Worldwide PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 03:17 PM BST

PDB ID	:	6OGX
Title	:	Ternary complex of OX40R (TNFRSF4) bound to Fab1 and Fab2
Authors	:	Ultsch, M.H.; Boenig, G.; Harris, S.F.
Deposited on	:	2019-04-03
Resolution	:	2.77 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 (i) symbol.

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

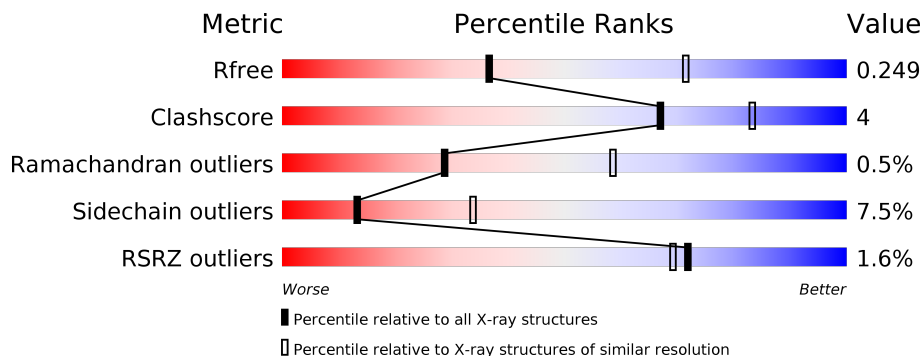|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.77 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		0.249
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		7.5%
RSRZ outliers		1.6%

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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	C	225	82% 13% · ·
2	D	214	87% 12% ·
3	G	163	2% 69% 15% · 14%
4	H	222	81% 11% 7%
5	L	214	3% 84% 13% · ·

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7776 atoms, of which 13 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 1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	218	Total 1647	C 1040	N 272	O 329	S 6	0	0	0

- Molecule 2 is a protein called Fab1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total 1647	C 1029	N 280	O 333	S 5	0	0	0

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	140	Total 1043	C 620	N 198	O 206	S 19	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	MET	-	initiating methionine	UNP P43489
G	9	GLY	-	expression tag	UNP P43489
G	10	SER	-	expression tag	UNP P43489
G	11	SER	-	expression tag	UNP P43489
G	12	HIS	-	expression tag	UNP P43489
G	13	HIS	-	expression tag	UNP P43489
G	14	HIS	-	expression tag	UNP P43489
G	15	HIS	-	expression tag	UNP P43489
G	16	HIS	-	expression tag	UNP P43489
G	17	HIS	-	expression tag	UNP P43489
G	18	SER	-	expression tag	UNP P43489
G	19	SER	-	expression tag	UNP P43489
G	20	GLY	-	expression tag	UNP P43489
G	21	LEU	-	expression tag	UNP P43489

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Chain	Residue	Modelled	Actual	Comment	Reference
G	22	VAL	-	expression tag	UNP P43489
G	23	PRO	-	expression tag	UNP P43489
G	24	ARG	-	expression tag	UNP P43489
G	25	GLY	-	expression tag	UNP P43489
G	26	SER	-	expression tag	UNP P43489
G	27	HIS	-	expression tag	UNP P43489
G	28	MET	-	expression tag	UNP P43489

- Molecule 4 is a protein called Fab2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	206	Total	C	N	O	S	0	0	0
			1546	981	254	307	4			

- Molecule 5 is a protein called Fab2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1623	1022	267	329	5			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
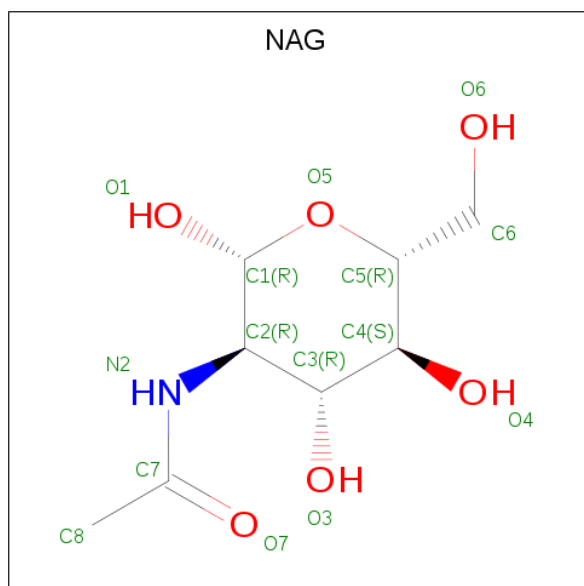
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

• Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	70	Total 70	O 70	0	0
7	D	61	Total 61	O 61	0	0
7	G	46	Total 46	O 46	0	0
7	H	33	Total 33	O 33	0	0
7	L	33	Total 33	O 33	0	0

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.
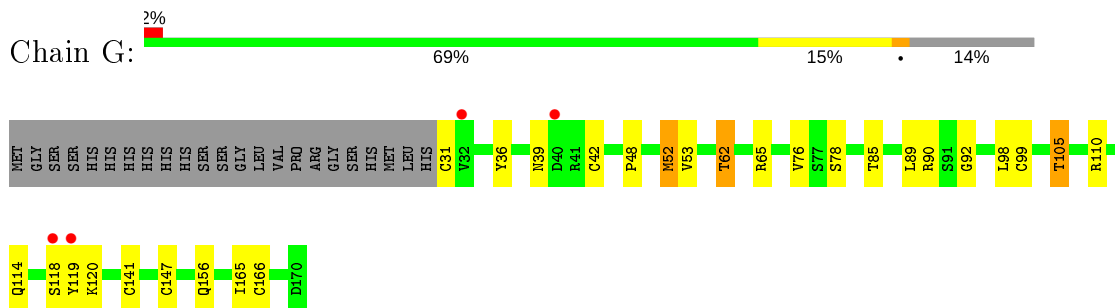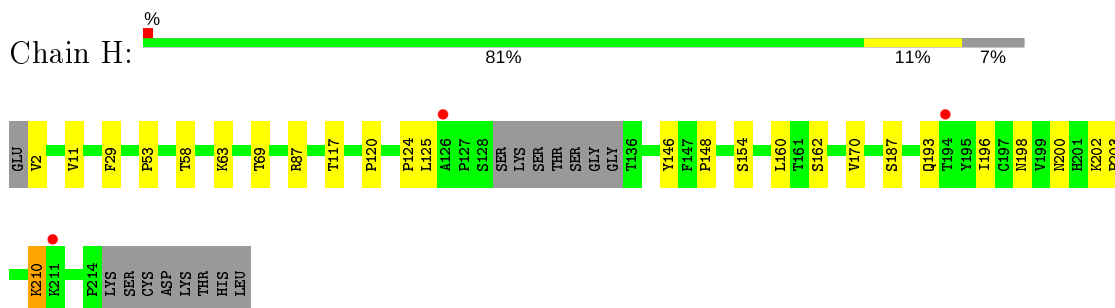
- Molecule 1: Fab 1 Heavy Chain
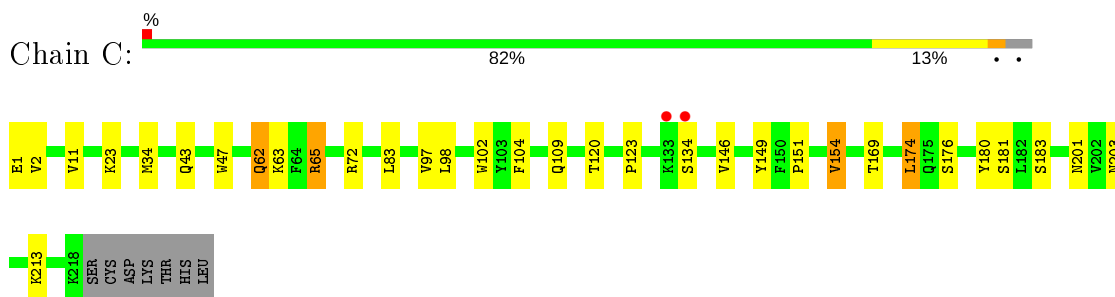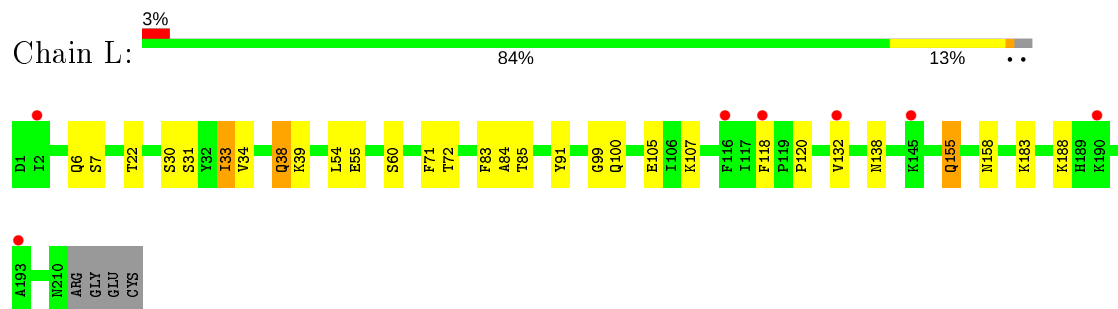
Chain C:

- Molecule 2: Fab1 Light Chain
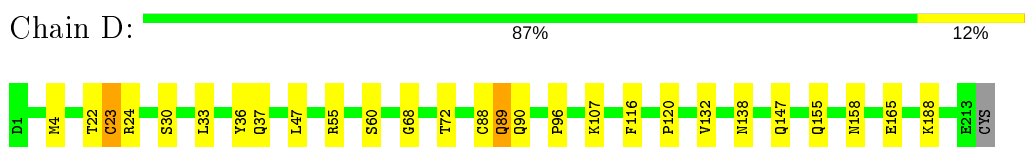
Chain D:

- Molecule 3: Tumor necrosis factor receptor superfamily member 4

Chain G:

- Molecule 4: Fab2 heavy chain

Chain H:

• Molecule 5: Fab2 light chain

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.77Å 125.25Å 197.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.77 105.77 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.27-2.77) 99.7 (105.77-2.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.203 , 0.254 0.199 , 0.249	Depositor DCC
R_{free} test set	2121 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å²)	53.6	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 54.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7776	wwPDB-VP
Average B, all atoms (Å²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: NAG

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	C	0.52	0/1688	0.74	0/2303
2	D	0.50	0/1683	0.70	0/2285
3	G	0.52	0/1068	0.71	0/1452
4	H	0.47	0/1582	0.72	0/2160
5	L	0.44	0/1662	0.69	0/2258
All	All	0.49	0/7683	0.71	0/10458

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	C	1647	0	1615	12	0
2	D	1647	0	1606	14	0
3	G	1043	0	961	17	0
4	H	1546	0	1522	9	0
5	L	1623	0	1559	11	0
6	G	14	13	13	0	0
7	C	70	0	0	0	0
7	D	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	46	0	0	0	0
7	H	33	0	0	0	0
7	L	33	0	0	0	0
All	All	7763	13	7276	55	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 4.

