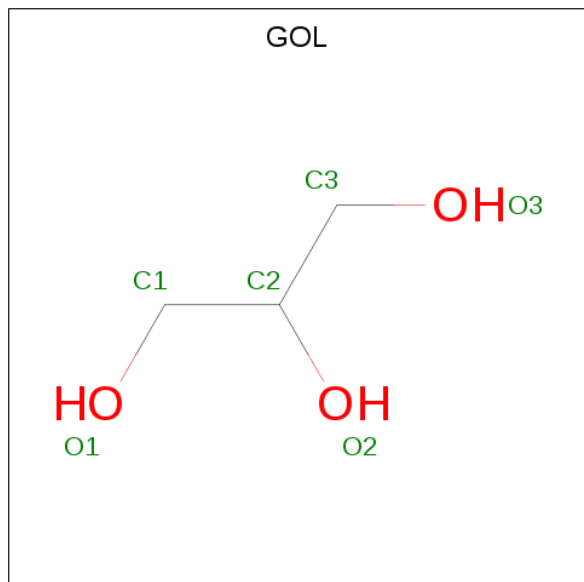
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 14	C 3	H 8	O 3	0	0
4	M	1	Total 14	C 3	H 8	O 3	0	0
4	R	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total 156	O 156	0	0

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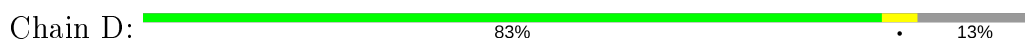| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	116	Total 116	O 116	0	0
5	C	26	Total 26	O 26	0	0
5	D	216	Total 216	O 216	0	0
5	E	172	Total 172	O 172	0	0
5	F	44	Total 44	O 44	0	0
5	G	204	Total 204	O 204	0	0
5	H	181	Total 181	O 181	0	0
5	I	237	Total 237	O 237	0	0
5	J	92	Total 92	O 92	0	0
5	K	196	Total 196	O 196	0	0
5	L	163	Total 163	O 163	0	0
5	M	227	Total 227	O 227	0	0
5	N	53	Total 53	O 53	0	0
5	O	191	Total 191	O 191	0	0
5	P	173	Total 173	O 173	0	0
5	Q	87	Total 87	O 87	0	0
5	R	70	Total 70	O 70	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.
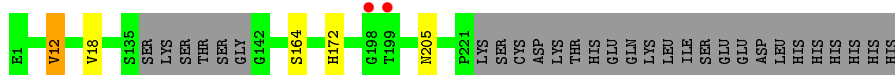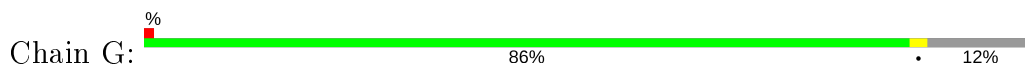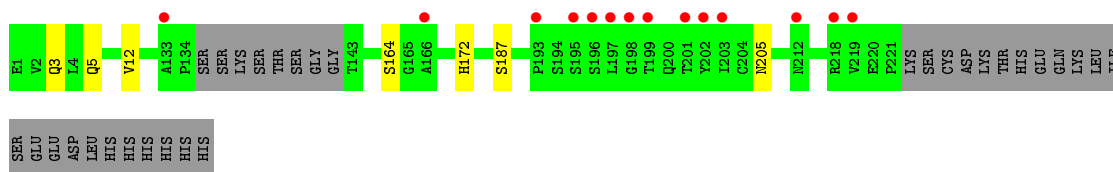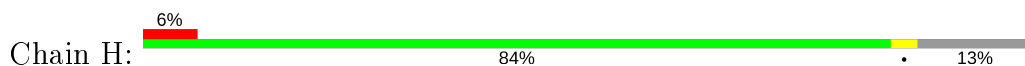
- Molecule 1: Fab_heavy_chain
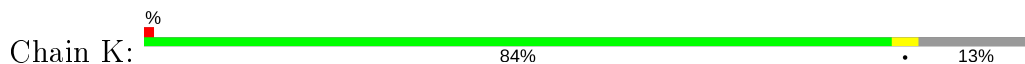
Chain A:

