



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:57 PM BST

PDB ID : 5UD7  
Title : Crystal Structure of Wild-Type Ig-like Domain  
Authors : Sudom, A.; Min, X.; Wang, Z.  
Deposited on : 2016-12-23  
Resolution : 2.20 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](mailto: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.

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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 : 2.13.1  
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

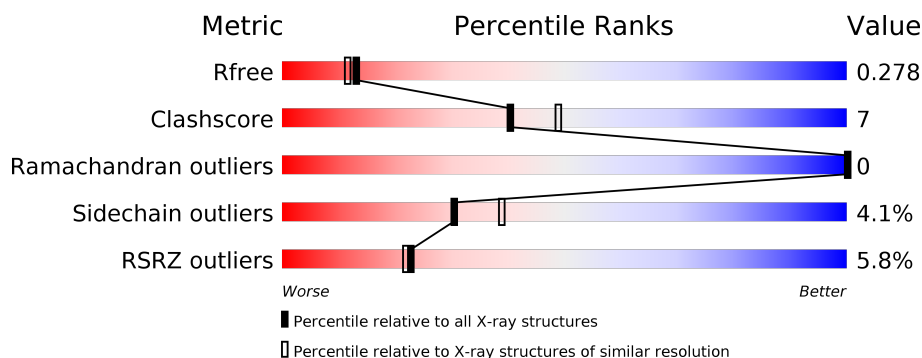
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	169	<div> <div>2%</div> <div>59% 5% • 36%</div> </div>
1	B	169	<div> <div>2%</div> <div>49% 13% • 37%</div> </div>
1	C	169	<div> <div>2%</div> <div>49% 15% 37%</div> </div>
1	D	169	<div> <div>9%</div> <div>50% 11% • 38%</div> </div>
1	E	169	<div> <div>5%</div> <div>52% 9% • 38%</div> </div>
1	F	169	<div> <div>•</div> <div>59% 5% • 35%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	203	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5304 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 Triggering receptor expressed on myeloid cells 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			857	536	160	156	5			
1	B	107	Total	C	N	O	S	0	0	0
			844	528	157	154	5			
1	C	107	Total	C	N	O	S	0	0	0
			840	526	157	152	5			
1	D	105	Total	C	N	O	S	0	0	0
			828	518	155	150	5			
1	E	105	Total	C	N	O	S	0	0	0
			828	518	155	150	5			
1	F	110	Total	C	N	O	S	0	0	0
			862	539	161	157	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASP	ASN	conflict	UNP Q9NZC2
A	175	GLU	-	expression tag	UNP Q9NZC2
A	176	ASN	-	expression tag	UNP Q9NZC2
A	177	LEU	-	expression tag	UNP Q9NZC2
A	178	TYR	-	expression tag	UNP Q9NZC2
A	179	PHE	-	expression tag	UNP Q9NZC2
A	180	GLN	-	expression tag	UNP Q9NZC2
A	181	GLY	-	expression tag	UNP Q9NZC2
A	182	HIS	-	expression tag	UNP Q9NZC2
A	183	HIS	-	expression tag	UNP Q9NZC2
A	184	HIS	-	expression tag	UNP Q9NZC2
A	185	HIS	-	expression tag	UNP Q9NZC2
A	186	HIS	-	expression tag	UNP Q9NZC2
A	187	HIS	-	expression tag	UNP Q9NZC2
B	20	ASP	ASN	conflict	UNP Q9NZC2
B	175	GLU	-	expression tag	UNP Q9NZC2
B	176	ASN	-	expression tag	UNP Q9NZC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LEU	-	expression tag	UNP Q9NZC2
B	178	TYR	-	expression tag	UNP Q9NZC2
B	179	PHE	-	expression tag	UNP Q9NZC2
B	180	GLN	-	expression tag	UNP Q9NZC2
B	181	GLY	-	expression tag	UNP Q9NZC2
B	182	HIS	-	expression tag	UNP Q9NZC2
B	183	HIS	-	expression tag	UNP Q9NZC2
