



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 10:13 PM BST

PDB ID : 5JOR
Title : Crystal structure of unbound anti-glycan antibody Fab14.22 at 2.2 Å
Authors : Sarkar, A.; Irimia, A.; Teyton, L.; Wilson, I.A.
Deposited on : 2016-05-02
Resolution : 2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.5 (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

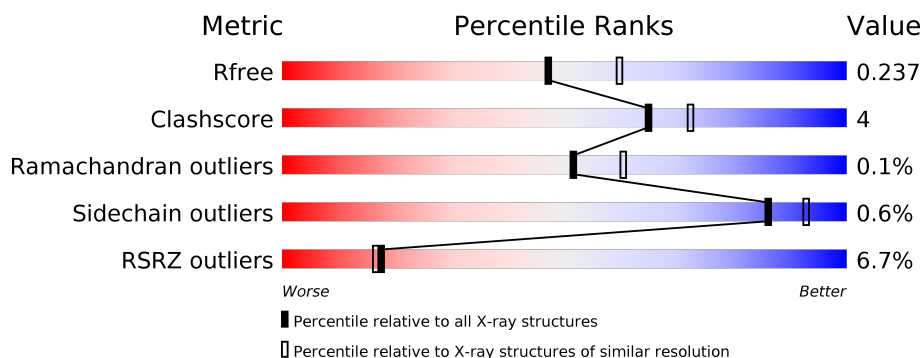
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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 ≥ 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	B	249	<div> <div>12%</div> <div>76%</div> <div>8%</div> <div>17%</div> </div>
1	D	249	<div> <div>16%</div> <div>76%</div> <div>7%</div> <div>16%</div> </div>
1	F	249	<div> <div>5%</div> <div>74%</div> <div>10%</div> <div>15%</div> </div>
1	H	249	<div> <div>4%</div> <div>76%</div> <div>8%</div> <div>15%</div> </div>
2	A	219	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>
2	C	219	<div> <div>%</div> <div>91%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	219	
2	L	219	

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	GOL	F	305	-	-	-	X
3	GOL	H	302	-	-	-	X
3	GOL	L	303	-	-	-	X
5	1PE	F	314	-	-	-	X
5	1PE	L	307	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14568 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 Fab14.22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	207	Total	C	N	O	S	0	1	0
			1580	1001	258	313	8			
1	F	211	Total	C	N	O	S	0	1	0
			1613	1018	266	321	8			
1	H	211	Total	C	N	O	S	0	3	0
			1619	1022	266	322	9			
1	D	208	Total	C	N	O	S	0	0	0
			1583	1002	259	314	8			

- Molecule 2 is a protein called Fab 14.22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	3	0
			1724	1083	290	343	8			
2	L	218	Total	C	N	O	S	0	0	0
			1712	1076	289	341	6			
2	C	218	Total	C	N	O	S	0	1	0
			1715	1078	289	342	6			
2	E	217	Total	C	N	O	S	0	0	0
			1703	1071	288	338	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

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



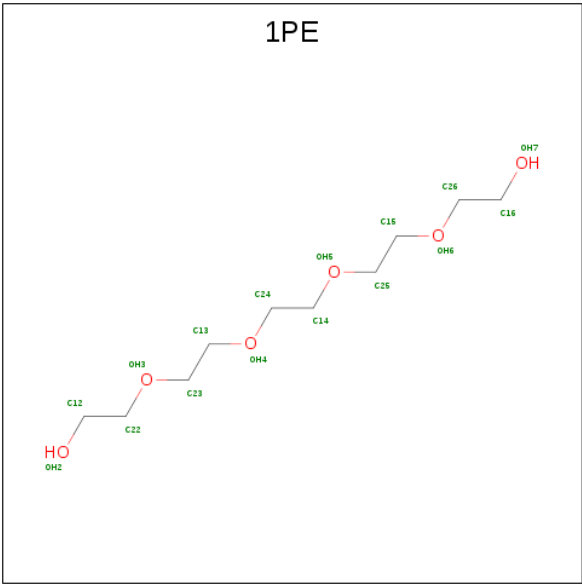
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total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

