



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 12, 2018 – 06:35 PM EDT

PDB ID : 6B8O
Title : WT Ig-like V Domain with Phosphatidylserine
Authors : Sudom, A.; Wang, Z.
Deposited on : 2017-10-09
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

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:

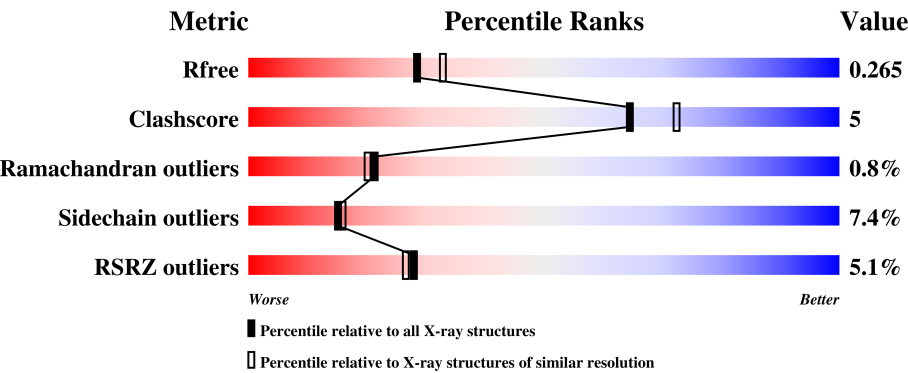
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031172
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

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 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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 ≥ 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	A	169	<div><div>12%</div><div>52%</div><div>9%</div><div>•</div><div>36%</div></div>
1	B	169	<div><div>53%</div><div>9%</div><div>•</div><div>37%</div></div>
1	C	169	<div><div>51%</div><div>11%</div><div>•</div><div>37%</div></div>
1	D	169	<div><div>12%</div><div>53%</div><div>8%</div><div>•</div><div>37%</div></div>
1	E	169	<div><div>4%</div><div>55%</div><div>6%</div><div>•</div><div>38%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	169	<div> <div> <div>%</div> <div> <div></div> <div>51%</div> <div>12%</div> <div>36%</div> </div> </div> <div>..</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
3	IOD	A	204	-	-	X	-
6	PSF	D	205	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5416 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	106	Total	C	N	O	S	0	0	0
			836	524	156	151	5			
1	E	105	Total	C	N	O	S	0	0	0
			828	518	155	150	5			
1	F	109	Total	C	N	O	S	0	0	0
			853	533	159	156	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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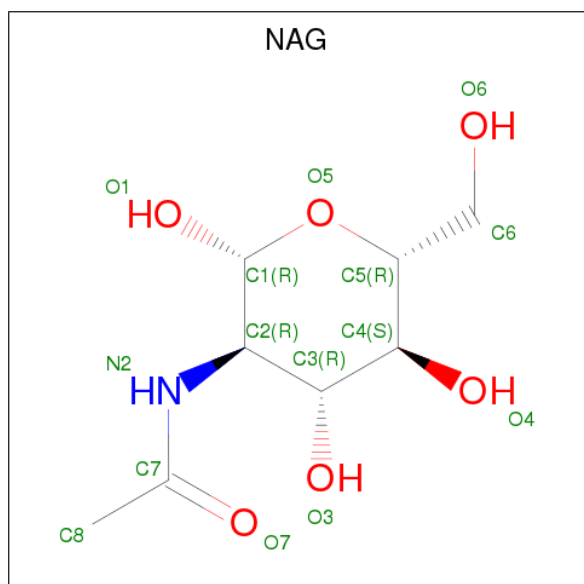
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	LEU	-	expression tag	UNP Q9NZC2
B	178	TYR	-	expression tag	UNP Q9NZC2
B	179	PHE	-	expression tag	UNP Q9NZC2
B	180	GLN	-	expression tag	UNP Q9NZC2
B	181	GLY	-	expression tag	UNP Q9NZC2
B	182	HIS	-	expression tag	UNP Q9NZC2
B	183	HIS	-	expression tag	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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

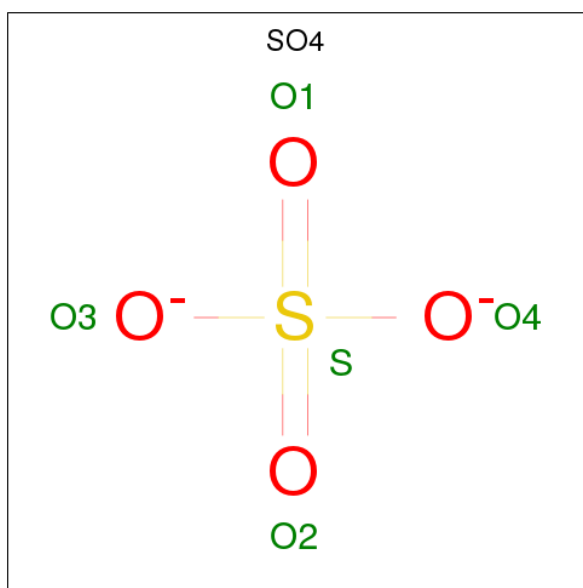


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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

