Full wwPDB X-ray Structure Validation Report (i)

May 13, 2024 – 12:13 PM EDT

PDB ID	:	8SFX
Title	:	High Affinity nanobodies against GFP
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Deposited on	:	2023-04-11
Resolution	:	1.95 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

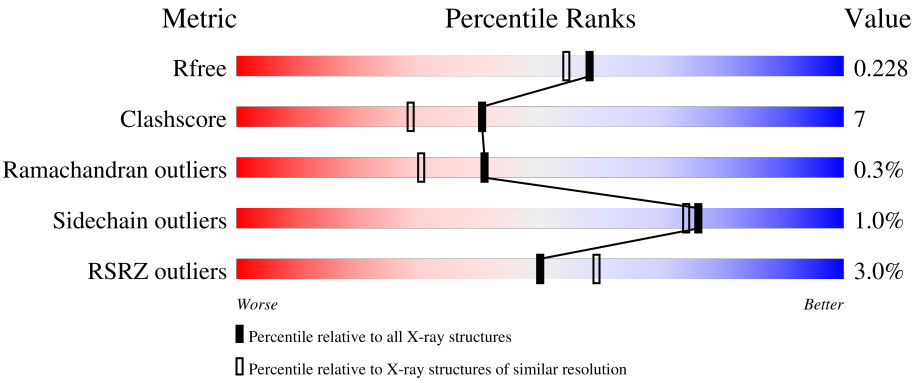
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	81% 7% • 10%
1	B	253	2% 84% 5% • 10%
2	C	142	5% 61% 20% • 16%
2	D	142	5% 64% 20% • 15%

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
6	PO4	A	308	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10879 atoms, of which 5191 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	0	0
			3561	1157	1745	307	346	6			
1	B	228	Total	C	H	N	O	S	1	0	0
			3544	1158	1725	308	347	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	insertion	UNP P42212
A	66	CR2	SER	chromophore	UNP P42212
A	66	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	72	ALA	SER	conflict	UNP P42212
A	177	HIS	GLN	conflict	UNP P42212
A	239	GLY	-	expression tag	UNP P42212
A	240	LEU	-	expression tag	UNP P42212
A	241	GLU	-	expression tag	UNP P42212
A	242	VAL	-	expression tag	UNP P42212
A	243	LEU	-	expression tag	UNP P42212
A	244	PHE	-	expression tag	UNP P42212
A	245	GLN	-	expression tag	UNP P42212
A	246	GLY	-	expression tag	UNP P42212
A	247	PRO	-	expression tag	UNP P42212
A	248	SER	-	expression tag	UNP P42212
A	249	HIS	-	expression tag	UNP P42212
A	250	HIS	-	expression tag	UNP P42212
A	251	HIS	-	expression tag	UNP P42212
A	252	HIS	-	expression tag	UNP P42212
A	253	HIS	-	expression tag	UNP P42212
A	254	HIS	-	expression tag	UNP P42212
B	1	ALA	-	insertion	UNP P42212
B	66	CR2	SER	chromophore	UNP P42212
B	66	CR2	TYR	chromophore	UNP P42212

