



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 09:29 PM UTC

PDB ID : 8SFZ / pdb_00008sfz
Title : High Affinity nanobodies against GFP
Authors : Ketaren, N.E.; Rout, M.P.; Bonanno, J.B.; Almo, S.C.
Deposited on : 2023-04-11
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

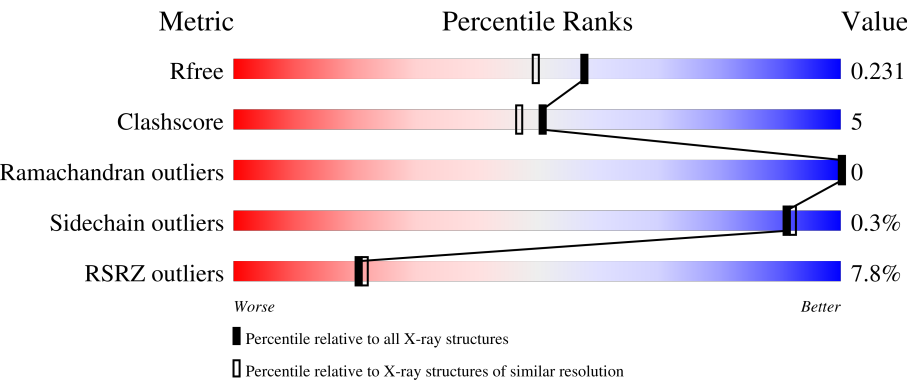
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 $\leq 5\%$. 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	145	17% 79%6%15%
1	B	145	79%10%12%
1	C	145	2% 79%9%11%
2	D	253	2% 81%9%10%
2	F	253	13% 78%11%11%

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Mol	Chain	Length	Quality of chain
3	E	253	6% 80% 9% 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16608 atoms, of which 7856 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 LaG35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	129	Total	C	H	N	O	S	0	0	0
			1941	629	942	172	194	4			
1	A	123	Total	C	H	N	O	S	0	0	0
			1845	596	893	166	186	4			
1	B	128	Total	C	H	N	O	S	0	0	0
			1910	617	924	172	192	5			

- Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	228	Total	C	H	N	O	S	0	0	0
			3534	1154	1724	306	344	6			
2	F	226	Total	C	H	N	O	S	0	0	0
			3470	1145	1679	303	337	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	insertion	UNP P42212
D	66	CR2	SER	chromophore	UNP P42212
D	66	CR2	TYR	chromophore	UNP P42212
D	66	CR2	GLY	chromophore	UNP P42212
D	72	ALA	SER	conflict	UNP P42212
D	177	HIS	GLN	conflict	UNP P42212
D	239	GLY	-	expression tag	UNP P42212
D	240	LEU	-	expression tag	UNP P42212
D	241	GLU	-	expression tag	UNP P42212
D	242	VAL	-	expression tag	UNP P42212
D	243	LEU	-	expression tag	UNP P42212
D	244	PHE	-	expression tag	UNP P42212
D	245	GLN	-	expression tag	UNP P42212
D	246	GLY	-	expression tag	UNP P42212

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

- Molecule 3 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	227	Total	C	H	N	O	S	0	0	0
			3497	1152	1694	307	338	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ALA	-	insertion	UNP P42212
E	66	CRO	SER	chromophore	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	66	CRO	TYR	chromophore	UNP P42212
E	66	CRO	GLY	chromophore	UNP P42212
E	72	ALA	SER	conflict	UNP P42212
E	177	HIS	GLN	conflict	UNP P42212
E	240	GLY	-	expression tag	UNP P42212
E	241	LEU	-	expression tag	UNP P42212
E	242	GLU	-	expression tag	UNP P42212
E	243	VAL	-	expression tag	UNP P42212
E	244	LEU	-	expression tag	UNP P42212
E	245	PHE	-	expression tag	UNP P42212
E	246	GLN	-	expression tag	UNP P42212
E	247	GLY	-	expression tag	UNP P42212
E	248	PRO	-	expression tag	UNP P42212
E	249	SER	-	expression tag	UNP P42212
E	250	HIS	-	expression tag	UNP P42212
E	251	HIS	-	expression tag	UNP P42212
E	252	HIS	-	expression tag	UNP P42212
E	253	HIS	-	expression tag	UNP P42212
E	254	HIS	-	expression tag	UNP P42212
E	255	HIS	-	expression tag	UNP P42212