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

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			11	7	4		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			12	8	4		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			6	4	2		
5	H	1	Total	C	O	0	0
			11	7	4		
5	H	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			11	7	4		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			12	8	4		

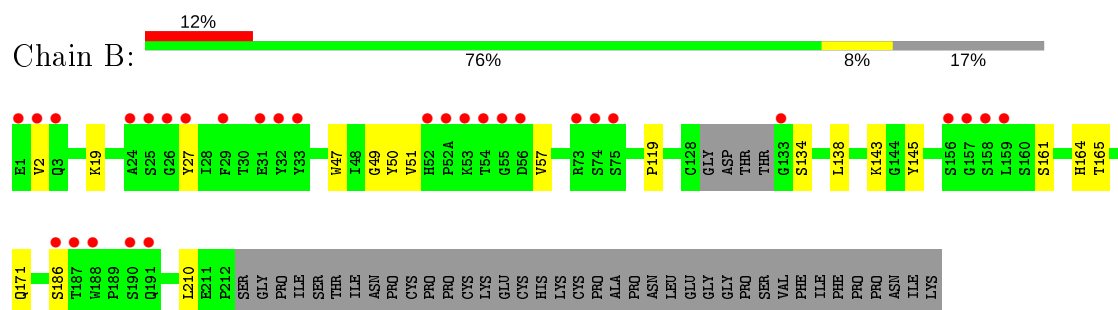
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	101	Total	O	0	0
			101	101		
6	A	135	Total	O	0	0
			135	135		
6	F	99	Total	O	0	0
			99	99		
6	H	118	Total	O	0	0
			118	118		
6	L	113	Total	O	0	0
			113	113		
6	C	122	Total	O	0	0
			122	122		
6	D	90	Total	O	0	0
			90	90		
6	E	101	Total	O	0	0
			101	101		

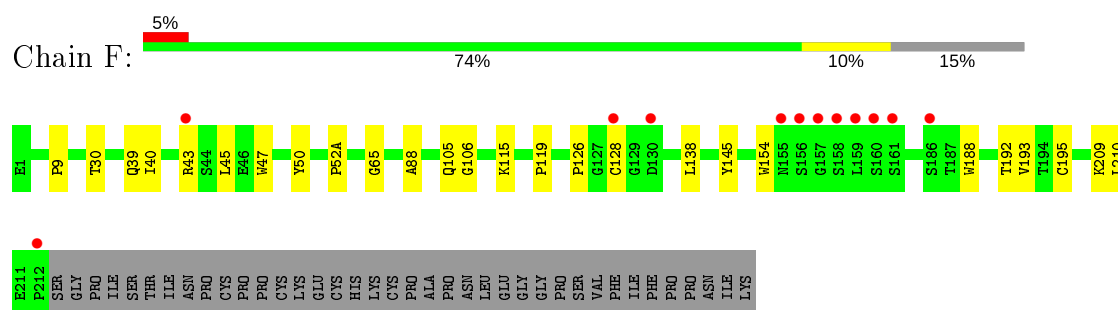
3 Residue-property plots [i](#)

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.