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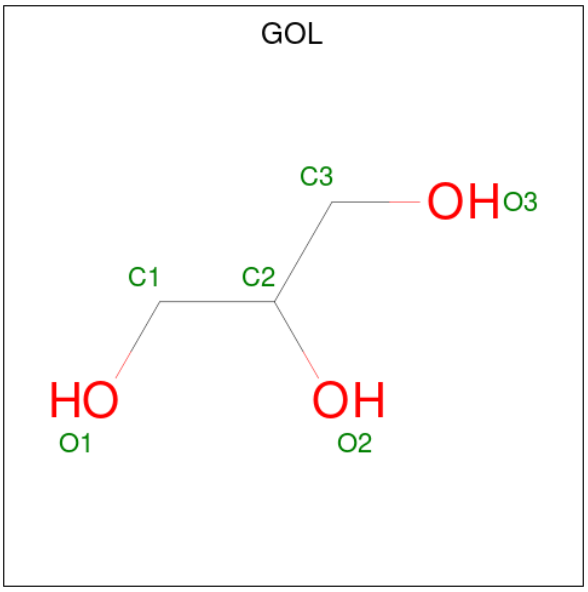
Chain	Residue	Modelled	Actual	Comment	Reference
B	66	CR2	GLY	chromophore	UNP P42212
B	72	ALA	SER	conflict	UNP P42212
B	177	HIS	GLN	conflict	UNP P42212
B	239	GLY	-	expression tag	UNP P42212
B	240	LEU	-	expression tag	UNP P42212
B	241	GLU	-	expression tag	UNP P42212
B	242	VAL	-	expression tag	UNP P42212
B	243	LEU	-	expression tag	UNP P42212
B	244	PHE	-	expression tag	UNP P42212
B	245	GLN	-	expression tag	UNP P42212
B	246	GLY	-	expression tag	UNP P42212
B	247	PRO	-	expression tag	UNP P42212
B	248	SER	-	expression tag	UNP P42212
B	249	HIS	-	expression tag	UNP P42212
B	250	HIS	-	expression tag	UNP P42212
B	251	HIS	-	expression tag	UNP P42212
B	252	HIS	-	expression tag	UNP P42212
B	253	HIS	-	expression tag	UNP P42212
B	254	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called LaG21.

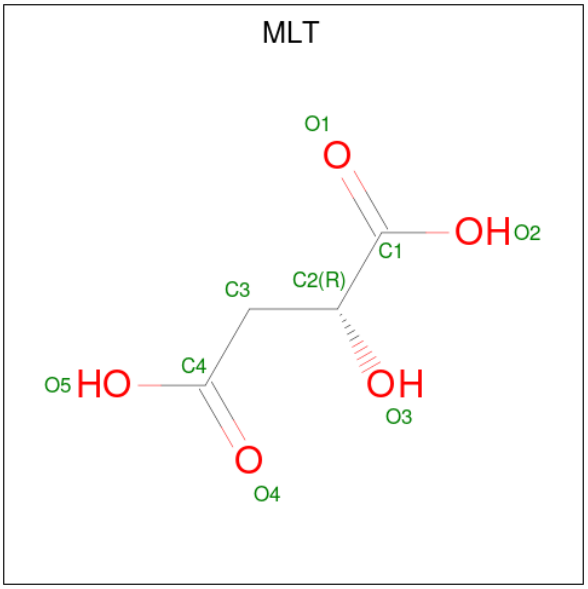
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	120	Total	C	H	N	O	S	6	0	0
			1740	558	838	160	179	5			
2	C	119	Total	C	H	N	O	S	17	0	0
			1738	560	835	160	178	5			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 14 3 8 3	0	0
3	A	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).

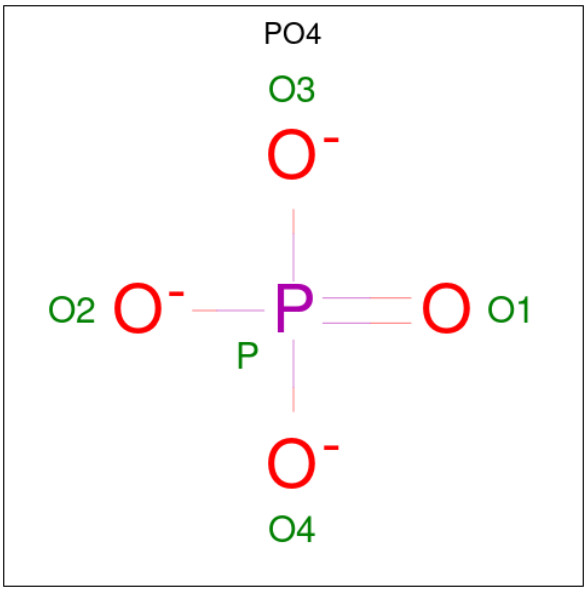


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 13 4 4 5	0	0
4	B	1	Total C H O 13 4 4 5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Na 4 4	0	0
5	B	10	Total Na 10 10	0	0
5	D	2	Total Na 2 2	0	0
5	C	3	Total Na 3 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0