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0

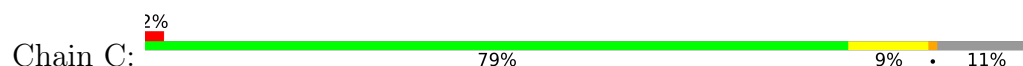
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	63	Total 63	O 63	0	0
6	A	77	Total 77	O 77	0	0
6	B	40	Total 40	O 40	0	0
6	D	97	Total 97	O 97	0	0
6	E	73	Total 73	O 73	0	0
6	F	56	Total 56	O 56	0	0

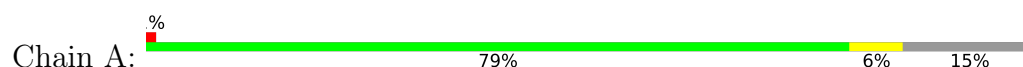
3 Residue-property plots [i](#)

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.

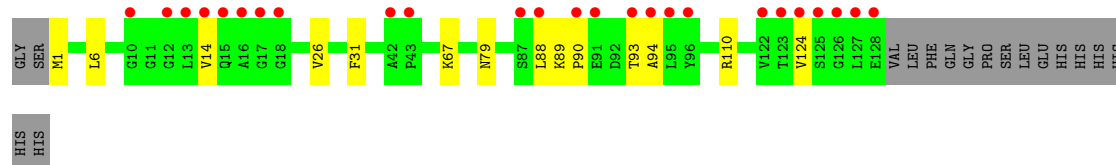
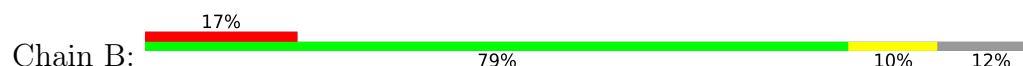
- Molecule 1: LaG35



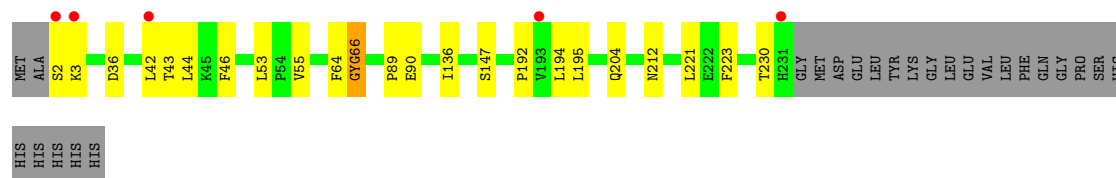
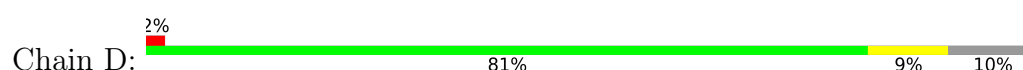
- Molecule 1: LaG35