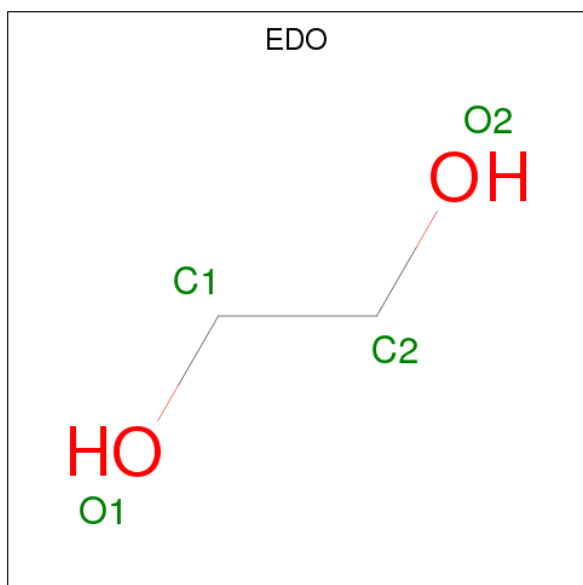
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	I	0	0
			2	2		
3	A	3	Total	I	0	0
			3	3		
3	C	1	Total	I	0	0
			1	1		
3	E	1	Total	I	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



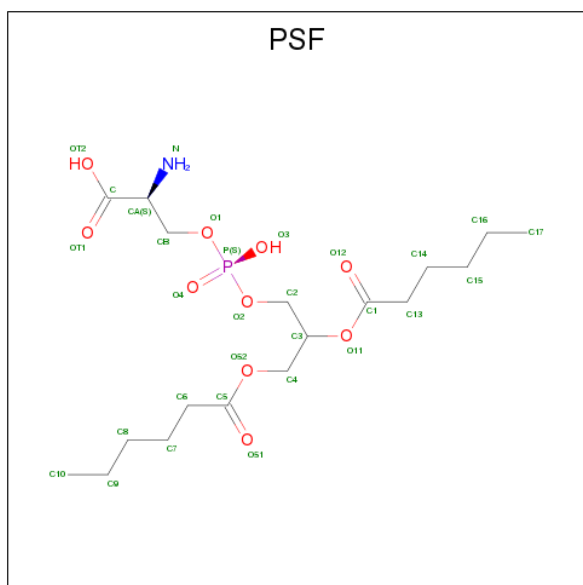
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: C₁₈H₃₄NO₁₀P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 30	C 18	N 1	O 10	P 1	0	0
6	C	1	Total 30	C 18	N 1	O 10	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			30	18	1	10	1		

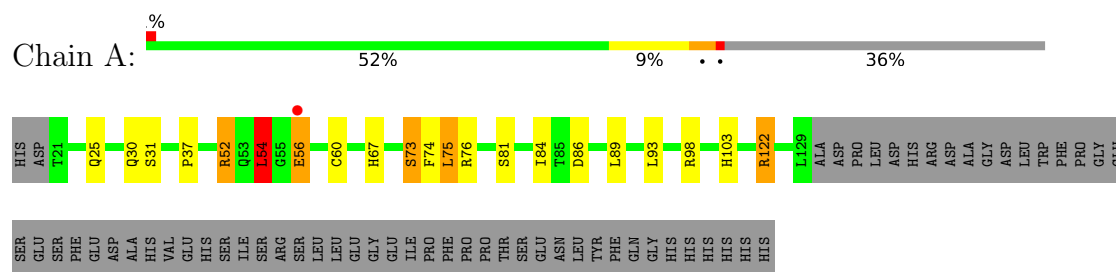
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	O	0	0
			15	15		
7	B	5	Total	O	0	0
			5	5		
7	C	14	Total	O	0	0
			14	14		
7	D	12	Total	O	0	0
			12	12		
7	E	15	Total	O	0	0
			15	15		
7	F	21	Total	O	0	0
			21	21		

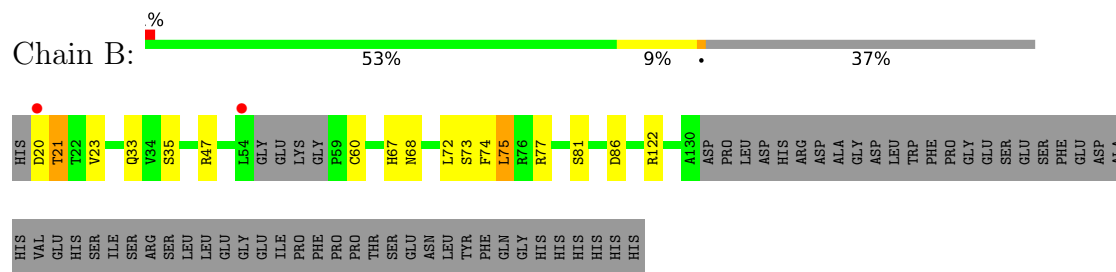
3 Residue-property plots [i](#)

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.