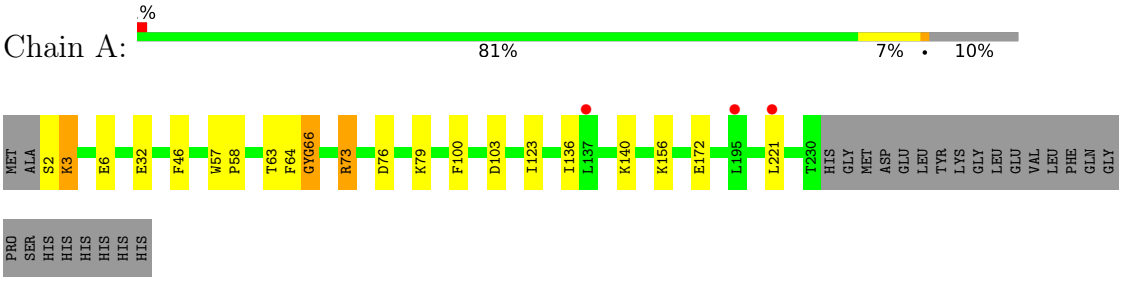
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	71	Total O 71 71	0	0
7	B	55	Total O 55 55	0	0
7	D	11	Total O 11 11	0	0
7	C	9	Total O 9 9	0	0

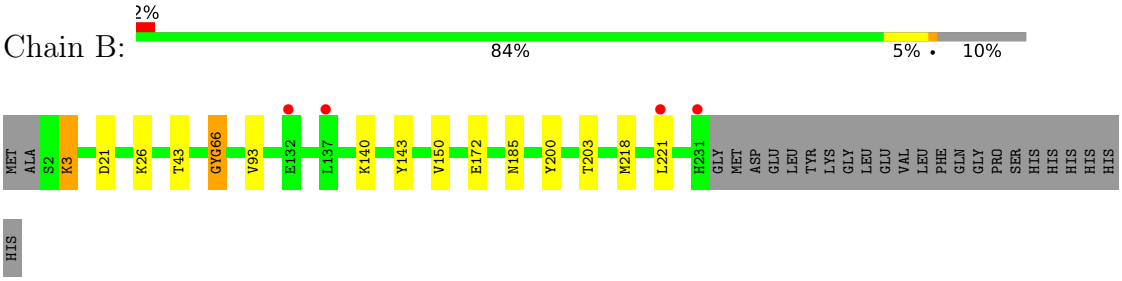
3 Residue-property plots (i)

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.