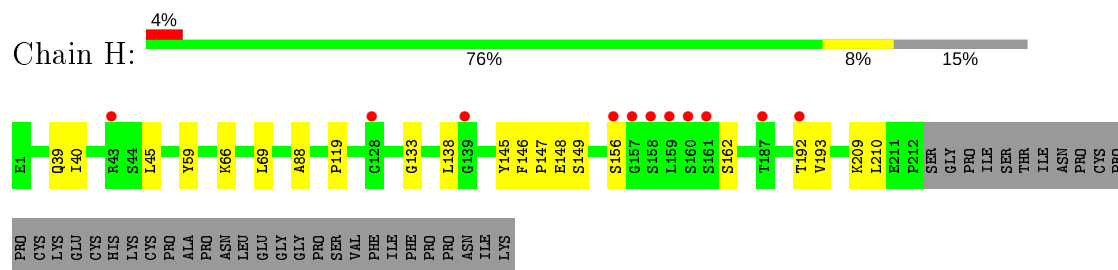
- Molecule 1: Fab14.22 heavy chain



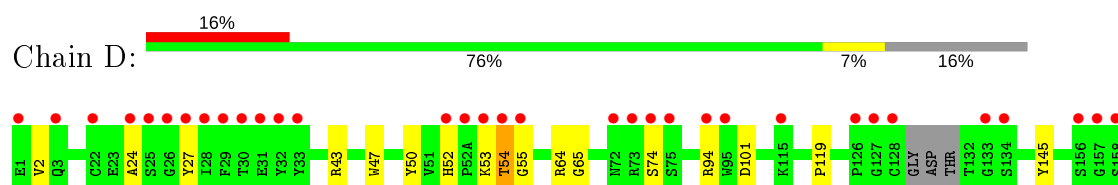
- Molecule 1: Fab14.22 heavy chain

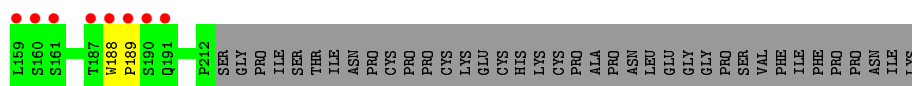


- Molecule 1: Fab14.22 heavy chain



- Molecule 1: Fab14.22 heavy chain

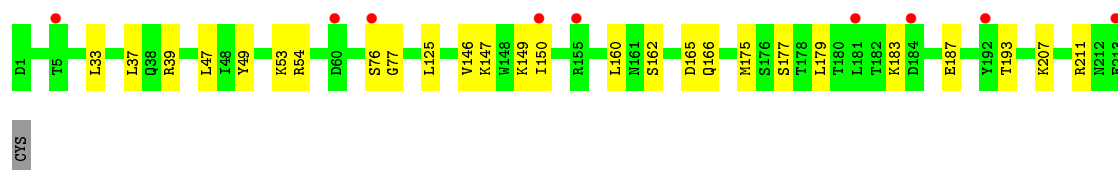
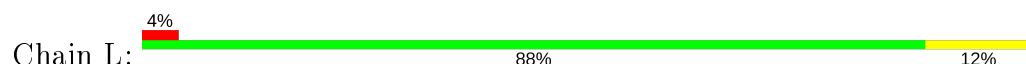




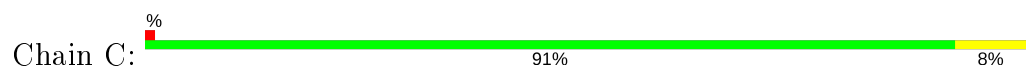
- Molecule 2: Fab 14.22 light chain



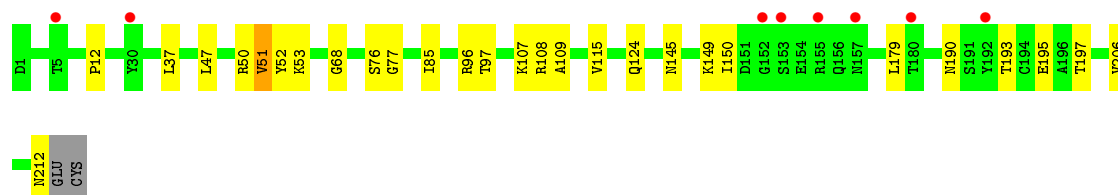
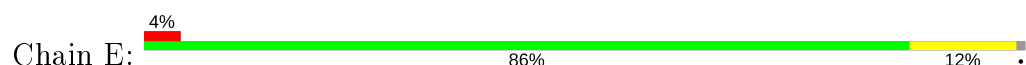
- Molecule 2: Fab 14.22 light chain



- Molecule 2: Fab 14.22 light chain



- Molecule 2: Fab 14.22 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.61Å 75.99Å 122.95Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	49.73 – 2.21 49.74 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.73-2.21) 98.9 (49.74-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: 000)	Depositor
R, R_{free}	0.205 , 0.237 0.205 , 0.237	Depositor DCC
R_{free} test set	5460 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14568	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0181e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 1PE

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	B	0.25	0/1626	0.45	0/2224
1	D	0.25	0/1626	0.45	0/2224
1	F	0.25	0/1657	0.46	0/2267
1	H	0.24	0/1669	0.45	0/2283
2	A	0.24	0/1770	0.45	0/2401
2	C	0.24	0/1758	0.44	0/2385
2	E	0.24	0/1743	0.44	0/2365
2	L	0.24	0/1752	0.43	0/2377
All	All	0.24	0/13601	0.45	0/18526