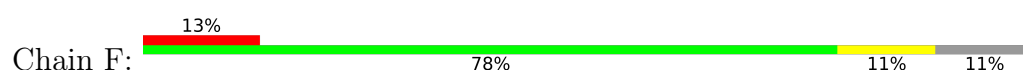
- Molecule 1: LaG35

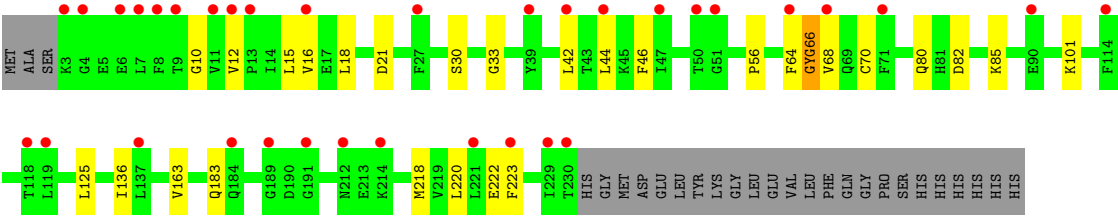


- Molecule 2: Green fluorescent protein

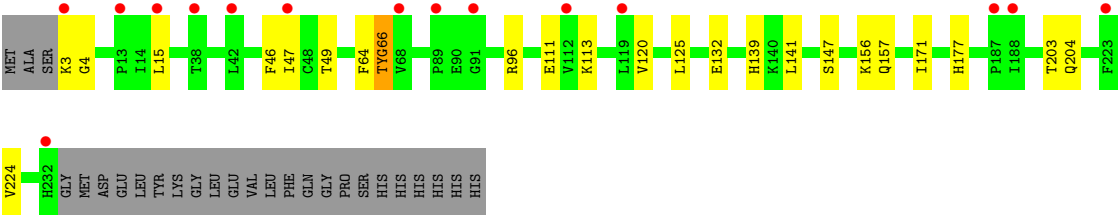
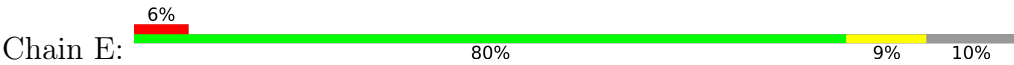


- Molecule 2: Green fluorescent protein





• Molecule 3: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	69.65Å 101.73Å 184.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 1.90 46.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.10-1.90) 99.3 (46.10-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.207 , 0.231 0.207 , 0.231	Depositor DCC
R_{free} test set	1999 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16608	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: CRO, NA, CR2, K

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	0.58	0/973	0.66	0/1317
1	B	0.50	0/1007	0.61	0/1362
1	C	0.61	1/1021 (0.1%)	0.66	0/1382
2	D	0.57	0/1833	0.63	0/2479
2	F	0.44	0/1814	0.51	0/2453
3	E	0.50	0/1827	0.58	0/2470
All	All	0.53	1/8475 (0.0%)	0.60	0/11463

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
3	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	MET	SD-CE	-8.25	1.58	1.79