B	184	HIS	-	expression tag	UNP Q9NZC2
B	185	HIS	-	expression tag	UNP Q9NZC2
B	186	HIS	-	expression tag	UNP Q9NZC2
B	187	HIS	-	expression tag	UNP Q9NZC2
C	20	ASP	ASN	conflict	UNP Q9NZC2
C	175	GLU	-	expression tag	UNP Q9NZC2
C	176	ASN	-	expression tag	UNP Q9NZC2
C	177	LEU	-	expression tag	UNP Q9NZC2
C	178	TYR	-	expression tag	UNP Q9NZC2
C	179	PHE	-	expression tag	UNP Q9NZC2
C	180	GLN	-	expression tag	UNP Q9NZC2
C	181	GLY	-	expression tag	UNP Q9NZC2
C	182	HIS	-	expression tag	UNP Q9NZC2
C	183	HIS	-	expression tag	UNP Q9NZC2
C	184	HIS	-	expression tag	UNP Q9NZC2
C	185	HIS	-	expression tag	UNP Q9NZC2
C	186	HIS	-	expression tag	UNP Q9NZC2
C	187	HIS	-	expression tag	UNP Q9NZC2
D	20	ASP	ASN	conflict	UNP Q9NZC2
D	175	GLU	-	expression tag	UNP Q9NZC2
D	176	ASN	-	expression tag	UNP Q9NZC2
D	177	LEU	-	expression tag	UNP Q9NZC2
D	178	TYR	-	expression tag	UNP Q9NZC2
D	179	PHE	-	expression tag	UNP Q9NZC2
D	180	GLN	-	expression tag	UNP Q9NZC2
D	181	GLY	-	expression tag	UNP Q9NZC2
D	182	HIS	-	expression tag	UNP Q9NZC2
D	183	HIS	-	expression tag	UNP Q9NZC2
D	184	HIS	-	expression tag	UNP Q9NZC2
D	185	HIS	-	expression tag	UNP Q9NZC2
D	186	HIS	-	expression tag	UNP Q9NZC2
D	187	HIS	-	expression tag	UNP Q9NZC2
E	20	ASP	ASN	conflict	UNP Q9NZC2
E	175	GLU	-	expression tag	UNP Q9NZC2
E	176	ASN	-	expression tag	UNP Q9NZC2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	177	LEU	-	expression tag	UNP Q9NZC2
E	178	TYR	-	expression tag	UNP Q9NZC2
E	179	PHE	-	expression tag	UNP Q9NZC2
E	180	GLN	-	expression tag	UNP Q9NZC2
E	181	GLY	-	expression tag	UNP Q9NZC2
E	182	HIS	-	expression tag	UNP Q9NZC2
E	183	HIS	-	expression tag	UNP Q9NZC2
E	184	HIS	-	expression tag	UNP Q9NZC2
E	185	HIS	-	expression tag	UNP Q9NZC2
E	186	HIS	-	expression tag	UNP Q9NZC2
E	187	HIS	-	expression tag	UNP Q9NZC2
F	20	ASP	ASN	conflict	UNP Q9NZC2
F	175	GLU	-	expression tag	UNP Q9NZC2
F	176	ASN	-	expression tag	UNP Q9NZC2
F	177	LEU	-	expression tag	UNP Q9NZC2
F	178	TYR	-	expression tag	UNP Q9NZC2
F	179	PHE	-	expression tag	UNP Q9NZC2
F	180	GLN	-	expression tag	UNP Q9NZC2
F	181	GLY	-	expression tag	UNP Q9NZC2
F	182	HIS	-	expression tag	UNP Q9NZC2
F	183	HIS	-	expression tag	UNP Q9NZC2
F	184	HIS	-	expression tag	UNP Q9NZC2
F	185	HIS	-	expression tag	UNP Q9NZC2
F	186	HIS	-	expression tag	UNP Q9NZC2
F	187	HIS	-	expression tag	UNP Q9NZC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	I	0	0
			1	1		
3	C	1	Total	I	0	0
			1	1		
3	E	3	Total	I	0	0
			3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