- Molecule 1: Fab_heavy_chain

Chain D:

- Molecule 1: Fab_heavy_chain

Chain G:

- Molecule 1: Fab_heavy_chain

Chain H:

- Molecule 1: Fab_heavy_chain

Chain K:

E1 V2 Q3 L11 S25 W47 I48 G49 P134 SER SER LYS SER THR SER GLY GLY T143 P155 S164 G165 A166 H172 N205 N212 P221 LYS SER CYS ASP LYS THR HIS GLU GLN LYS LEU ILE SER GLU GLU ASP LEU HIS HIS HIS HIS HIS

• Molecule 1: Fab_heavy_chain

Chain O:

3%

83%　　　　5%　　13%

E1 V2 Q3 L4 Q5 R13 W47 P62 Q65 P134 SER SER LYS SER THR SER GLY GLY T143 S164 H172 P175 P193 S194 S195 S196 L197 G198 T199 Q200 N205 R218 P221 LYS SER CYS ASP LYS THR HIS GLU GLN LYS LEU ILE SER GLU GLU

ASP LEU HIS HIS HIS HIS HIS

• Molecule 2: Fab_light_chain

Chain B:

4%

87%　　　　•　　10%

MET GLY TRP SER LEU ILE LEU LEU PHE LEU VAL ALA VAL ALA THR ARG VAL LEU SER D1 I2 Q3 Q37 Q40 L47 F83 H90 F91 W92 I107 N138 L155 L182 A185 D186 Y187 K191 V192 F210 ASN ARG GLU GLU CYS

• Molecule 2: Fab_light_chain

Chain E:

%

86%　　　　•　　9%

MET GLY TRP SER LEU ILE LEU LEU PHE LEU VAL ALA VAL ALA THR ARG VAL LEU SER D1 I2 Q3 C23 Q37 L47 F83 H90 F91 W92 I107 P121 A131 N138 R212 GLY GLU CYS

• Molecule 2: Fab_light_chain

Chain I:

88%　　　　•　　9%

MET GLY TRP SER LEU ILE LEU LEU PHE LEU VAL ALA VAL ALA THR ARG VAL LEU SER D1 F83 H90 F91 W92 I107 N138 R212 GLY GLU CYS

• Molecule 2: Fab_light_chain

Chain L:

2%

86%　　　　•　　9%

MET GLY TRP SER LEU ILE LEU LEU PHE LEU VAL ALA VAL ALA THR ARG VAL LEU SER D1 L78 H90 F91 W92 L126 K127 N138 K146 L155 Y187 E188 K189 H190 K191 T198 N211 R212 GLY GLU CYS

• Molecule 2: Fab_light_chain

Chain M:

88%　　　　•　　9%

MET GLY TRP SER LEU ILE LEU LEU PHE LEU VAL ALA VAL ALA THR ARG VAL LEU SER D1 A50 N53 F83 H90 F91 W92 I107 N138 R212 GLY GLU CYS

• Molecule 2: Fab_light_chain

Chain P:

• Molecule 3: Myeloid-derived growth factor

Chain C:

• Molecule 3: Myeloid-derived growth factor

Chain F:

• Molecule 3: Myeloid-derived growth factor

Chain J:

• Molecule 3: Myeloid-derived growth factor

Chain N:

• Molecule 3: Myeloid-derived growth factor

Chain Q:

• Molecule 3: Myeloid-derived growth factor

Chain R:

4%

85%

15%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.52Å 107.43Å 109.37Å 71.54° 86.25° 73.38°	Depositor
Resolution (Å)	97.82 – 1.58 97.82 – 1.58	Depositor EDS
% Data completeness (in resolution range)	62.6 (97.82-1.58) 62.6 (97.82-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	1.70 (at 1.58Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.181 , 0.206 0.183 , 0.181	Depositor DCC
R_{free} test set	16198 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27628	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.48	0/1685	0.66	0/2298
1	D	0.51	0/1676	0.68	0/2285
1	G	0.52	0/1680	0.65	0/2290
1	H	0.52	0/1670	0.68	0/2277
1	K	0.53	0/1662	0.66	0/2267
1	O	0.54	0/1670	0.68	0/2277
2	B	0.45	0/1666	0.62	0/2265
2	E	0.51	0/1676	0.63	0/2278
2	I	0.54	0/1676	0.64	0/2278
2	L	0.51	0/1676	0.66	0/2278
2	M	0.54	0/1676	0.66	0/2278
2	P	0.53	0/1490	0.67	0/2026
3	C	0.40	0/763	0.65	0/1027
3	F	0.40	0/923	0.63	0/1245
3	J	0.50	0/1020	0.63	0/1378
3	N	0.43	0/1007	0.63	0/1361
3	Q	0.47	0/996	0.64	0/1345
3	R	0.49	0/967	0.65	0/1306
All	All	0.50	0/25579	0.65	0/34759