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	96	ARG	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	952	893	893	7	0
1	B	986	924	932	12	0
1	C	999	942	942	9	0
2	D	1810	1724	1737	20	0
2	F	1791	1679	1719	24	0
3	E	1803	1694	1735	17	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	77	0	0	1	0
6	B	40	0	0	0	0
6	C	63	0	0	1	0
6	D	97	0	0	1	0
6	E	73	0	0	3	0
6	F	56	0	0	1	0
All	All	8752	7856	7958	83	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 (83) 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:F:70:CYS:O	2:F:85:LYS:NZ	2.01	0.93
1:C:21:LEU:HG	1:C:84:MET:HE2	1.56	0.87
1:A:101:ARG:NH1	1:B:1:MET:O	2.10	0.84
2:F:82:ASP:OD2	2:F:85:LYS:HD2	1.88	0.74
1:B:6:LEU:HD22	1:B:26:VAL:HG22	1.71	0.73
3:E:111:GLU:OE1	3:E:113:LYS:NZ	2.23	0.72
3:E:171:ILE:HD11	3:E:177:HIS:HB2	1.75	0.67
1:B:93:THR:HG22	1:B:124:VAL:H	1.58	0.66
1:A:13:VAL:HG11	1:A:87:LEU:HD13	1.78	0.65
2:F:101:LYS:NZ	6:F:401:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:MET:HE3	2:F:220:LEU:HB2	1.82	0.61
1:B:89:LYS:O	1:B:124:VAL:HG11	2.01	0.60
2:D:36:ASP:OD1	6:D:401:HOH:O	2.16	0.58
1:A:19:LEU:HD22	1:A:87:LEU:HD11	1.85	0.58
2:F:46:PHE:CZ	2:F:64:PHE:HB3	2.39	0.57
3:E:15:LEU:HD12	3:E:120:VAL:HG13	1.85	0.57
1:B:110:ARG:NH2	2:D:195:LEU:O	2.38	0.56
2:F:33:GLY:HA3	2:F:44:LEU:HD23	1.87	0.55
3:E:3:LYS:HG3	3:E:4:GLY:N	2.23	0.54
1:C:78:ASN:OD1	2:D:230:THR:HG21	2.08	0.54
2:D:90:GLU:CD	2:D:90:GLU:H	2.15	0.54
2:D:2:SER:OG	2:D:3:LYS:N	2.39	0.53
3:E:47:ILE:HD11	3:E:49:THR:HG22	1.91	0.53
3:E:132:GLU:OE1	6:E:301:HOH:O	2.18	0.53
1:A:13:VAL:HG11	1:A:87:LEU:CD1	2.37	0.53
1:B:93:THR:O	1:B:94:ALA:HB2	2.09	0.53
1:B:89:LYS:HB3	1:B:90:PRO:CD	2.39	0.52
3:E:47:ILE:HD12	3:E:47:ILE:C	2.33	0.52
1:C:35:MET:HE1	1:C:99:ALA:HB2	1.92	0.52
2:F:66:CR2:HD2	2:F:66:CR2:N2	2.24	0.52
3:E:147:SER:OG	3:E:204:GLN:HG2	2.10	0.52
1:B:67:LYS:HE2	2:D:192:PRO:O	2.11	0.51
2:D:42:LEU:C	2:D:42:LEU:HD23	2.35	0.51
2:F:223:PHE:CD1	2:F:223:PHE:N	2.79	0.51
2:D:42:LEU:HD21	2:D:44:LEU:CD1	2.41	0.51
1:B:6:LEU:CD2	1:B:26:VAL:HG22	2.40	0.50
1:C:76:ALA:O	2:D:230:THR:HG22	2.11	0.49
1:A:104:ASP:HB2	6:A:359:HOH:O	2.13	0.49
2:F:44:LEU:HD13	2:F:46:PHE:CZ	2.47	0.49
1:B:110:ARG:HD3	2:D:194:LEU:HD22	1.95	0.49
2:F:42:LEU:HD21	2:F:44:LEU:HD12	1.94	0.49
3:E:139:HIS:HD2	6:E:369:HOH:O	1.96	0.48
2:F:18:LEU:C	2:F:18:LEU:HD23	2.39	0.48
2:F:56:PRO:HD3	2:F:136:ILE:O	2.14	0.48
2:F:82:ASP:CG	2:F:85:LYS:HD2	2.38	0.48
2:D:42:LEU:HD21	2:D:44:LEU:HD12	1.96	0.47
1:C:21:LEU:CG	1:C:84:MET:HE2	2.38	0.47
2:D:147:SER:OG	2:D:204:GLN:HG2	2.15	0.47
1:B:14:VAL:HG11	1:B:88:LEU:HD13	1.96	0.47
2:F:44:LEU:HD13	2:F:46:PHE:HZ	1.77	0.47