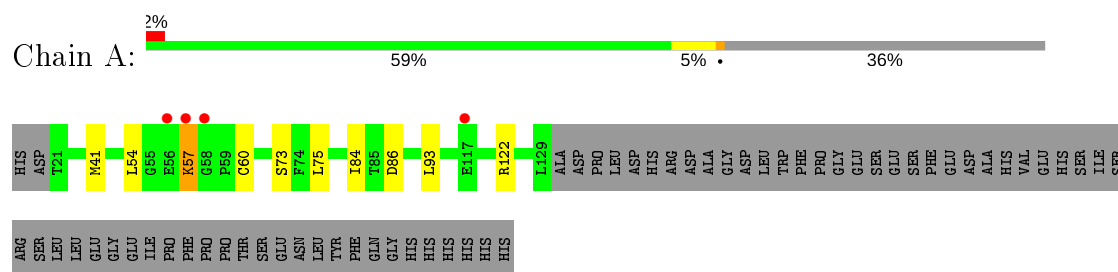
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	18	Total	O	0	0
			18	18		
5	C	22	Total	O	0	0
			22	22		
5	D	19	Total	O	0	0
			19	19		
5	E	25	Total	O	0	0
			25	25		
5	F	40	Total	O	0	0
			40	40		



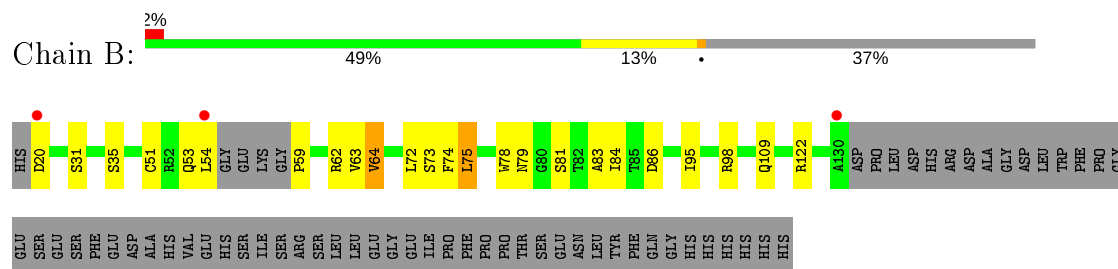
### 3 Residue-property plots

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.

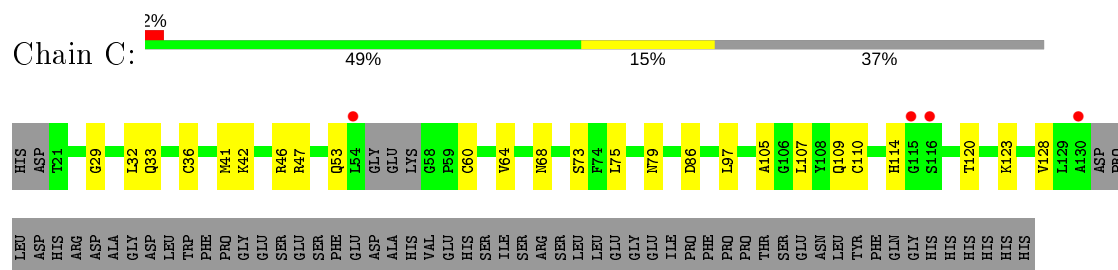
- Molecule 1: Triggering receptor expressed on myeloid cells 2



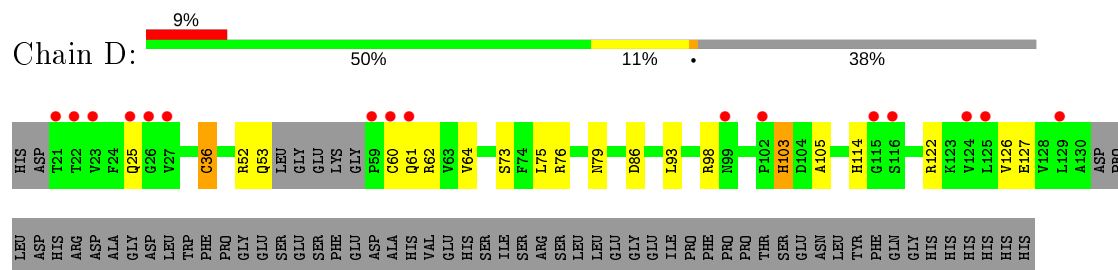
- Molecule 1: Triggering receptor expressed on myeloid cells 2