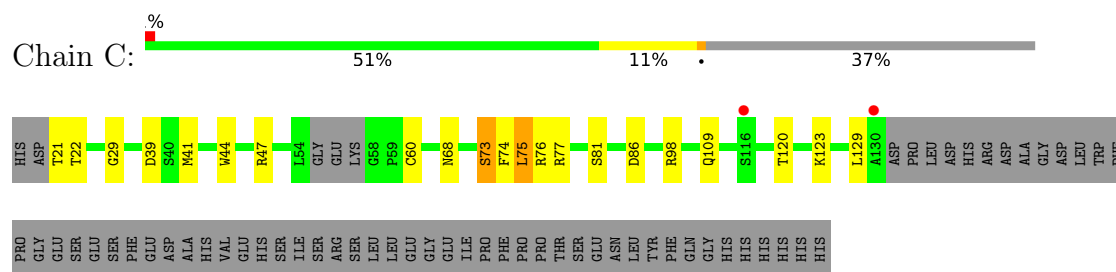
- Molecule 1: Triggering receptor expressed on myeloid cells 2



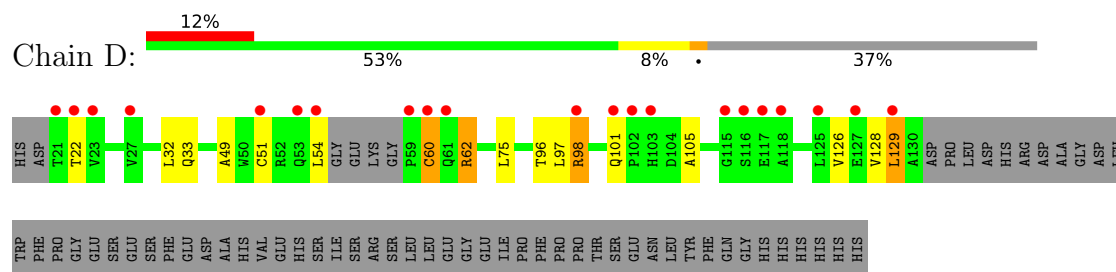
- Molecule 1: Triggering receptor expressed on myeloid cells 2



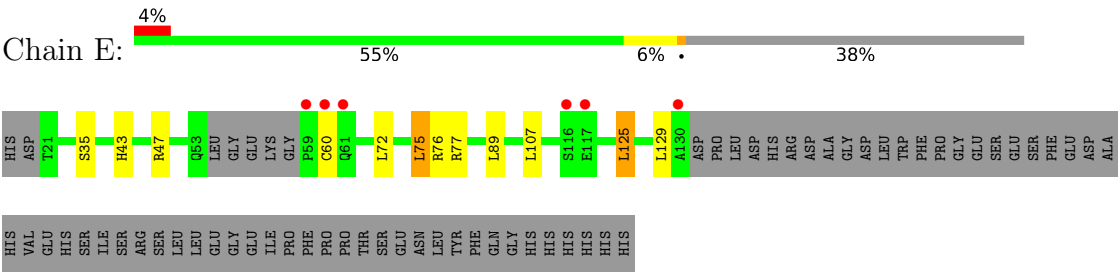
- Molecule 1: Triggering receptor expressed on myeloid cells 2



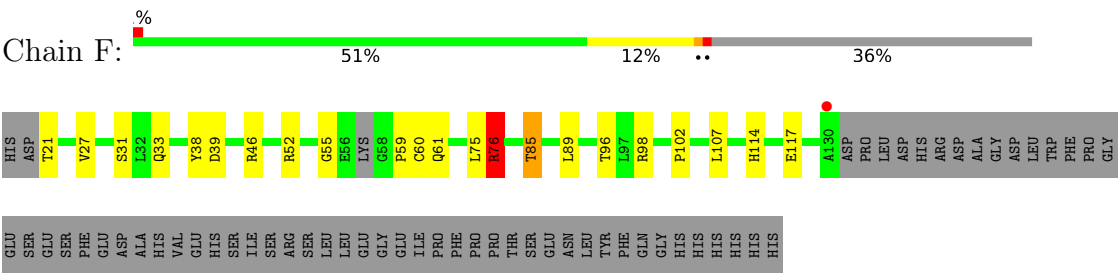
- Molecule 1: Triggering receptor expressed on myeloid cells 2