1:A:69:PHE:CZ	1:A:84:MET:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:LEU:HD21	2:F:44:LEU:CD1	2.45	0.47
3:E:66:CRO:HD1	3:E:66:CRO:N2	2.30	0.46
2:D:53:LEU:HD23	2:D:55:VAL:O	2.16	0.46
1:C:23:CYS:HB3	1:C:80:VAL:HG13	1.97	0.45
2:F:10:GLY:O	2:F:12:VAL:HG23	2.17	0.45
2:F:80:GLN:OE1	2:F:80:GLN:N	2.43	0.45
2:F:42:LEU:C	2:F:42:LEU:HD23	2.43	0.44
1:C:69:PHE:HA	1:C:83:GLN:O	2.17	0.44
1:C:13:VAL:HG11	1:C:19:LEU:HG	1.99	0.44
1:C:104:ASP:HB2	6:C:333:HOH:O	2.17	0.44
3:E:46:PHE:CZ	3:E:64:PHE:HB3	2.52	0.44
2:F:15:LEU:HD13	2:F:16:VAL:N	2.32	0.44
2:D:212:ASN:C	2:D:212:ASN:OD1	2.60	0.43
2:D:46:PHE:CZ	2:D:64:PHE:HB3	2.53	0.43
2:D:66:CR2:HD2	2:D:66:CR2:N2	2.33	0.43
2:F:68:VAL:HG23	2:F:68:VAL:O	2.18	0.43
2:F:222:GLU:C	2:F:223:PHE:CD1	2.96	0.43
2:D:89:PRO:HD2	2:D:90:GLU:OE2	2.19	0.43
3:E:125:LEU:C	3:E:125:LEU:HD23	2.44	0.42
2:F:21:ASP:OD1	2:F:21:ASP:C	2.61	0.42
1:A:19:LEU:CD2	1:A:87:LEU:HD11	2.49	0.42
3:E:15:LEU:CD2	6:E:304:HOH:O	2.66	0.42
2:F:163:VAL:HB	2:F:183:GLN:HB3	2.00	0.42
2:D:221:LEU:HD21	2:D:223:PHE:HE2	1.84	0.42
3:E:47:ILE:HD11	3:E:49:THR:CG2	2.50	0.42
2:F:125:LEU:C	2:F:125:LEU:HD23	2.45	0.41
3:E:203:THR:HG23	3:E:224:VAL:HG22	2.03	0.41
2:D:136:ILE:N	2:D:136:ILE:HD12	2.35	0.41
2:D:42:LEU:HD23	2:D:43:THR:N	2.36	0.40
3:E:156:LYS:O	3:E:157:GLN:C	2.63	0.40
1:B:31:PHE:CD2	1:B:79:ASN:HA	2.56	0.40
3:E:141:LEU:CD2	3:E:171:ILE:CD1	3.00	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	121/145 (83%)	120 (99%)	1 (1%)	0	100	100
1	B	126/145 (87%)	119 (94%)	7 (6%)	0	100	100
1	C	127/145 (88%)	125 (98%)	2 (2%)	0	100	100
2	D	223/253 (88%)	221 (99%)	2 (1%)	0	100	100
2	F	221/253 (87%)	211 (96%)	10 (4%)	0	100	100
3	E	222/253 (88%)	218 (98%)	4 (2%)	0	100	100
All	All	1040/1194 (87%)	1014 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/116 (84%)	96 (99%)	1 (1%)	73	74
1	B	100/116 (86%)	100 (100%)	0	100	100
1	C	102/116 (88%)	101 (99%)	1 (1%)	73	74
2	D	194/219 (89%)	194 (100%)	0	100	100
2	F	189/219 (86%)	188 (100%)	1 (0%)	86	88
3	E	192/219 (88%)	192 (100%)	0	100	100
All	All	874/1005 (87%)	871 (100%)	3 (0%)	91	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	GLU
1	A	22	SER
2	F	30	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	GLN
1	A	4	GLN
1	B	59	HIS
2	D	157	GLN
2	D	184	GLN
3	E	139	HIS
3	E	159	ASN
2	F	77	HIS
2	F	149	ASN
2	F	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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$
2	CR2	D	66	2	20,20,21	2.63	6 (30%)	25,27,29	2.88	10 (40%)
3	CRO	E	66	3	20,20,24	2.71	9 (45%)	25,27,34	3.12	6 (24%)
2	CR2	F	66	2	20,20,21	2.67	8 (40%)	25,27,29	2.72	9 (36%)