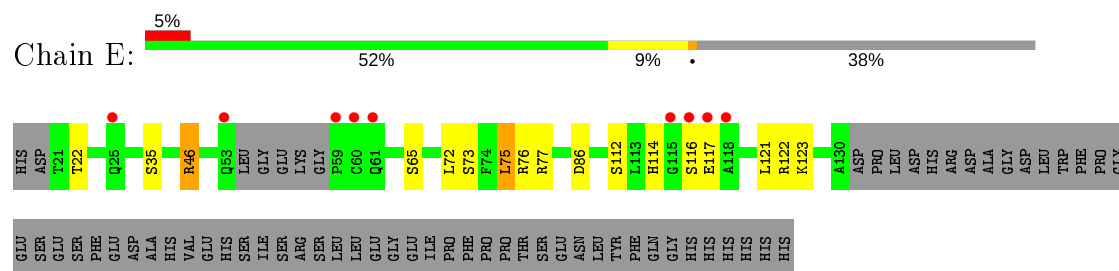
- Molecule 1: Triggering receptor expressed on myeloid cells 2



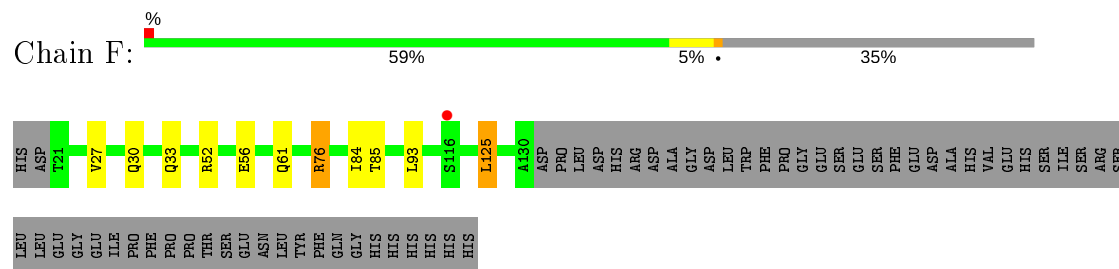
- Molecule 1: Triggering receptor expressed on myeloid cells 2



- Molecule 1: Triggering receptor expressed on myeloid cells 2



- Molecule 1: Triggering receptor expressed on myeloid cells 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.66 Å 160.66 Å 86.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 2.20 47.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.49-2.20) 100.0 (47.49-2.20)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.241 , 0.277 0.241 , 0.278	Depositor DCC
$R_{free}$ test set	2944 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: IOD, NAG, SO4

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	0/875	0.63	0/1187
1	B	0.39	0/861	0.57	0/1168
1	C	0.49	1/857 (0.1%)	0.66	1/1163 (0.1%)
1	D	0.37	0/845	0.57	0/1146
1	E	0.38	0/845	0.58	0/1146
1	F	0.50	0/880	0.68	1/1194 (0.1%)
All	All	0.44	1/5163 (0.0%)	0.62	2/7004 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	CYS	CB-SG	-5.64	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	125	LEU	CA-CB-CG	5.52	128.01	115.30
1	C	110	CYS	CA-CB-SG	5.46	123.82	114.00

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	A	857	0	850	5	0
1	B	844	0	834	13	0
1	C	840	0	832	28	0
1	D	828	0	819	12	0
1	E	828	0	819	22	0
1	F	862	0	855	7	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	1	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	E	3	0	0	0	0
4	C	5	0	0	2	0
5	A	27	0	0	0	0
5	B	18	0	0	1	0
5	C	22	0	0	1	0
5	D	19	0	0	1	0
5	E	25	0	0	1	0
5	F	40	0	0	1	0
All	All	5304	0	5087	74	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 7.