- 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, α , β , γ	160.33Å 160.33Å 86.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.36 – 2.20 47.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.36-2.20) 100.0 (47.36-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.222 , 0.261 0.228 , 0.265	Depositor DCC
R_{free} test set	2768 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	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	0.94	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: SO4, IOD, PSF, NAG, EDO

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	0.98	1/875 (0.1%)	1.10	3/1187 (0.3%)
1	B	0.94	0/861	1.03	2/1168 (0.2%)
1	C	0.94	1/857 (0.1%)	1.11	6/1163 (0.5%)
1	D	0.86	1/853 (0.1%)	0.90	0/1157
1	E	0.83	0/845	0.94	1/1146 (0.1%)
1	F	1.00	0/870	1.08	2/1180 (0.2%)
All	All	0.93	3/5161 (0.1%)	1.03	14/7001 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	SER	CB-OG	-7.66	1.32	1.42
1	D	98	ARG	CZ-NH1	-6.66	1.24	1.33
1	A	73	SER	CB-OG	-5.83	1.34	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	B	77	ARG	NE-CZ-NH1	9.64	125.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	C	77	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	C	98	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	B	77	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	A	98	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	98	ARG	NE-CZ-NH2	8.55	124.57	120.30
1	A	122	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	C	39	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	39	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	F	76	ARG	CB-CA-C	5.18	120.77	110.40
1	E	77	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	76	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	56	GLU	Peptide
1	B	20	ASP	Peptide

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	15	0
1	B	844	0	834	8	0
1	C	840	0	832	6	0
1	D	836	0	830	6	0
1	E	828	0	819	5	0
1	F	853	0	841	11	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	3	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	10	0	0	1	0
4	D	15	0	0	0	0
4	E	15	0	0	1	0
4	F	15	0	0	1	0
5	A	20	0	29	3	0
5	B	16	0	24	0	0
5	F	4	0	6	0	0
6	B	30	0	32	3	0
6	C	30	0	32	2	0
6	D	30	0	32	2	0
7	A	15	0	0	0	0
7	B	5	0	0	0	0
7	C	14	0	0	1	0
7	D	12	0	0	0	0
7	E	15	0	0	0	0
7	F	21	0	0	0	0
All	All	5416	0	5239	48	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 5.