All (55) 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:D:4:MET:HE3	2:D:90:GLN:HB3	1.45	0.95
2:D:23:CYS:HG	2:D:88:CYS:HG	1.24	0.83
3:G:99:CYS:HB3	3:G:105:THR:HG22	1.65	0.78
3:G:147:CYS:HG	3:G:166:CYS:HG	0.79	0.75
1:C:97:VAL:HG11	1:C:104:PHE:HB3	1.68	0.75
5:L:155:GLN:HG3	5:L:158:ASN:HD21	1.56	0.71
4:H:154:SER:HB2	4:H:198:ASN:HB2	1.77	0.66
3:G:52:MET:HG3	3:G:78:SER:HA	1.78	0.64
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.81	0.61
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.83	0.61
4:H:120:PRO:HB3	4:H:146:TYR:HB3	1.85	0.58
4:H:11:VAL:HG21	4:H:203:PRO:HB3	1.85	0.57
3:G:156:GLN:HB2	3:G:165:ILE:HB	1.86	0.57
5:L:33:ILE:HG21	5:L:71:PHE:CD1	2.40	0.56
2:D:36:TYR:CE1	2:D:89:GLN:HG2	2.40	0.56
1:C:11:VAL:HB	1:C:151:PRO:HG3	1.87	0.56
5:L:6:GLN:HG3	5:L:99:GLY:HA3	1.88	0.56
1:C:2:VAL:HG23	3:G:119:TYR:HB2	1.88	0.55
1:C:134:SER:HA	2:D:116:PHE:HD1	1.74	0.52
4:H:11:VAL:CG2	4:H:203:PRO:HB3	2.38	0.52
1:C:62:GLN:HG3	1:C:65:ARG:HE	1.75	0.50
3:G:92:GLY:O	3:G:110:ARG:HG2	2.12	0.49
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.94	0.49
5:L:39:LYS:HG2	5:L:84:ALA:HB2	1.95	0.49
3:G:53:VAL:HG21	3:G:65:ARG:HB2	1.94	0.49
1:C:146:VAL:HG11	1:C:154:VAL:HG11	1.95	0.48
2:D:155:GLN:HE21	2:D:158:ASN:HD21	1.61	0.47
2:D:22:THR:HG22	2:D:72:THR:HG22	1.96	0.47
1:C:134:SER:HA	2:D:116:PHE:CD1	2.50	0.47
4:H:200:ASN:HD21	4:H:202:LYS:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:PRO:HB3	1:C:149:TYR:HB3	1.96	0.46
1:C:98:LEU:HD21	3:G:118:SER:HB2	1.96	0.46
5:L:22:THR:HG22	5:L:72:THR:HG22	1.97	0.46
2:D:23:CYS:CB	2:D:88:CYS:HG	2.27	0.45
4:H:29:PHE:CE2	4:H:53:PRO:HB3	2.50	0.45
3:G:36:TYR:CE1	3:G:62:THR:HG21	2.52	0.45
2:D:36:TYR:HE1	2:D:89:GLN:CG	2.30	0.45
3:G:90:ARG:CZ	5:L:54:LEU:HD23	2.46	0.45
5:L:155:GLN:HG3	5:L:158:ASN:ND2	2.27	0.45
3:G:36:TYR:HE1	3:G:62:THR:HG21	1.82	0.45
4:H:117:THR:HG22	4:H:148:PRO:HD3	1.99	0.44
3:G:147:CYS:CB	3:G:166:CYS:HG	2.30	0.44
3:G:48:PRO:HD3	3:G:76:VAL:HG12	2.00	0.44
3:G:114:GLN:HB3	3:G:141:CYS:SG	2.57	0.43
3:G:53:VAL:CG2	3:G:65:ARG:HB2	2.49	0.43
4:H:124:PRO:HD3	4:H:210:LYS:HD3	2.01	0.43
5:L:38:GLN:HG3	5:L:85:THR:HB	2.00	0.42
1:C:47:TRP:CD2	2:D:96:PRO:HD2	2.54	0.42
5:L:34:VAL:HG23	5:L:91:TYR:CE1	2.54	0.42
3:G:85:THR:O	3:G:105:THR:HG21	2.19	0.42
4:H:125:LEU:HB3	5:L:118:PHE:CD1	2.55	0.42
1:C:174:LEU:HG	1:C:180:TYR:CE1	2.55	0.42
1:C:102:TRP:CG	2:D:96:PRO:HG3	2.55	0.41
2:D:36:TYR:HE1	2:D:89:GLN:HG2	1.83	0.41
3:G:156:GLN:HB2	3:G:165:ILE:HD12	2.02	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	C	216/225 (96%)	206 (95%)	9 (4%)	1 (0%)	29	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	211/214 (99%)	202 (96%)	7 (3%)	2 (1%)	17	44
3	G	138/163 (85%)	133 (96%)	4 (3%)	1 (1%)	22	50
4	H	202/222 (91%)	194 (96%)	8 (4%)	0	100	100
5	L	208/214 (97%)	200 (96%)	7 (3%)	1 (0%)	29	58
All	All	975/1038 (94%)	935 (96%)	35 (4%)	5 (0%)	29	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	39	ASN
1	C	65	ARG
5	L	138	ASN
2	D	138	ASN
2	D	68	GLY