All (74) 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:C:41:MET:CE	1:E:76:ARG:NE	2.13	1.12
1:C:41:MET:HE2	1:E:76:ARG:NE	1.92	0.83
1:F:76:ARG:HH21	1:F:76:ARG:HB3	1.46	0.81
1:C:41:MET:HE1	1:E:76:ARG:NE	1.95	0.80
1:C:41:MET:CE	1:E:76:ARG:HE	2.01	0.72
1:C:41:MET:HE1	1:E:76:ARG:CD	2.19	0.72
1:C:41:MET:CE	1:E:76:ARG:CZ	2.68	0.71
1:B:53:GLN:NE2	1:B:109:GLN:HE21	1.90	0.69
1:A:122:ARG:NH2	1:C:29:GLY:O	2.18	0.69
1:D:52:ARG:NH2	1:D:105:ALA:O	2.29	0.66
1:F:52:ARG:HB3	1:F:61:GLN:HG2	1.80	0.64
1:C:41:MET:HE2	1:E:76:ARG:CZ	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:HB2	4:C:203:SO4:O2	1.99	0.63
1:C:41:MET:CE	1:E:76:ARG:CD	2.76	0.63
1:B:73:SER:HB3	1:B:86:ASP:HB3	1.81	0.62
1:C:53:GLN:HE22	1:C:123:LYS:NZ	1.96	0.62
1:B:72:LEU:HB3	1:B:75:LEU:HD22	1.81	0.62
1:C:53:GLN:OE1	1:C:107:LEU:HB3	2.01	0.60
1:C:73:SER:HB3	1:C:86:ASP:HB3	1.82	0.60
1:B:64:VAL:HG13	1:B:79:ASN:HB2	1.82	0.60
1:B:54:LEU:HD12	1:B:59:PRO:HG2	1.83	0.60
1:C:32:LEU:HD23	1:C:97:LEU:HD12	1.84	0.60
1:F:76:ARG:HA	1:F:85:THR:HG22	1.84	0.59
1:C:46:ARG:HD3	1:C:114:HIS:HB3	1.85	0.59
1:F:27:VAL:HG13	1:F:30:GLN:HG3	1.84	0.59
2:C:202:NAG:H81	5:F:301:HOH:O	2.02	0.59
1:A:73:SER:HB3	1:A:86:ASP:HB3	1.86	0.58
1:B:98:ARG:HG3	4:C:203:SO4:O3	2.03	0.57
1:B:51:CYS:HB3	1:B:62:ARG:HA	1.88	0.55
1:C:41:MET:HE2	1:E:76:ARG:HE	1.60	0.55
1:C:47:ARG:HD3	1:C:68:ASN:HA	1.87	0.55
1:D:103:HIS:ND1	1:D:103:HIS:O	2.40	0.54
1:F:76:ARG:HH21	1:F:76:ARG:CB	2.18	0.54
1:E:73:SER:HB3	1:E:86:ASP:HB3	1.91	0.52
1:D:53:GLN:HG2	1:D:60:CYS:SG	2.50	0.52
2:A:201:NAG:H82	5:D:304:HOH:O	2.09	0.52
1:C:47:ARG:HG2	5:C:317:HOH:O	2.11	0.51
1:C:42:LYS:HG2	5:E:302:HOH:O	2.11	0.51
1:B:35:SER:OG	5:B:301:HOH:O	2.19	0.50
1:D:25:GLN:HB3	1:D:127:GLU:HB2	1.93	0.50
1:E:112:SER:HB2	1:E:121:LEU:HD21	1.93	0.49
1:C:41:MET:HE3	1:E:76:ARG:CZ	2.42	0.49
1:C:53:GLN:HG3	1:C:60:CYS:SG	2.52	0.49
1:C:105:ALA:HB2	1:C:128:VAL:HG23	1.96	0.48
1:A:84:ILE:HD11	1:A:93:LEU:HD11	1.96	0.48