All (48) 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:D:51:CYS:HG	1:D:60:CYS:HG	1.18	0.88
1:D:33:GLN:NE2	1:D:96:THR:OG1	2.12	0.77
1:A:67:HIS:CE1	6:D:205:PSF:H2	2.07	0.71
6:C:203:PSF:H21	1:F:89:LEU:HD13	1.73	0.71
1:B:74:PHE:CE2	1:B:75:LEU:HD13	2.28	0.69
1:A:74:PHE:CE1	1:A:75:LEU:HD13	2.30	0.67
1:A:67:HIS:HE1	6:D:205:PSF:H2	1.44	0.65
1:D:49:ALA:HB1	1:D:62:ARG:HD2	1.81	0.62
1:C:73:SER:HB3	1:C:86:ASP:HB3	1.83	0.60
1:C:74:PHE:CE1	1:C:75:LEU:HD13	2.37	0.59
1:C:47:ARG:HD3	1:C:68:ASN:HA	1.85	0.58
1:A:31:SER:OG	3:A:204:IOD:I	2.91	0.58
1:C:41:MET:CE	1:E:76:ARG:NE	2.68	0.57
1:F:59:PRO:HB2	1:F:61:GLN:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:IOD:I	1:B:35:SER:HB2	2.77	0.55
1:B:73:SER:HB3	1:B:86:ASP:HB3	1.87	0.55
6:B:204:PSF:O3	1:E:89:LEU:HA	2.06	0.55
1:B:67:HIS:HE2	6:B:204:PSF:H21	1.73	0.54
1:A:73:SER:HB3	1:A:86:ASP:HB3	1.89	0.53
1:D:32:LEU:HD23	1:D:97:LEU:HD12	1.91	0.53
1:A:103:HIS:N	4:A:205:SO4:O4	2.38	0.52
1:A:122:ARG:NH2	1:C:29:GLY:O	2.26	0.52
1:F:33:GLN:HE21	1:F:96:THR:HG23	1.74	0.52
1:F:76:ARG:HB2	1:F:85:THR:HG23	1.90	0.52
1:A:37:PRO:HD3	3:A:203:IOD:I	2.81	0.49
1:E:43:HIS:CD2	4:E:204:SO4:O4	2.65	0.49
1:C:109:GLN:NE2	1:C:120:THR:OG1	2.47	0.48
1:A:76:ARG:H	5:A:211:EDO:H11	1.78	0.48
1:B:47:ARG:NE	1:B:68:ASN:HA	2.29	0.47
1:F:52:ARG:HD2	1:F:107:LEU:O	2.13	0.47
1:B:72:LEU:HB3	1:B:75:LEU:HD22	1.97	0.47
1:F:46:ARG:HD2	1:F:114:HIS:HB3	1.96	0.47
1:A:52:ARG:HG2	1:A:54:LEU:HD13	1.97	0.46
1:E:107:LEU:HD13	1:E:125:LEU:HD22	1.97	0.46
1:A:76:ARG:H	5:A:211:EDO:C1	2.29	0.46
1:A:30:GLN:NE2	1:B:23:VAL:O	2.49	0.46
1:B:67:HIS:CE1	6:B:204:PSF:HA	2.51	0.45
1:A:89:LEU:HD23	7:C:311:HOH:O	2.16	0.45
1:F:38:TYR:HB2	4:F:204:SO4:O3	2.17	0.44
1:D:128:VAL:HG12	1:D:129:LEU:N	2.31	0.44
1:D:105:ALA:HB2	1:D:128:VAL:HG23	2.00	0.43
1:A:76:ARG:NH1	5:A:207:EDO:H11	2.33	0.43
1:E:72:LEU:HB3	1:E:75:LEU:HD22	2.01	0.43
1:A:84:ILE:HD11	1:A:93:LEU:HD11	2.01	0.41
6:C:203:PSF:C2	1:F:89:LEU:HD13	2.47	0.41
1:F:31:SER:HA	1:F:98:ARG:O	2.19	0.41
1:F:114:HIS:CE1	1:F:117:GLU:HB2	2.54	0.41
1:F:33:GLN:NE2	1:F:96:THR:OG1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/169 (63%)	104 (97%)	1 (1%)	2 (2%)	9	5
1	B	103/169 (61%)	102 (99%)	0	1 (1%)	17	15
1	C	103/169 (61%)	100 (97%)	2 (2%)	1 (1%)	17	15
1	D	102/169 (60%)	100 (98%)	2 (2%)	0	100	100
1	E	101/169 (60%)	100 (99%)	1 (1%)	0	100	100
1	F	105/169 (62%)	103 (98%)	1 (1%)	1 (1%)	17	15
All	All	621/1014 (61%)	609 (98%)	7 (1%)	5 (1%)	21	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	56	GLU
1	F	55	GLY
1	C	129	LEU
1	B	21	THR

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%)	88 (94%)	6 (6%)	19	22
1	B	93/147 (63%)	87 (94%)	6 (6%)	19	21
1	C	92/147 (63%)	85 (92%)	7 (8%)	14	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	92/147 (63%)	83 (90%)	9 (10%)	9	8
1	E	91/147 (62%)	85 (93%)	6 (7%)	18	20
1	F	93/147 (63%)	86 (92%)	7 (8%)	15	15
All	All	555/882 (63%)	514 (93%)	41 (7%)	15	16

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	52	ARG
1	A	54	LEU
1	A	60	CYS
1	A	75	LEU
1	A	81	SER
1	B	21	THR
1	B	33	GLN
1	B	60	CYS
1	B	75	LEU
1	B	81	SER
1	B	122	ARG
1	C	21	THR
1	C	22	THR
1	C	44	TRP
1	C	60	CYS
1	C	75	LEU
1	C	81	SER
1	C	123	LYS
1	D	22	THR
1	D	54	LEU
1	D	60	CYS
1	D	62	ARG
1	D	75	LEU
1	D	98	ARG
1	D	101	GLN
1	D	126	VAL
1	D	129	LEU
1	E	35	SER
1	E	47	ARG
1	E	60	CYS
1	E	75	LEU
1	E	125	LEU

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Mol	Chain	Res	Type
1	E	129	LEU
1	F	21	THR
1	F	27	VAL
1	F	60	CYS
1	F	75	LEU
1	F	76	ARG
1	F	85	THR
1	F	102	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	67	HIS
1	B	33	GLN
1	C	33	GLN
1	C	109	GLN
1	C	111	GLN
1	D	33	GLN
1	D	53	GLN
1	D	101	GLN
1	D	109	GLN
1	E	25	GLN
1	E	109	GLN
1	F	33	GLN
1	F	61	GLN