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	B	1580	0	1534	11	0
1	D	1583	0	1534	15	0
1	F	1613	0	1561	19	0
1	H	1619	0	1570	12	0
2	A	1724	0	1668	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1715	0	1659	11	0
2	E	1703	0	1646	18	0
2	L	1712	0	1654	18	0
3	A	18	0	24	1	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
3	D	36	0	48	0	0
3	E	36	0	48	2	0
3	F	48	0	63	5	0
3	H	12	0	16	2	0
3	L	24	0	32	1	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	15	0	0	1	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	20	0	0	0	0
4	H	10	0	0	0	0
4	L	10	0	0	1	0
5	A	7	0	9	0	0
5	B	69	0	88	4	0
5	C	11	0	13	2	0
5	D	7	0	9	0	0
5	E	12	0	15	1	0
5	F	13	0	16	1	0
5	H	15	0	18	1	0
5	L	13	0	16	1	0
6	A	135	0	0	1	0
6	B	101	0	0	1	0
6	C	122	0	0	1	0
6	D	90	0	0	0	0
6	E	101	0	0	1	0
6	F	99	0	0	0	0
6	H	118	0	0	1	0
6	L	113	0	0	3	0
All	All	14568	0	13273	111	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.

The worst 5 of 111 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:E:108:ARG:HH22	5:E:309:1PE:H141	1.51	0.75
5:B:306:1PE:H121	2:C:40:PRO:HA	1.74	0.69
1:B:119:PRO:HB3	1:B:145:TYR:HB3	1.77	0.65
1:F:105:GLN:HE21	3:F:305:GOL:H31	1.62	0.64
1:F:128:CYS:SG	6:E:456:HOH:O	2.51	0.64

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	B	204/249 (82%)	198 (97%)	6 (3%)	0	100	100
1	D	204/249 (82%)	197 (97%)	7 (3%)	0	100	100
1	F	210/249 (84%)	204 (97%)	6 (3%)	0	100	100
1	H	212/249 (85%)	205 (97%)	7 (3%)	0	100	100
2	A	219/219 (100%)	214 (98%)	5 (2%)	0	100	100
2	C	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
2	E	215/219 (98%)	211 (98%)	2 (1%)	2 (1%)	17	16
2	L	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
All	All	1697/1872 (91%)	1653 (97%)	42 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	51	VAL
2	E	68	GLY

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	B	182/218 (84%)	179 (98%)	3 (2%)	62	76
1	D	182/218 (84%)	180 (99%)	2 (1%)	73	85
1	F	185/218 (85%)	185 (100%)	0	100	100
1	H	187/218 (86%)	186 (100%)	1 (0%)	88	94
2	A	197/195 (101%)	196 (100%)	1 (0%)	88	94
2	C	195/195 (100%)	194 (100%)	1 (0%)	88	94
2	E	193/195 (99%)	193 (100%)	0	100	100
2	L	194/195 (100%)	193 (100%)	1 (0%)	88	94
All	All	1515/1652 (92%)	1506 (99%)	9 (1%)	86	93

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	162	SER
1	D	74	SER
2	C	33	LEU
1	B	186	SER
2	L	33	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	212	ASN

5.3.3 RNA

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](#)