There are no bond length outliers.

There are no bond angle outliers.

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	1645	0	1582	12	0
1	D	1636	0	1580	7	0
1	G	1640	0	1585	6	0
1	H	1630	0	1577	7	0
1	K	1622	0	1569	7	0
1	O	1630	0	1577	9	0
2	B	1628	0	1567	6	0
2	E	1638	0	1579	6	0
2	I	1638	0	1579	5	0
2	L	1638	0	1579	8	0
2	M	1638	0	1579	6	0
2	P	1458	0	1400	7	0
3	C	747	0	726	1	0
3	F	903	0	877	1	0
3	J	995	0	950	2	0
3	N	981	0	941	1	0
3	Q	972	0	937	2	0
3	R	943	0	913	0	0
4	E	6	8	8	0	0
4	M	6	8	8	0	0
4	R	6	8	8	0	0
5	A	156	0	0	0	0
5	B	116	0	0	0	0
5	C	26	0	0	0	0
5	D	216	0	0	0	0
5	E	172	0	0	0	0
5	F	44	0	0	0	0
5	G	204	0	0	0	0
5	H	181	0	0	0	0
5	I	237	0	0	0	0
5	J	92	0	0	0	0
5	K	196	0	0	0	0
5	L	163	0	0	0	0
5	M	227	0	0	0	0
5	N	53	0	0	0	0
5	O	191	0	0	0	0
5	P	173	0	0	0	0
5	Q	87	0	0	0	0
5	R	70	0	0	0	0
All	All	27604	24	24121	78	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 78 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:A:18[B]:VAL:HG23	1:A:86:LEU:HD11	1.57	0.85
2:L:90:HIS:HD2	2:L:92:TRP:H	1.30	0.79
2:M:90:HIS:HD2	2:M:92:TRP:H	1.32	0.77
1:D:164:SER:H	1:D:205:ASN:HD21	1.34	0.75
2:P:90:HIS:HD2	2:P:92:TRP:H	1.35	0.75

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	212/244 (87%)	210 (99%)	2 (1%)	0	100	100
1	D	211/244 (86%)	209 (99%)	2 (1%)	0	100	100
1	G	212/244 (87%)	210 (99%)	2 (1%)	0	100	100
1	H	210/244 (86%)	210 (100%)	0	0	100	100
1	K	209/244 (86%)	208 (100%)	1 (0%)	0	100	100
1	O	210/244 (86%)	208 (99%)	2 (1%)	0	100	100
2	B	209/234 (89%)	205 (98%)	4 (2%)	0	100	100
2	E	210/234 (90%)	206 (98%)	4 (2%)	0	100	100
2	I	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	L	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	M	210/234 (90%)	207 (99%)	3 (1%)	0	100	100
2	P	185/234 (79%)	182 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	83/142 (58%)	81 (98%)	1 (1%)	1 (1%)	13	2
3	F	108/142 (76%)	107 (99%)	1 (1%)	0	100	100
3	J	122/142 (86%)	118 (97%)	4 (3%)	0	100	100
3	N	118/142 (83%)	116 (98%)	2 (2%)	0	100	100
3	Q	117/142 (82%)	114 (97%)	3 (3%)	0	100	100
3	R	114/142 (80%)	111 (97%)	3 (3%)	0	100	100
All	All	3160/3720 (85%)	3116 (99%)	43 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	115	THR