1:C:41:MET:HE3	1:E:76:ARG:NE	2.20	0.47
1:E:72:LEU:HB3	1:E:75:LEU:HD22	1.95	0.47
1:E:22:THR:HG21	1:E:122:ARG:NH1	2.30	0.47
1:B:84:ILE:HG13	1:B:95:ILE:HG13	1.98	0.46
1:B:74:PHE:CE2	1:B:75:LEU:HD13	2.52	0.45
1:D:36:CYS:HB3	1:D:93:LEU:HB3	1.98	0.45
1:C:53:GLN:HE22	1:C:123:LYS:HZ1	1.63	0.45
1:D:105:ALA:HA	1:D:126:VAL:HG13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:HG13	1:D:79:ASN:CB	2.48	0.44
1:D:114:HIS:ND1	1:D:114:HIS:O	2.50	0.43
1:F:84:ILE:HD11	1:F:93:LEU:HD11	2.00	0.43
1:D:75:LEU:HA	1:D:75:LEU:HD12	1.86	0.43
1:C:109:GLN:OE1	1:C:120:THR:OG1	2.37	0.42
1:D:52:ARG:O	1:D:61:GLN:N	2.52	0.42
1:E:65:SER:O	1:E:77:ARG:HD3	2.20	0.42
1:E:123:LYS:HB2	1:E:123:LYS:HE2	1.92	0.42
1:D:73:SER:HB3	1:D:86:ASP:HB3	2.02	0.41
1:C:41:MET:CE	1:E:76:ARG:HD2	2.50	0.41
1:E:116:SER:OG	1:E:117:GLU:OE1	2.34	0.41
1:C:41:MET:HE1	1:E:76:ARG:HD2	1.98	0.41
1:E:72:LEU:O	1:E:75:LEU:HB2	2.21	0.41
1:E:46:ARG:HD3	1:E:114:HIS:HB3	2.03	0.41
1:B:78:TRP:CD2	1:B:83:ALA:HB2	2.56	0.40
1:A:41:MET:CE	1:F:76:ARG:HD2	2.51	0.40
1:A:57:LYS:HA	1:A:57:LYS:HE2	2.02	0.40
1:B:51:CYS:HA	1:B:63:VAL:HG23	2.04	0.40
1:D:122:ARG:HG3	1:D:122:ARG:NH1	2.37	0.40
1:C:64:VAL:HG13	1:C:79:ASN:HB3	2.03	0.40
1:C:64:VAL:CG1	1:C:79:ASN:HB3	2.51	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	A	107/169 (63%)	103 (96%)	4 (4%)	0	100	100
1	B	103/169 (61%)	102 (99%)	1 (1%)	0	100	100
1	C	103/169 (61%)	100 (97%)	3 (3%)	0	100	100
1	D	101/169 (60%)	99 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	101/169 (60%)	98 (97%)	3 (3%)	0	100	100
1	F	108/169 (64%)	106 (98%)	2 (2%)	0	100	100
All	All	623/1014 (61%)	608 (98%)	15 (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	94/147 (64%)	90 (96%)	4 (4%)	29	36
1	B	93/147 (63%)	88 (95%)	5 (5%)	22	26
1	C	92/147 (63%)	90 (98%)	2 (2%)	52	65
1	D	91/147 (62%)	86 (94%)	5 (6%)	21	26
1	E	91/147 (62%)	88 (97%)	3 (3%)	38	49
1	F	94/147 (64%)	90 (96%)	4 (4%)	29	36
All	All	555/882 (63%)	532 (96%)	23 (4%)	30	39