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 37 ligands modelled in this entry, 7 are monoatomic - leaving 30 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	0.90	0	17,19,21	2.18	5 (29%)
4	SO4	A	205	-	4,4,4	0.65	0	6,6,6	0.45	0
4	SO4	A	206	-	4,4,4	0.71	0	6,6,6	3.23	3 (50%)
5	EDO	A	207	-	3,3,3	1.21	0	2,2,2	0.92	0
5	EDO	A	208	-	3,3,3	0.44	0	2,2,2	0.89	0
5	EDO	A	209	-	3,3,3	0.39	0	2,2,2	0.57	0
5	EDO	A	210	-	3,3,3	0.44	0	2,2,2	1.18	0
5	EDO	A	211	-	3,3,3	0.66	0	2,2,2	1.12	0
2	NAG	B	201	1	14,14,15	1.00	0	17,19,21	2.01	7 (41%)
6	PSF	B	204	-	25,29,29	1.62	2 (8%)	28,36,36	1.93	8 (28%)
5	EDO	B	205	-	3,3,3	0.53	0	2,2,2	0.39	0
5	EDO	B	206	-	3,3,3	0.37	0	2,2,2	0.43	0
5	EDO	B	207	-	3,3,3	0.65	0	2,2,2	0.27	0
5	EDO	B	208	-	3,3,3	0.63	0	2,2,2	0.54	0
2	NAG	C	201	1	14,14,15	0.50	0	17,19,21	0.99	2 (11%)
6	PSF	C	203	-	25,29,29	1.54	2 (8%)	28,36,36	2.25	7 (25%)
2	NAG	D	201	1	14,14,15	0.77	0	17,19,21	1.93	5 (29%)
4	SO4	D	202	-	4,4,4	0.36	0	6,6,6	0.58	0
4	SO4	D	203	-	4,4,4	0.58	0	6,6,6	0.89	0
4	SO4	D	204	-	4,4,4	0.49	0	6,6,6	0.55	0
6	PSF	D	205	-	25,29,29	1.68	2 (8%)	28,36,36	1.80	6 (21%)
2	NAG	E	201	1	14,14,15	0.52	0	17,19,21	2.53	5 (29%)
4	SO4	E	203	-	4,4,4	0.57	0	6,6,6	0.34	0
4	SO4	E	204	-	4,4,4	0.60	0	6,6,6	0.81	0
4	SO4	E	205	-	4,4,4	0.56	0	6,6,6	0.58	0
2	NAG	F	201	1	14,14,15	0.51	0	17,19,21	1.46	2 (11%)
4	SO4	F	202	-	4,4,4	0.32	0	6,6,6	1.77	1 (16%)
4	SO4	F	203	-	4,4,4	0.46	0	6,6,6	0.38	0
4	SO4	F	204	-	4,4,4	0.65	0	6,6,6	0.77	0
5	EDO	F	205	-	3,3,3	0.61	0	2,2,2	0.20	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	A	201	1	-	0/6/23/26	0/1/1/1
4	SO4	A	205	-	-	0/0/0/0	0/0/0/0
4	SO4	A	206	-	-	0/0/0/0	0/0/0/0
5	EDO	A	207	-	-	0/1/1/1	0/0/0/0
5	EDO	A	208	-	-	0/1/1/1	0/0/0/0
5	EDO	A	209	-	-	0/1/1/1	0/0/0/0
5	EDO	A	210	-	-	0/1/1/1	0/0/0/0
5	EDO	A	211	-	-	0/1/1/1	0/0/0/0
2	NAG	B	201	1	-	0/6/23/26	0/1/1/1
6	PSF	B	204	-	-	0/31/35/35	0/0/0/0
5	EDO	B	205	-	-	0/1/1/1	0/0/0/0
5	EDO	B	206	-	-	0/1/1/1	0/0/0/0
5	EDO	B	207	-	-	0/1/1/1	0/0/0/0
5	EDO	B	208	-	-	0/1/1/1	0/0/0/0
2	NAG	C	201	1	-	0/6/23/26	0/1/1/1
6	PSF	C	203	-	-	2/31/35/35	0/0/0/0
2	NAG	D	201	1	-	0/6/23/26	0/1/1/1
4	SO4	D	202	-	-	0/0/0/0	0/0/0/0
4	SO4	D	203	-	-	0/0/0/0	0/0/0/0
4	SO4	D	204	-	-	0/0/0/0	0/0/0/0
6	PSF	D	205	-	-	0/31/35/35	0/0/0/0
2	NAG	E	201	1	-	0/6/23/26	0/1/1/1
4	SO4	E	203	-	-	0/0/0/0	0/0/0/0
4	SO4	E	204	-	-	0/0/0/0	0/0/0/0
4	SO4	E	205	-	-	0/0/0/0	0/0/0/0
2	NAG	F	201	1	-	0/6/23/26	0/1/1/1
4	SO4	F	202	-	-	0/0/0/0	0/0/0/0
4	SO4	F	203	-	-	0/0/0/0	0/0/0/0
4	SO4	F	204	-	-	0/0/0/0	0/0/0/0