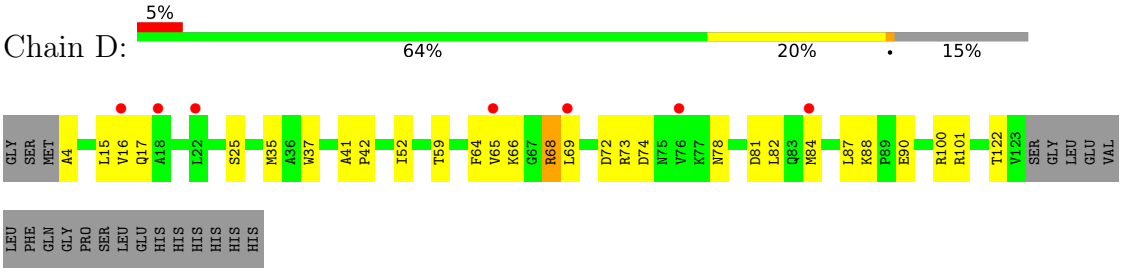
• Molecule 1: Green fluorescent protein



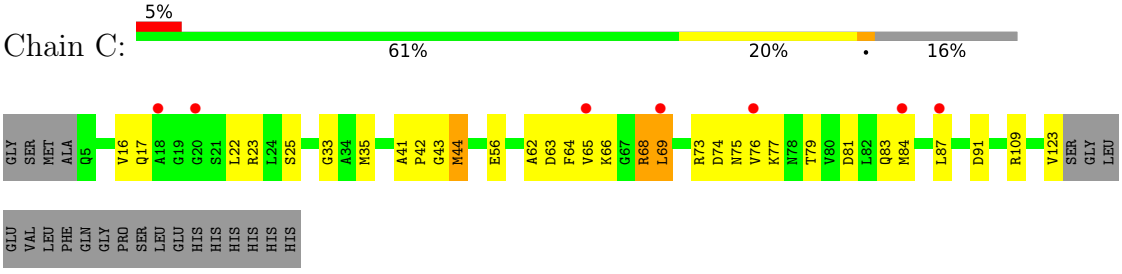
• Molecule 1: Green fluorescent protein



• Molecule 2: LaG21



• Molecule 2: LaG21



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	111.12Å 111.12Å 194.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.67 – 1.95 36.67 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.4 (36.67-1.95) 94.4 (36.67-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.210 , 0.228 0.210 , 0.228	Depositor DCC
R_{free} test set	1991 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10879	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, PO4, MLT, GOL, NA

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	0.63	1/1839 (0.1%)	0.68	1/2485 (0.0%)
1	B	0.61	0/1843	0.67	0/2493
2	C	0.56	0/919	0.95	1/1245 (0.1%)
2	D	0.53	0/918	0.70	0/1245
All	All	0.60	1/5519 (0.0%)	0.73	2/7468 (0.0%)