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	57	LYS
1	A	60	CYS
1	A	75	LEU
1	B	20	ASP
1	B	64	VAL
1	B	75	LEU
1	B	81	SER
1	B	122	ARG
1	C	33	GLN
1	C	75	LEU
1	D	36	CYS

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Mol	Chain	Res	Type
1	D	62	ARG
1	D	76	ARG
1	D	98	ARG
1	D	103	HIS
1	E	35	SER
1	E	46	ARG
1	E	75	LEU
1	F	33	GLN
1	F	56	GLU
1	F	76	ARG
1	F	125	LEU

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

Mol	Chain	Res	Type
1	B	53	GLN
1	C	53	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](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z  > 2$
2	NAG	A	201	1	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	C	202	1	14,14,15	0.43	0	17,19,21	0.51	0
2	NAG	D	201	1	14,14,15	0.35	0	17,19,21	0.43	0
4	SO4	C	203	-	4,4,4	0.58	0	6,6,6	1.11	0
2	NAG	B	202	1	14,14,15	0.32	0	17,19,21	0.54	0
2	NAG	F	201	1	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	E	204	1	14,14,15	0.44	0	17,19,21	0.44	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
2	NAG	C	202	1	-	0/6/23/26	0/1/1/1
2	NAG	D	201	1	-	2/6/23/26	0/1/1/1
2	NAG	A	201	1	-	1/6/23/26	0/1/1/1
2	NAG	B	202	1	-	2/6/23/26	0/1/1/1
2	NAG	F	201	1	-	0/6/23/26	0/1/1/1
2	NAG	E	204	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	201	NAG	C4-C5-C6-O6
2	B	202	NAG	O5-C5-C6-O6
2	D	201	NAG	O5-C5-C6-O6
2	B	202	NAG	C4-C5-C6-O6
2	E	204	NAG	O5-C5-C6-O6
2	A	201	NAG	O5-C5-C6-O6
2	E	204	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	NAG	1	0
2	C	202	NAG	1	0
4	C	203	SO4	2	0

## 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/169 (64%)	0.39	4 (3%) 41 39	34, 43, 71, 81	0
1	B	107/169 (63%)	0.31	3 (2%) 53 51	36, 50, 71, 84	0
1	C	107/169 (63%)	0.23	4 (3%) 41 39	33, 47, 69, 77	0
1	D	105/169 (62%)	0.78	16 (15%) 2 2	38, 63, 86, 91	0
1	E	105/169 (62%)	0.32	9 (8%) 10 9	33, 52, 76, 87	0
1	F	110/169 (65%)	-0.01	1 (0%) 84 83	31, 43, 66, 75	0
All	All	643/1014 (63%)	0.34	37 (5%) 23 22	31, 48, 80, 91	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	115	GLY	7.6
1	E	60	CYS	5.4
1	B	54	LEU	5.2
1	D	59	PRO	4.7
1	A	57	LYS	4.4
1	E	116	SER	4.2
1	D	116	SER	3.8
1	D	115	GLY	3.7
1	A	56	GLU	3.7
1	D	60	CYS	3.7
1	C	130	ALA	3.7
1	F	116	SER	3.4
1	B	20	ASP	3.3
1	D	61	GLN	3.3
1	E	117	GLU	3.0
1	D	23	VAL	3.0
1	D	21	THR	2.9
1	D	22	THR	2.9
1	D	124	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	102	PRO	2.8
1	D	125	LEU	2.8
1	B	130	ALA	2.7
1	A	117	GLU	2.7
1	C	115	GLY	2.7
1	D	129	LEU	2.6
1	D	27	VAL	2.5
1	D	26	GLY	2.4
1	C	116	SER	2.4
1	C	54	LEU	2.3
1	E	61	GLN	2.3
1	E	59	PRO	2.3
1	E	118	ALA	2.3
1	D	25	GLN	2.2
1	D	99	ASN	2.1
1	A	58	GLY	2.0
1	E	25	GLN	2.0
1	E	53	GLN	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	C	202	14/15	0.79	0.17	51,64,74,74	0
2	NAG	E	204	14/15	0.79	0.35	72,81,88,89	0
2	NAG	B	202	14/15	0.80	0.21	59,64,69,71	0
3	IOD	E	203	1/1	0.80	0.11	161,161,161,161	0
2	NAG	F	201	14/15	0.85	0.16	58,67,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	201	14/15	0.86	0.24	77,83,86,88	0
2	NAG	A	201	14/15	0.91	0.12	50,57,66,72	0
3	IOD	E	202	1/1	0.93	0.05	130,130,130,130	0
4	SO4	C	203	5/5	0.99	0.24	24,45,47,56	0
3	IOD	B	201	1/1	1.00	0.17	39,39,39,39	0
3	IOD	E	201	1/1	1.00	0.18	36,36,36,36	0
3	IOD	C	201	1/1	1.00	0.17	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.