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	C	188/195 (96%)	169 (90%)	19 (10%)	7	20
2	D	189/190 (100%)	178 (94%)	11 (6%)	20	47
3	G	122/142 (86%)	114 (93%)	8 (7%)	16	41
4	H	174/188 (93%)	162 (93%)	12 (7%)	15	38
5	L	186/189 (98%)	172 (92%)	14 (8%)	13	34
All	All	859/904 (95%)	795 (92%)	64 (8%)	13	34

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	GLU
1	C	23	LYS
1	C	34	MET

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Mol	Chain	Res	Type
1	C	43	GLN
1	C	62	GLN
1	C	63	LYS
1	C	72	ARG
1	C	83	LEU
1	C	109	GLN
1	C	120	THR
1	C	154	VAL
1	C	169	THR
1	C	174	LEU
1	C	176	SER
1	C	181	SER
1	C	183	SER
1	C	201	ASN
1	C	203	ASN
1	C	213	LYS
2	D	23	CYS
2	D	24	ARG
2	D	30	SER
2	D	33	LEU
2	D	55	ARG
2	D	60	SER
2	D	89	GLN
2	D	107	LYS
2	D	147	GLN
2	D	165	GLU
2	D	188	LYS
3	G	31	CYS
3	G	42	CYS
3	G	52	MET
3	G	62	THR
3	G	89	LEU
3	G	98	LEU
3	G	105	THR
3	G	120	LYS
4	H	2	VAL
4	H	58	THR
4	H	63	LYS
4	H	69	THR
4	H	87	ARG
4	H	160	LEU
4	H	162	SER

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Mol	Chain	Res	Type
4	H	170	VAL
4	H	187	SER
4	H	193	GLN
4	H	196	ILE
4	H	210	LYS
5	L	7	SER
5	L	30	SER
5	L	31	SER
5	L	33	ILE
5	L	38	GLN
5	L	55	GLU
5	L	60	SER
5	L	83	PHE
5	L	100	GLN
5	L	105	GLU
5	L	107	LYS
5	L	155	GLN
5	L	183	LYS
5	L	188	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	155	GLN
5	L	155	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)

1 ligand is 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	#$|Z| > 2$
6	NAG	G	501	3	14,14,15	0.30	0	17,19,21	0.78	1 (5%)

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
6	NAG	G	501	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	501	NAG	C1-O5-C5	2.49	115.56	112.19

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	C	218/225 (96%)	-0.01	2 (0%)	84	82	35, 50, 80, 104	0
2	D	213/214 (99%)	-0.02	0	100	100	37, 51, 70, 100	0
3	G	140/163 (85%)	0.03	4 (2%)	51	46	35, 57, 95, 111	0
4	H	206/222 (92%)	0.04	3 (1%)	73	71	43, 64, 114, 131	0
5	L	210/214 (98%)	0.36	7 (3%)	46	41	44, 73, 107, 122	0
All	All	987/1038 (95%)	0.09	16 (1%)	72	69	35, 57, 102, 131	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	211	LYS	3.6
1	C	134	SER	3.6
3	G	118	SER	2.7
3	G	32	VAL	2.6
4	H	194	THR	2.5
5	L	116	PHE	2.5
5	L	190	LYS	2.5
1	C	133	LYS	2.4
3	G	40	ASP	2.4
5	L	193	ALA	2.4
4	H	126	ALA	2.3
5	L	132	VAL	2.3
3	G	119	TYR	2.2
5	L	118	PHE	2.2
5	L	145	LYS	2.1
5	L	2	ILE	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 monosaccharides 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
6	NAG	G	501	14/15	0.88	0.18	85,90,92,93	0

6.5 Other polymers (i)

There are no such residues in this entry.