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
2	C	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CB-CG	-5.19	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	69	LEU	CB-CG-CD2	22.25	148.83	111.00
1	A	221	LEU	CB-CG-CD1	5.01	119.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	68	ARG	Sidechain
2	D	68	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	1745	1755	15	0
1	B	1819	1725	1742	10	0
2	C	903	835	860	35	0
2	D	902	838	847	17	0
3	A	12	16	16	0	0
3	B	12	16	16	0	0
3	C	6	8	8	1	0
4	A	9	4	4	0	0
4	B	9	4	4	0	0
5	A	4	0	0	0	0
5	B	10	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
6	A	10	0	0	2	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	10	0	0	0	0
7	A	71	0	0	1	0
7	B	55	0	0	0	0
7	C	9	0	0	0	0
7	D	11	0	0	0	0
All	All	5688	5191	5252	77	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 (77) 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:C:23:ARG:HD2	2:C:83:GLN:HG3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:VAL:HG21	2:C:22:LEU:HG	1.70	0.74
1:A:156:LYS:HD2	1:A:156:LYS:H	1.52	0.73
1:B:21:ASP:OD2	1:B:26:LYS:NZ	2.20	0.73
2:C:56:GLU:OE2	2:C:75:ASN:ND2	2.23	0.72
2:D:15:LEU:HD23	2:D:122:THR:HB	1.76	0.68
2:C:25:SER:OG	2:C:81:ASP:OD1	2.11	0.68
2:C:65:VAL:CG1	2:C:69:LEU:HD12	2.26	0.64
2:C:65:VAL:HG12	2:C:69:LEU:CD1	2.27	0.64
2:C:64:PHE:CE1	2:C:65:VAL:HG13	2.33	0.63
2:D:64:PHE:CE1	2:D:65:VAL:HG13	2.33	0.63
2:C:69:LEU:HD22	2:C:84:MET:HA	1.81	0.61
1:A:3:LYS:H	1:A:3:LYS:HD2	1.65	0.60
1:A:103:ASP:OD2	7:A:401:HOH:O	2.16	0.60
1:A:156:LYS:H	1:A:156:LYS:CD	2.14	0.60
2:C:68:ARG:NH2	2:C:91:ASP:OD2	2.33	0.60
2:D:41:ALA:HB1	2:D:42:PRO:HD2	1.85	0.59
2:C:41:ALA:HB1	2:C:42:PRO:HD2	1.84	0.59
2:D:25:SER:OG	2:D:81:ASP:OD1	2.15	0.56
2:C:65:VAL:CG1	2:C:69:LEU:CD1	2.83	0.55
2:D:84:MET:HB2	2:D:87:LEU:HD21	1.89	0.55
2:C:16:VAL:HG21	2:C:22:LEU:CG	2.36	0.55
1:B:3:LYS:H	1:B:3:LYS:HD2	1.72	0.54
2:D:65:VAL:CG1	2:D:69:LEU:HD22	2.40	0.52
2:C:65:VAL:HG12	2:C:69:LEU:HD12	1.86	0.51
2:D:68:ARG:HB2	2:D:69:LEU:HD13	1.92	0.51
2:C:65:VAL:HB	2:C:69:LEU:HD12	1.93	0.51
2:D:68:ARG:C	2:D:69:LEU:HD12	2.31	0.51
2:D:16:VAL:HG12	2:D:17:GLN:N	2.25	0.51
2:C:16:VAL:HG12	2:C:17:GLN:N	2.27	0.50
2:C:43:GLY:H	2:C:44:MET:HE1	1.77	0.50
1:A:73:ARG:NH2	6:A:308:PO4:O2	2.42	0.50
2:D:88:LYS:HB2	2:D:90:GLU:OE1	2.13	0.48
1:B:140:LYS:O	1:B:172:GLU:HG2	2.14	0.48
2:C:109:ARG:HH12	3:C:201:GOL:H12	1.78	0.48
2:C:74:ASP:OD1	2:C:76:VAL:HG13	2.13	0.48
1:B:21:ASP:HB2	1:B:26:LYS:HZ2	1.78	0.48
2:D:68:ARG:O	2:D:69:LEU:HD12	2.14	0.47
1:A:140:LYS:O	1:A:172:GLU:HG2	2.15	0.47