67 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	$\# Z > 2$
5	1PE	B	308	-	6,6,15	0.62	0	5,5,14	0.26	0
4	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	B	311	-	12,12,15	0.75	0	11,11,14	0.25	0
4	SO4	L	306	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	L	307	2	12,12,15	0.74	0	11,11,14	0.24	0
5	1PE	B	309	-	11,11,15	0.78	0	10,10,14	0.23	0
3	GOL	A	303	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	C	302	-	5,5,5	0.38	0	5,5,5	0.28	0
5	1PE	F	313	-	6,6,15	0.63	0	5,5,14	0.26	0
4	SO4	F	312	5	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	D	304	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GOL	E	306	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	L	302	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	H	301	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	A	301	-	5,5,5	0.37	0	5,5,5	0.27	0
5	1PE	B	310	-	12,12,15	0.77	0	11,11,14	0.22	0
5	1PE	B	307	-	10,10,15	0.80	0	9,9,14	0.22	0
3	GOL	D	306	-	5,5,5	0.36	0	5,5,5	0.35	0
3	GOL	F	306	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	E	303	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	D	303	-	5,5,5	0.37	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	E	308	2	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	L	304	-	5,5,5	0.38	0	5,5,5	0.22	0
4	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	302	-	5,5,5	0.39	0	5,5,5	0.22	0
3	GOL	F	308	-	5,5,5	0.37	0	5,5,5	0.26	0
4	SO4	F	310	-	4,4,4	0.15	0	6,6,6	0.05	0
3	GOL	E	301	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	F	301	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	H	302	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	D	301	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	F	305	-	5,5,5	0.32	0	5,5,5	0.45	0
4	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	B	302	-	5,5,5	0.37	0	5,5,5	0.22	0
4	SO4	E	307	-	4,4,4	0.14	0	6,6,6	0.04	0
3	GOL	E	304	-	5,5,5	0.38	0	5,5,5	0.24	0
3	GOL	F	303	-	5,5,5	0.36	0	5,5,5	0.30	0
5	1PE	D	308	-	6,6,15	0.63	0	5,5,14	0.28	0
3	GOL	F	307	-	5,5,5	0.38	0	5,5,5	0.21	0
4	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	F	311	-	4,4,4	0.15	0	6,6,6	0.05	0
5	1PE	H	305	-	10,10,15	0.79	0	9,9,14	0.17	0
4	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	307	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	H	306	-	3,3,15	0.54	0	2,2,14	0.35	0
5	1PE	A	306	-	6,6,15	0.54	0	5,5,14	0.31	0
5	1PE	B	306	-	12,12,15	0.75	0	11,11,14	0.23	0
3	GOL	B	301	-	5,5,5	0.37	0	5,5,5	0.28	0
4	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	F	302	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	L	303	-	5,5,5	0.36	0	5,5,5	0.20	0
3	GOL	C	301	-	5,5,5	0.40	0	5,5,5	0.18	0
4	SO4	H	304	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	E	309	-	11,11,15	0.78	0	10,10,14	0.21	0
4	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	E	302	-	5,5,5	0.36	0	5,5,5	0.25	0
3	GOL	F	304	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	L	301	-	5,5,5	0.36	0	5,5,5	0.25	0