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	CR2	D	66	2	-	1/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CRO	E	66	3	-	1/6/25/32	0/2/2/2
2	CR2	F	66	2	-	0/6/25/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	66	CRO	C1-N3	6.10	1.47	1.37
2	D	66	CR2	C1-N3	5.62	1.46	1.37
2	F	66	CR2	CA2-C2	5.31	1.54	1.48
2	D	66	CR2	CA2-C2	5.20	1.54	1.48
2	F	66	CR2	C1-N2	5.13	1.41	1.32
3	E	66	CRO	CG2-CB2	5.10	1.56	1.46
2	D	66	CR2	C1-N2	4.92	1.41	1.32
2	F	66	CR2	C1-N3	4.91	1.45	1.37
3	E	66	CRO	C1-N2	4.51	1.40	1.32
3	E	66	CRO	CA1-C1	4.27	1.54	1.49
2	D	66	CR2	CB2-CA2	-4.24	1.31	1.35
2	F	66	CR2	CB2-CA2	-3.89	1.31	1.35
3	E	66	CRO	OH-CZ	3.69	1.45	1.37
2	F	66	CR2	C2-N3	3.28	1.47	1.40
2	F	66	CR2	CA1-C1	3.17	1.53	1.49
2	F	66	CR2	CG2-CB2	3.10	1.52	1.46
2	D	66	CR2	CG2-CB2	2.82	1.52	1.46
2	D	66	CR2	C2-N3	2.76	1.46	1.40
3	E	66	CRO	C2-N3	2.54	1.45	1.40
3	E	66	CRO	CA2-C2	2.51	1.51	1.48
3	E	66	CRO	CA2-N2	2.44	1.43	1.38
2	F	66	CR2	O2-C2	-2.11	1.18	1.23
3	E	66	CRO	O2-C2	-2.04	1.18	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	66	CRO	O2-C2-CA2	-10.72	124.18	131.02
2	D	66	CR2	C2-N3-C1	-9.44	103.83	108.08
2	F	66	CR2	C3-CA3-N3	-7.35	95.70	112.43
3	E	66	CRO	C2-N3-C1	-6.92	104.97	108.08
2	F	66	CR2	O2-C2-CA2	-6.20	127.07	131.02
2	D	66	CR2	O2-C2-CA2	-5.45	127.54	131.02
3	E	66	CRO	CG2-CB2-CA2	-4.93	124.01	129.87
3	E	66	CRO	CA2-C2-N3	4.89	107.61	103.50
2	D	66	CR2	CA2-C2-N3	4.84	107.56	103.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	66	CR2	C2-N3-C1	-4.69	105.97	108.08
2	F	66	CR2	CG2-CB2-CA2	-4.52	124.50	129.87
2	D	66	CR2	C1-CA1-N1	-3.70	104.67	112.85
2	F	66	CR2	CA2-C2-N3	3.49	106.43	103.50
2	F	66	CR2	C2-CA2-N2	-3.20	106.66	108.95
2	D	66	CR2	C3-CA3-N3	3.16	119.62	112.43
2	D	66	CR2	CG2-CB2-CA2	-2.57	126.81	129.87
2	F	66	CR2	CE2-CD2-CG2	-2.49	118.00	121.22
2	D	66	CR2	CA3-N3-C2	2.49	129.14	123.67
2	F	66	CR2	CD2-CG2-CD1	2.36	121.16	117.65
2	D	66	CR2	N3-C1-N2	2.17	114.27	111.75
3	E	66	CRO	C2-CA2-N2	-2.11	107.44	108.95
3	E	66	CRO	C1-CA1-N1	-2.10	108.21	112.85
2	D	66	CR2	O3-C3-CA3	-2.10	116.03	125.47
2	D	66	CR2	C2-CA2-N2	-2.05	107.48	108.95
2	F	66	CR2	C1-CA1-N1	-2.01	108.41	112.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	66	CR2	C3-CA3-N3-C2
3	E	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	66	CR2	1	0
3	E	66	CRO	1	0
2	F	66	CR2	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	123/145 (84%)	-0.01	1 (0%) 82 84	32, 41, 65, 83	0