2:C:65:VAL:CB	2:C:69:LEU:HD12	2.43	0.47
2:C:64:PHE:CD1	2:C:65:VAL:HG13	2.50	0.47
1:B:66:CR2:CE1	1:B:203:THR:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:TRP:CD1	2:D:82:LEU:HD12	2.50	0.46
1:A:100:PHE:CD2	1:A:136:ILE:HD11	2.51	0.46
2:C:77:LYS:HB3	2:C:79:THR:HG23	1.97	0.46
2:C:84:MET:HB3	2:C:87:LEU:HD21	1.98	0.46
2:C:16:VAL:O	2:C:123:VAL:HA	2.15	0.45
2:C:84:MET:CB	2:C:87:LEU:HD21	2.46	0.45
2:C:33:GLY:O	2:C:73:ARG:NH1	2.42	0.45
1:B:66:CR2:CZ	1:B:203:THR:HG21	2.47	0.44
1:A:76:ASP:HA	1:A:79:LYS:HG2	1.99	0.44
2:D:52:ILE:CD1	2:D:59:THR:OG1	2.66	0.44
1:A:79:LYS:HD2	1:A:79:LYS:HA	1.85	0.44
2:C:41:ALA:HB1	2:C:42:PRO:CD	2.48	0.44
2:C:35:MET:HG3	2:C:73:ARG:NH1	2.32	0.44
2:C:62:ALA:O	2:C:65:VAL:HG23	2.18	0.43
2:C:16:VAL:CG2	2:C:22:LEU:HD21	2.48	0.43
1:A:66:CR2:N2	1:A:66:CR2:HD1	2.33	0.43
2:C:69:LEU:HD22	2:C:84:MET:HG2	2.00	0.43
2:C:69:LEU:CD2	2:C:84:MET:HA	2.46	0.43
2:D:4:ALA:O	2:D:101:ARG:NH1	2.52	0.42
1:A:63:THR:CG2	1:A:123:ILE:HG21	2.50	0.42
1:B:43:THR:HG22	1:B:221:LEU:HG	2.01	0.42
1:B:150:VAL:O	1:B:200:TYR:HA	2.20	0.41
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.55	0.41
2:D:74:ASP:O	2:D:78:ASN:N	2.54	0.41
2:D:35:MET:HG3	2:D:73:ARG:NH1	2.36	0.41
2:C:16:VAL:HG23	2:C:22:LEU:HD11	2.01	0.41
2:C:63:ASP:N	2:C:63:ASP:OD1	2.54	0.41
1:A:2:SER:O	1:A:6:GLU:HB2	2.21	0.41
2:D:88:LYS:CB	2:D:90:GLU:OE1	2.69	0.41
2:C:65:VAL:HG12	2:C:69:LEU:HD11	1.98	0.41
1:A:57:TRP:N	1:A:58:PRO:CD	2.84	0.40
2:C:35:MET:HG3	2:C:73:ARG:CZ	2.51	0.40
1:B:93:VAL:O	1:B:185:ASN:HA	2.21	0.40
1:A:73:ARG:NH1	6:A:308:PO4:O2	2.53	0.40
1:B:143:TYR:OH	1:B:218:MET:HG3	2.21	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	222/253 (88%)	219 (99%)	3 (1%)	0	100 100
1	B	223/253 (88%)	220 (99%)	3 (1%)	0	100 100
2	C	117/142 (82%)	112 (96%)	4 (3%)	1 (1%)	17 8
2	D	118/142 (83%)	114 (97%)	3 (2%)	1 (1%)	19 9
All	All	680/790 (86%)	665 (98%)	13 (2%)	2 (0%)	41 30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	66	LYS
2	D	66	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	197/219 (90%)	195 (99%)	2 (1%)	76 74
1	B	196/219 (90%)	195 (100%)	1 (0%)	88 88
2	C	93/113 (82%)	92 (99%)	1 (1%)	73 71
2	D	91/113 (80%)	89 (98%)	2 (2%)	52 44
All	All	577/664 (87%)	571 (99%)	6 (1%)	76 74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	73	ARG
1	B	3	LYS
2	D	72	ASP
2	D	100	ARG
2	C	44	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CR2	A	66	1	20,20,21	2.55	7 (35%)	25,27,29	2.38	8 (32%)
1	CR2	B	66	5,1	20,20,21	2.69	7 (35%)	25,27,29	2.18	7 (28%)