4	SO4	F	309	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	C	306	-	10,10,15	0.79	0	9,9,14	0.21	0
3	GOL	E	305	-	5,5,5	0.34	0	5,5,5	0.31	0
5	1PE	F	314	4	5,5,15	0.62	0	4,4,14	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	302	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	D	305	-	5,5,5	0.33	0	5,5,5	0.43	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
5	1PE	B	308	-	-	0/4/4/13	-
5	1PE	B	311	-	-	7/10/10/13	-
5	1PE	L	307	2	-	8/10/10/13	-
3	GOL	A	303	-	-	2/4/4/4	-
5	1PE	F	313	-	-	2/4/4/13	-
3	GOL	D	304	-	-	2/4/4/4	-
3	GOL	E	306	-	-	2/4/4/4	-
3	GOL	L	302	-	-	2/4/4/4	-
3	GOL	H	301	-	-	2/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
5	1PE	B	310	-	-	6/10/10/13	-
5	1PE	B	307	-	-	2/8/8/13	-
3	GOL	D	306	-	-	2/4/4/4	-
3	GOL	F	306	-	-	2/4/4/4	-
3	GOL	E	303	-	-	1/4/4/4	-
3	GOL	D	303	-	-	2/4/4/4	-
5	1PE	B	309	-	-	4/9/9/13	-
3	GOL	L	304	-	-	0/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	F	308	-	-	2/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
3	GOL	E	301	-	-	0/4/4/4	-
3	GOL	F	301	-	-	2/4/4/4	-
3	GOL	H	302	-	-	0/4/4/4	-
3	GOL	D	301	-	-	2/4/4/4	-
3	GOL	F	305	-	-	0/4/4/4	-
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	E	304	-	-	2/4/4/4	-
3	GOL	F	303	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	D	308	-	-	2/4/4/13	-
3	GOL	F	307	-	-	2/4/4/4	-
5	1PE	H	305	-	-	5/8/8/13	-
5	1PE	H	306	-	-	1/1/1/13	-
5	1PE	B	306	-	-	6/10/10/13	-
5	1PE	A	306	-	-	2/4/4/13	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	F	302	-	-	0/4/4/4	-
3	GOL	L	303	-	-	0/4/4/4	-
3	GOL	C	301	-	-	2/4/4/4	-
5	1PE	E	309	-	-	6/9/9/13	-
3	GOL	E	302	-	-	2/4/4/4	-
3	GOL	F	304	-	-	2/4/4/4	-
3	GOL	L	301	-	-	2/4/4/4	-
5	1PE	C	306	-	-	6/8/8/13	-
3	GOL	E	305	-	-	2/4/4/4	-
5	1PE	F	314	4	-	0/3/3/13	-
3	GOL	D	302	-	-	2/4/4/4	-
3	GOL	D	305	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	GOL	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-C3
3	D	304	GOL	O1-C1-C2-C3
3	A	301	GOL	O1-C1-C2-C3
3	D	306	GOL	O1-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	308	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	311	1PE	2	0
5	L	307	1PE	1	0
5	F	313	1PE	1	0
3	E	306	GOL	1	0
3	A	301	GOL	1	0
3	L	304	GOL	1	0
4	C	304	SO4	1	0
3	F	308	GOL	1	0
3	F	301	GOL	1	0
3	H	302	GOL	2	0
3	F	305	GOL	3	0
4	L	305	SO4	1	0
5	H	305	1PE	1	0
5	B	306	1PE	1	0
5	E	309	1PE	1	0
5	C	306	1PE	2	0
3	E	305	GOL	1	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, 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	B	207/249 (83%)	0.92	30 (14%) 2 2	23, 39, 89, 113	1 (0%)
1	D	208/249 (83%)	1.03	41 (19%) 1 1	26, 40, 90, 106	0
1	F	211/249 (84%)	0.40	12 (5%) 23 22	24, 39, 81, 121	0
1	H	211/249 (84%)	0.42	11 (5%) 27 26	24, 37, 83, 111	0
2	A	218/219 (99%)	0.18	2 (0%) 84 83	24, 35, 52, 90	0
2	C	218/219 (99%)	0.11	2 (0%) 84 83	23, 34, 52, 92	0
2	E	217/219 (99%)	0.34	8 (3%) 41 39	24, 38, 63, 92	0
2	L	218/219 (99%)	0.37	9 (4%) 37 35	24, 38, 66, 106	0
All	All	1708/1872 (91%)	0.46	115 (6%) 17 16	23, 37, 80, 121	1 (0%)