1	B	128/145 (88%)	1.00	25 (19%) 4 3	31, 54, 86, 100	0
1	C	129/145 (88%)	0.24	3 (2%) 61 63	31, 44, 69, 103	0
2	D	227/253 (89%)	0.20	5 (2%) 62 64	31, 43, 67, 87	0
2	F	225/253 (88%)	1.08	34 (15%) 6 6	38, 62, 83, 130	0
3	E	226/253 (89%)	0.49	15 (6%) 26 27	31, 50, 72, 134	0
All	All	1058/1194 (88%)	0.53	83 (7%) 20 21	31, 48, 78, 134	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	5.4
2	F	230	THR	4.7
2	F	7	LEU	4.4
3	E	15	LEU	4.1
2	D	2	SER	4.0
1	B	16	ALA	4.0
2	F	8	PHE	3.9
1	B	42	ALA	3.9
1	B	17	GLY	3.9
1	B	126	GLY	3.8
3	E	232	HIS	3.7
3	E	47	ILE	3.4
2	F	42	LEU	3.4
2	F	212	ASN	3.4
1	B	93	THR	3.4
2	F	12	VAL	3.4
1	B	125	SER	3.4
2	D	231	HIS	3.3
1	B	123	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	14	VAL	3.3
3	E	187	PRO	3.2
1	B	94	ALA	3.2
1	B	124	VAL	3.2
1	B	13	LEU	3.1
1	C	27	GLY	3.1
1	B	122	VAL	3.1
2	F	114	PHE	3.1
2	F	9	THR	3.1
1	B	10	GLY	3.0
2	F	119	LEU	3.0
2	F	118	THR	3.0
2	D	3	LYS	3.0
3	E	119	LEU	3.0
1	B	18	GLY	2.9
3	E	188	ILE	2.9
2	F	221	LEU	2.9
2	F	50	THR	2.9
3	E	3	LYS	2.9
3	E	91	GLY	2.8
2	F	68	VAL	2.8
2	F	229	ILE	2.8
1	B	43	PRO	2.8
2	F	90	GLU	2.8
2	F	11	VAL	2.7
1	B	95	LEU	2.7
2	F	44	LEU	2.7
2	F	39	TYR	2.7
2	F	13	PRO	2.6
3	E	112	VAL	2.6
2	F	214	LYS	2.6
1	B	15	GLN	2.6
2	F	6	GLU	2.6
2	F	4	GLY	2.6
3	E	223	PHE	2.5
2	F	137	LEU	2.4
1	B	128	GLU	2.4
1	B	90	PRO	2.4
2	F	16	VAL	2.4
2	F	47	ILE	2.4
1	C	2	ASP	2.4
1	B	12	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	191	GLY	2.4
2	F	27	PHE	2.3
1	A	124	SER	2.3
3	E	13	PRO	2.2
2	D	193	VAL	2.2
3	E	42	LEU	2.2
1	B	96	TYR	2.2
1	B	87	SER	2.2
2	F	3	LYS	2.1
3	E	38	THR	2.1
2	F	189	GLY	2.1
2	F	64	PHE	2.1
2	F	223	PHE	2.1
3	E	89	PRO	2.1
2	F	51	GLY	2.1
3	E	68	VAL	2.0
1	C	41	ALA	2.0
1	B	91	GLU	2.0
2	F	184	GLN	2.0
1	B	88	LEU	2.0
2	D	42	LEU	2.0
2	F	71	PHE	2.0

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

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
2	CR2	F	66	19/20	0.88	0.11	45,56,63,68	0
3	CRO	E	66	19/23	0.91	0.10	32,40,50,54	0
2	CR2	D	66	19/20	0.94	0.08	32,37,45,46	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	201	1/1	0.78	0.16	48,48,48,48	0
5	K	B	201	1/1	0.92	0.08	58,58,58,58	0
4	NA	C	201	1/1	0.94	0.10	39,39,39,39	0
5	K	D	301	1/1	0.99	0.06	40,40,40,40	0
5	K	F	301	1/1	1.00	0.04	38,38,38,38	1

6.5 Other polymers [i](#)

There are no such residues in this entry.