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
1	CR2	A	66	1	-	1/6/25/26	0/2/2/2
1	CR2	B	66	5,1	-	1/6/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CR2	CA2-C2	6.19	1.54	1.48
1	B	66	CR2	C1-N3	5.47	1.45	1.37
1	A	66	CR2	C1-N3	5.24	1.45	1.37
1	A	66	CR2	CA2-C2	4.80	1.53	1.48
1	A	66	CR2	CB2-CA2	-4.67	1.31	1.35
1	B	66	CR2	C1-N2	4.43	1.40	1.32
1	B	66	CR2	CB2-CA2	-4.35	1.31	1.35
1	A	66	CR2	C1-N2	3.95	1.39	1.32
1	A	66	CR2	CG2-CB2	3.54	1.53	1.46
1	B	66	CR2	CG2-CB2	3.20	1.53	1.46
1	B	66	CR2	C2-N3	3.11	1.47	1.39
1	A	66	CR2	C2-N3	2.95	1.46	1.39
1	B	66	CR2	CA2-N2	2.90	1.44	1.38
1	A	66	CR2	CA1-C1	2.84	1.52	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CR2	O2-C2-CA2	-6.76	127.17	130.96
1	B	66	CR2	O2-C2-CA2	-5.94	127.62	130.96
1	A	66	CR2	CA2-C2-N3	4.89	105.69	103.37
1	B	66	CR2	CA2-C2-N3	4.43	105.47	103.37
1	A	66	CR2	O3-C3-CA3	-4.20	113.72	126.39
1	B	66	CR2	O3-C3-CA3	-3.97	114.41	126.39
1	A	66	CR2	C2-N3-C1	-3.55	106.25	107.99
1	B	66	CR2	C1-CA1-N1	-3.30	105.56	112.85
1	B	66	CR2	CA3-N3-C1	-2.91	123.84	127.86
1	A	66	CR2	CA3-N3-C1	-2.78	124.02	127.86
1	B	66	CR2	C2-N3-C1	-2.72	106.66	107.99
1	A	66	CR2	C1-CA1-N1	-2.62	107.05	112.85
1	A	66	CR2	CA3-N3-C2	2.58	129.72	123.80
1	B	66	CR2	CA3-N3-C2	2.48	129.49	123.80
1	A	66	CR2	CG2-CB2-CA2	-2.08	127.40	129.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CR2	C3-CA3-N3-C2
1	B	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CR2	1	0
1	B	66	CR2	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 19 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
3	GOL	B	301	-	5,5,5	0.83	0	5,5,5	0.98	0
6	PO4	A	308	-	4,4,4	1.18	0	6,6,6	0.49	0
6	PO4	B	315	-	4,4,4	0.72	0	6,6,6	0.57	0
3	GOL	A	302	5	5,5,5	0.83	0	5,5,5	1.06	0
4	MLT	B	303	-	8,8,8	1.00	0	10,10,10	1.60	1 (10%)
6	PO4	B	314	-	4,4,4	0.96	0	6,6,6	0.43	0
3	GOL	A	301	-	5,5,5	0.86	0	5,5,5	0.93	0
6	PO4	A	309	-	4,4,4	0.73	0	6,6,6	0.46	0
3	GOL	C	201	-	5,5,5	0.89	0	5,5,5	1.10	0
6	PO4	D	204	-	4,4,4	0.83	0	6,6,6	0.26	0
3	GOL	B	302	5	5,5,5	0.63	0	5,5,5	0.98	0
4	MLT	A	303	-	8,8,8	0.96	0	10,10,10	1.63	2 (20%)
6	PO4	D	203	-	4,4,4	0.99	0	6,6,6	0.31	0
6	PO4	C	205	5	4,4,4	0.80	0	6,6,6	0.38	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
3	GOL	B	301	-	-	0/4/4/4	-
3	GOL	A	302	5	-	3/4/4/4	-
4	MLT	B	303	-	-	6/8/8/8	-
3	GOL	A	301	-	-	1/4/4/4	-
3	GOL	C	201	-	-	2/4/4/4	-
3	GOL	B	302	5	-	2/4/4/4	-
4	MLT	A	303	-	-	2/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	303	MLT	O2-C1-C2	3.49	120.40	112.72
4	A	303	MLT	O2-C1-C2	3.46	120.33	112.72
4	A	303	MLT	O5-C4-C3	2.24	121.24	114.07