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	GLY	15.2
1	H	156	SER	9.2
1	F	128	CYS	8.3
1	H	157	GLY	7.7
1	B	29	PHE	6.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	1PE	L	307	13/16	0.44	0.56	51,59,86,88	0
5	1PE	F	314	6/16	0.48	0.40	72,77,89,95	0
5	1PE	B	309	12/16	0.59	0.32	58,69,72,72	0
5	1PE	B	307	11/16	0.64	0.32	76,79,80,81	0
3	GOL	D	304	6/6	0.64	0.31	89,89,90,90	0
4	SO4	F	312	5/5	0.66	0.39	103,107,108,109	0
5	1PE	B	310	13/16	0.66	0.37	55,63,64,64	0
5	1PE	B	306	13/16	0.66	0.27	64,72,76,77	0
3	GOL	E	302	6/6	0.67	0.25	54,60,63,63	0
3	GOL	A	303	6/6	0.67	0.30	64,68,70,72	0
5	1PE	C	306	11/16	0.68	0.31	59,61,66,67	0
5	1PE	H	305	11/16	0.69	0.29	65,70,73,74	0
3	GOL	E	303	6/6	0.69	0.25	73,74,79,79	0
3	GOL	L	303	6/6	0.70	0.47	79,81,82,84	0
3	GOL	H	302	6/6	0.71	0.54	73,74,75,77	0
5	1PE	F	313	7/16	0.74	0.26	62,68,69,71	0
3	GOL	E	304	6/6	0.74	0.22	77,79,79,79	0
3	GOL	F	307	6/6	0.74	0.17	60,61,62,62	0
3	GOL	F	306	6/6	0.74	0.39	67,70,71,71	0
3	GOL	F	305	6/6	0.76	0.48	39,41,48,52	0
3	GOL	L	301	6/6	0.77	0.29	87,87,88,88	0
3	GOL	A	301	6/6	0.77	0.30	66,69,71,73	0
4	SO4	E	308	5/5	0.77	0.31	76,85,87,88	0
4	SO4	H	304	5/5	0.78	0.24	111,111,112,112	0
3	GOL	D	302	6/6	0.78	0.20	61,65,65,67	0
4	SO4	F	311	5/5	0.79	0.27	103,104,105,106	0
4	SO4	B	304	5/5	0.79	0.29	127,127,127,128	0
3	GOL	L	304	6/6	0.79	0.25	50,59,62,62	0
5	1PE	B	311	13/16	0.79	0.29	44,60,68,68	0
5	1PE	E	309	12/16	0.79	0.23	56,61,63,63	0
3	GOL	E	305	6/6	0.81	0.26	68,68,71,73	0
3	GOL	A	302	6/6	0.81	0.26	75,75,76,76	0
4	SO4	L	306	5/5	0.81	0.39	117,118,118,118	0
3	GOL	C	301	6/6	0.82	0.24	32,37,42,43	0
5	1PE	D	308	7/16	0.82	0.30	73,74,75,76	0
5	1PE	B	308	7/16	0.83	0.23	43,45,56,57	0
3	GOL	C	302	6/6	0.83	0.30	71,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	1PE	A	306	7/16	0.83	0.29	65,66,70,71	0
3	GOL	F	303	6/6	0.83	0.26	71,72,74,74	0
3	GOL	E	306	6/6	0.84	0.32	69,70,71,72	0
3	GOL	F	304	6/6	0.85	0.17	57,59,63,65	0
4	SO4	A	305	5/5	0.85	0.23	102,103,103,104	0
3	GOL	D	303	6/6	0.86	0.31	73,78,79,80	0
4	SO4	B	305	5/5	0.86	0.48	112,112,112,113	0
4	SO4	C	304	5/5	0.86	0.32	102,102,104,105	0
5	1PE	H	306	4/16	0.87	0.14	61,61,62,62	0
4	SO4	L	305	5/5	0.87	0.26	116,117,117,118	0
4	SO4	C	303	5/5	0.87	0.23	73,76,77,81	0
3	GOL	F	301	6/6	0.87	0.16	55,61,64,66	0
4	SO4	H	303	5/5	0.87	0.64	115,116,116,117	0
3	GOL	F	302	6/6	0.87	0.44	64,69,70,71	0
3	GOL	D	305	6/6	0.87	0.27	37,39,44,47	0
3	GOL	D	306	6/6	0.88	0.21	41,52,58,61	0
3	GOL	B	302	6/6	0.88	0.19	64,65,66,67	0
4	SO4	A	304	5/5	0.90	0.18	81,82,83,86	0
3	GOL	B	301	6/6	0.90	0.17	34,39,45,49	0
3	GOL	H	301	6/6	0.90	0.20	64,65,66,67	0
4	SO4	E	307	5/5	0.90	0.26	113,113,114,114	0
3	GOL	L	302	6/6	0.91	0.26	66,68,70,72	0
4	SO4	C	305	5/5	0.91	0.16	95,95,96,96	0
3	GOL	E	301	6/6	0.92	0.30	35,35,41,42	0
3	GOL	F	308	6/6	0.93	0.29	70,70,72,74	0
4	SO4	F	310	5/5	0.94	0.12	86,88,89,90	0
3	GOL	D	301	6/6	0.94	0.15	30,31,32,33	0
4	SO4	D	307	5/5	0.94	0.25	99,99,100,101	0
4	SO4	B	303	5/5	0.95	0.20	102,102,102,103	0
4	SO4	F	309	5/5	0.96	0.14	65,65,67,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.