5	EDO	F	205	-	-	0/1/1/1	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	203	PSF	O52-C5	4.19	1.45	1.33
6	B	204	PSF	O11-C1	5.05	1.48	1.34
6	C	203	PSF	O11-C1	5.10	1.49	1.34
6	B	204	PSF	O52-C5	5.19	1.48	1.33
6	D	205	PSF	O11-C1	5.45	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	205	PSF	O52-C5	5.49	1.49	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	206	SO4	O2-S-O1	-5.84	69.34	109.86
6	C	203	PSF	O11-C1-O12	-4.70	112.10	123.69
2	A	201	NAG	O5-C5-C6	-4.07	100.70	107.15
6	C	203	PSF	O52-C5-O51	-3.83	114.23	123.58
2	F	201	NAG	O5-C1-C2	-3.71	106.39	111.52
2	A	201	NAG	O5-C1-C2	-3.69	106.43	111.52
2	A	201	NAG	C8-C7-N2	-3.68	109.66	116.10
2	E	201	NAG	O5-C1-C2	-3.39	106.84	111.52
6	B	204	PSF	O52-C5-O51	-3.20	115.78	123.58
6	B	204	PSF	O3-P-O2	-2.88	94.38	107.75
2	B	201	NAG	C4-C3-C2	-2.87	106.81	111.02
6	D	205	PSF	O1-CB-CA	-2.60	105.77	108.07
2	B	201	NAG	C8-C7-N2	-2.47	111.77	116.10
6	D	205	PSF	O52-C5-O51	-2.40	117.73	123.58
2	B	201	NAG	C1-O5-C5	-2.38	108.92	112.19
2	E	201	NAG	C6-C5-C4	-2.37	107.40	112.99
2	E	201	NAG	C4-C3-C2	-2.29	107.67	111.02
6	C	203	PSF	C4-C3-C2	-2.20	106.90	111.86
2	D	201	NAG	O6-C6-C5	-2.15	103.79	111.29
6	B	204	PSF	O11-C1-O12	-2.11	118.48	123.69
2	C	201	NAG	C4-C3-C2	-2.04	108.03	111.02
2	E	201	NAG	O5-C5-C6	2.09	110.45	107.15
2	C	201	NAG	C3-C4-C5	2.12	114.04	110.24
4	A	206	SO4	O3-S-O2	2.12	120.72	109.24
2	A	201	NAG	O4-C4-C5	2.20	114.81	109.31
6	C	203	PSF	O3-P-O4	2.27	123.68	112.14
6	B	204	PSF	O11-C3-C4	2.37	117.03	108.43
2	D	201	NAG	O5-C5-C6	2.40	110.94	107.15
6	D	205	PSF	C3-O11-C1	2.51	123.80	117.88
2	B	201	NAG	C2-N2-C7	2.60	126.74	122.94
2	D	201	NAG	C4-C3-C2	2.63	114.87	111.02
2	F	201	NAG	C1-O5-C5	2.86	116.12	112.19
2	B	201	NAG	O3-C3-C4	2.96	117.26	110.34
2	D	201	NAG	C1-C2-N2	2.98	115.57	110.49
6	B	204	PSF	C4-O52-C5	3.04	126.20	117.13
6	B	204	PSF	O11-C1-C13	3.25	118.39	111.55
2	B	201	NAG	O7-C7-N2	3.29	128.16	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	202	SO4	O4-S-O3	3.51	124.47	108.83
6	D	205	PSF	C4-O52-C5	3.58	127.83	117.13
2	B	201	NAG	O5-C5-C6	3.63	112.89	107.15
6	C	203	PSF	O52-C5-C6	3.63	122.42	111.92
2	A	201	NAG	O7-C7-N2	4.05	129.59	121.94
6	D	205	PSF	O52-C5-C6	4.37	124.56	111.92
6	B	204	PSF	O52-C5-C6	4.46	124.80	111.92
4	A	206	SO4	O4-S-O2	4.50	133.57	109.24
6	B	204	PSF	O1-CB-CA	4.64	112.18	108.07
6	D	205	PSF	O11-C1-C13	4.82	121.72	111.55
6	C	203	PSF	O11-C1-C13	4.93	121.93	111.55
2	D	201	NAG	C2-N2-C7	4.99	130.22	122.94
6	C	203	PSF	O1-CB-CA	6.24	113.60	108.07
2	E	201	NAG	C1-O5-C5	8.35	123.67	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	203	PSF	C3-O11-C1-O12
6	C	203	PSF	C3-O11-C1-C13