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
4	A	303	MLT	C1-C2-C3-C4
4	A	303	MLT	O3-C2-C3-C4
4	B	303	MLT	O1-C1-C2-O3
4	B	303	MLT	O2-C1-C2-O3
3	C	201	GOL	C1-C2-C3-O3
3	B	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
4	B	303	MLT	O1-C1-C2-C3
4	B	303	MLT	O2-C1-C2-C3
3	C	201	GOL	O2-C2-C3-O3
4	B	303	MLT	O3-C2-C3-C4
3	A	301	GOL	O2-C2-C3-O3
4	B	303	MLT	C2-C3-C4-O5
3	A	302	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	308	PO4	2	0
3	C	201	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, 95^{th} 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	226/253 (89%)	0.38	3 (1%)	77	83	30, 45, 69, 87	0
1	B	227/253 (89%)	0.42	4 (1%)	68	76	30, 45, 69, 111	0
2	C	119/142 (83%)	0.60	7 (5%)	22	30	37, 56, 84, 98	2 (1%)
2	D	120/142 (84%)	0.63	7 (5%)	23	31	36, 56, 87, 100	1 (0%)
All	All	692/790 (87%)	0.48	21 (3%)	50	59	30, 48, 78, 111	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	65	VAL	4.5
2	D	69	LEU	4.2
2	D	76	VAL	4.1
2	C	69	LEU	4.1
2	C	76	VAL	3.4
2	D	65	VAL	3.1
1	B	231	HIS	2.6
2	C	18	ALA	2.6
1	A	195	LEU	2.5
2	D	22	LEU	2.5
2	C	84	MET	2.3
2	D	16	VAL	2.3
1	B	221	LEU	2.3
1	B	137	LEU	2.3
2	C	20	GLY	2.2
2	D	84	MET	2.2
2	C	87	LEU	2.2
2	D	18	ALA	2.1
1	A	137	LEU	2.1
1	A	221	LEU	2.0
1	B	132	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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
1	CR2	A	66	19/20	0.97	0.14	31,39,47,48	0
1	CR2	B	66	19/20	0.97	0.14	32,38,47,47	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MLT	B	303	9/9	0.59	0.16	87,101,122,129	0
4	MLT	A	303	9/9	0.63	0.21	74,98,128,128	0
6	PO4	B	315	5/5	0.78	0.15	79,86,110,121	0
6	PO4	A	309	5/5	0.79	0.21	82,90,115,125	0
3	GOL	A	301	6/6	0.83	0.31	65,96,119,125	0
3	GOL	B	301	6/6	0.83	0.26	63,83,102,122	0
3	GOL	A	302	6/6	0.84	0.21	63,83,100,100	0
3	GOL	B	302	6/6	0.84	0.19	71,91,112,112	0
6	PO4	D	204	5/5	0.84	0.18	93,103,125,131	0
5	NA	A	305	1/1	0.85	0.20	58,58,58,58	0
6	PO4	C	205	5/5	0.86	0.12	96,98,120,125	0
5	NA	B	309	1/1	0.88	0.19	63,63,63,63	0
5	NA	B	306	1/1	0.90	0.24	57,57,57,57	0
5	NA	B	313	1/1	0.91	0.10	52,52,52,52	0
5	NA	C	204	1/1	0.91	0.28	66,66,66,66	0
5	NA	C	202	1/1	0.92	0.22	56,56,56,56	0
5	NA	B	304	1/1	0.94	0.16	60,60,60,60	0
3	GOL	C	201	6/6	0.95	0.11	65,78,88,89	0
6	PO4	A	308	5/5	0.95	0.15	67,77,92,95	0
6	PO4	B	314	5/5	0.96	0.13	71,77,90,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	D	202	1/1	0.96	0.16	49,49,49,49	0
5	NA	C	203	1/1	0.97	0.12	45,45,45,45	0
5	NA	A	304	1/1	0.97	0.12	42,42,42,42	0
5	NA	B	305	1/1	0.98	0.09	43,43,43,43	0
5	NA	B	310	1/1	0.98	0.10	40,40,40,40	0
5	NA	B	311	1/1	0.98	0.17	55,55,55,55	0
6	PO4	D	203	5/5	0.98	0.12	71,80,91,99	0
5	NA	A	307	1/1	0.98	0.13	32,32,32,32	1
5	NA	D	201	1/1	0.98	0.12	43,43,43,43	0
5	NA	B	307	1/1	0.99	0.12	45,45,45,45	0
5	NA	B	308	1/1	0.99	0.15	30,30,30,30	1
5	NA	B	312	1/1	0.99	0.10	52,52,52,52	0
5	NA	A	306	1/1	0.99	0.11	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.