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	185/211 (88%)	185 (100%)	0	100	100
1	D	184/211 (87%)	184 (100%)	0	100	100
1	G	184/211 (87%)	183 (100%)	1 (0%)	88	80
1	H	183/211 (87%)	181 (99%)	2 (1%)	73	55
1	K	182/211 (86%)	181 (100%)	1 (0%)	88	80
1	O	183/211 (87%)	182 (100%)	1 (0%)	88	80
2	B	184/203 (91%)	184 (100%)	0	100	100
2	E	185/203 (91%)	184 (100%)	1 (0%)	88	80
2	I	185/203 (91%)	185 (100%)	0	100	100
2	L	185/203 (91%)	183 (99%)	2 (1%)	73	55
2	M	185/203 (91%)	185 (100%)	0	100	100
2	P	166/203 (82%)	164 (99%)	2 (1%)	71	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	79/118 (67%)	79 (100%)	0	100	100
3	F	94/118 (80%)	94 (100%)	0	100	100
3	J	104/118 (88%)	102 (98%)	2 (2%)	57	31
3	N	103/118 (87%)	102 (99%)	1 (1%)	76	59
3	Q	101/118 (86%)	101 (100%)	0	100	100
3	R	99/118 (84%)	99 (100%)	0	100	100
All	All	2771/3192 (87%)	2758 (100%)	13 (0%)	88	80

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	81	VAL
1	K	3	GLN
1	O	194	SER
3	J	31	THR
3	N	5	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	79	GLN
1	K	58	ASN
2	P	138	ASN
2	I	89	GLN
2	I	138	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	GOL	R	201	-	5,5,5	0.27	0	5,5,5	0.58	0
4	GOL	M	301	-	5,5,5	0.28	0	5,5,5	0.33	0
4	GOL	E	301	-	5,5,5	0.20	0	5,5,5	0.46	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	GOL	R	201	-	-	0/4/4/4	-
4	GOL	M	301	-	-	0/4/4/4	-
4	GOL	E	301	-	-	0/4/4/4	-

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	A	212/244 (86%)	0.07	5 (2%)	59	60	17, 32, 63, 74	0
1	D	213/244 (87%)	-0.16	0	100	100	15, 24, 45, 60	0
1	G	215/244 (88%)	-0.15	2 (0%)	84	85	15, 24, 47, 58	0
1	H	213/244 (87%)	0.19	14 (6%)	18	18	12, 29, 62, 83	0
1	K	213/244 (87%)	-0.11	2 (0%)	84	85	13, 23, 55, 61	0
1	O	213/244 (87%)	0.06	8 (3%)	40	41	11, 28, 60, 76	0
2	B	210/234 (89%)	0.14	9 (4%)	35	35	21, 37, 72, 88	0
2	E	212/234 (90%)	0.03	2 (0%)	84	85	15, 31, 58, 72	0
2	I	212/234 (90%)	-0.17	0	100	100	14, 22, 41, 65	0
2	L	212/234 (90%)	0.07	4 (1%)	66	68	14, 32, 62, 84	0
2	M	212/234 (90%)	-0.13	0	100	100	13, 22, 48, 69	0
2	P	191/234 (81%)	0.11	12 (6%)	20	20	13, 26, 59, 80	0
3	C	95/142 (66%)	0.65	12 (12%)	3	3	25, 52, 80, 107	0
3	F	116/142 (81%)	0.70	16 (13%)	2	2	24, 46, 82, 107	0
3	J	126/142 (88%)	0.08	7 (5%)	24	24	17, 28, 63, 77	0
3	N	123/142 (86%)	0.56	19 (15%)	2	1	17, 45, 79, 87	0
3	Q	123/142 (86%)	0.16	8 (6%)	18	19	15, 28, 55, 78	0
3	R	120/142 (84%)	0.13	5 (4%)	36	36	14, 28, 62, 70	0
All	All	3231/3720 (86%)	0.08	125 (3%)	39	40	11, 29, 64, 107	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	GLY	8.0
3	F	96	ALA	8.0
3	F	83	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
3	F	95	ALA	6.1
3	Q	30	TYR	6.0

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
4	GOL	E	301	6/6	0.92	0.12	20,22,27,27	0
4	GOL	M	301	6/6	0.93	0.10	20,25,27,28	0
4	GOL	R	201	6/6	0.94	0.11	17,23,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.