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	205	SO4	1	0
5	A	207	EDO	1	0
5	A	211	EDO	2	0
6	B	204	PSF	3	0
6	C	203	PSF	2	0
6	D	205	PSF	2	0
4	E	204	SO4	1	0
4	F	204	SO4	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	109/169 (64%)	0.21	1 (0%) 84 83	32, 43, 79, 97	0
1	B	107/169 (63%)	0.19	2 (1%) 66 65	35, 49, 80, 112	0
1	C	107/169 (63%)	0.13	2 (1%) 66 65	32, 48, 77, 91	0
1	D	106/169 (62%)	1.01	21 (19%) 1 1	37, 64, 95, 107	0
1	E	105/169 (62%)	0.22	6 (5%) 24 22	32, 54, 84, 92	0
1	F	109/169 (64%)	-0.07	1 (0%) 84 83	30, 43, 70, 86	0
All	All	643/1014 (63%)	0.28	33 (5%) 28 26	30, 49, 85, 112	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54	LEU	7.7
1	D	116	SER	5.6
1	F	130	ALA	5.5
1	D	60	CYS	5.5
1	E	60	CYS	5.0
1	B	54	LEU	4.7
1	B	20	ASP	4.4
1	D	61	GLN	4.4
1	E	116	SER	4.4
1	D	102	PRO	4.2
1	D	125	LEU	4.0
1	D	115	GLY	3.5
1	C	130	ALA	3.5
1	D	101	GLN	3.2
1	D	59	PRO	3.1
1	D	51	CYS	3.1
1	D	23	VAL	2.9
1	D	27	VAL	2.8
1	E	130	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	21	THR	2.7
1	D	98	ARG	2.6
1	C	116	SER	2.6
1	E	59	PRO	2.6
1	E	117	GLU	2.5
1	D	22	THR	2.5
1	D	53	GLN	2.4
1	E	61	GLN	2.4
1	D	129	LEU	2.3
1	A	56	GLU	2.2
1	D	118	ALA	2.1
1	D	127	GLU	2.1
1	D	103	HIS	2.1
1	D	117	GLU	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(\AA^2)	Q<0.9
6	PSF	D	205	30/30	0.55	0.47	41,87,116,148	0
6	PSF	C	203	30/30	0.60	0.34	36,72,106,119	0
6	PSF	B	204	30/30	0.65	0.36	33,76,102,134	0
2	NAG	B	201	14/15	0.75	0.24	64,72,81,82	0
5	EDO	F	205	4/4	0.82	0.17	69,73,79,82	0
5	EDO	B	208	4/4	0.82	0.23	55,62,63,70	0
5	EDO	B	207	4/4	0.85	0.15	62,69,71,74	0
2	NAG	C	201	14/15	0.86	0.18	67,76,86,91	0
5	EDO	B	206	4/4	0.87	0.30	42,44,52,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	208	4/4	0.88	0.25	42,47,62,67	0
2	NAG	E	201	14/15	0.88	0.26	79,89,102,107	0
2	NAG	D	201	14/15	0.88	0.26	96,106,116,119	0
2	NAG	A	201	14/15	0.89	0.12	52,62,74,79	0
2	NAG	F	201	14/15	0.90	0.14	66,76,94,99	0
4	SO4	E	203	5/5	0.90	0.30	77,79,93,95	0
5	EDO	A	207	4/4	0.90	0.39	22,34,54,59	0
5	EDO	A	210	4/4	0.90	0.32	37,47,58,59	0
5	EDO	A	209	4/4	0.92	0.13	56,59,63,70	0
5	EDO	B	205	4/4	0.92	0.28	49,58,64,65	0
5	EDO	A	211	4/4	0.93	0.30	46,51,58,60	0
4	SO4	F	202	5/5	0.93	0.18	47,51,68,92	0
4	SO4	E	205	5/5	0.96	0.16	53,69,74,82	0
4	SO4	F	204	5/5	0.96	0.28	59,59,80,83	0
4	SO4	D	204	5/5	0.97	0.19	58,72,80,96	0
3	IOD	E	202	1/1	0.97	0.09	74,74,74,74	0
4	SO4	D	203	5/5	0.97	0.11	59,69,76,79	0
4	SO4	F	203	5/5	0.98	0.17	51,58,66,78	0
4	SO4	A	206	5/5	0.99	0.18	34,34,54,58	0
4	SO4	D	202	5/5	0.99	0.17	41,54,72,75	0
4	SO4	A	205	5/5	0.99	0.16	36,51,72,76	0
4	SO4	E	204	5/5	0.99	0.23	41,66,68,85	0
3	IOD	B	203	1/1	0.99	0.15	57,57,57,57	0
3	IOD	A	204	1/1	0.99	0.14	58,58,58,58	0
3	IOD	A	203	1/1	1.00	0.14	52,52,52,52	0
3	IOD	C	202	1/1	1.00	0.20	35,35,35,35	0
3	IOD	B	202	1/1	1.00	0.19	40,40,40,40	0
3	IOD	A	202	1/1	1.00	0.20	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.