



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:11 PM UTC

PDB ID : 9AWE / pdb_00009awe
Title : The crystal structure of an engineered Protein GF with Human Kappa Fab
Authors : Slezak, T.; Kossiakoff, A.A.
Deposited on : 2024-03-05
Resolution : 2.80 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

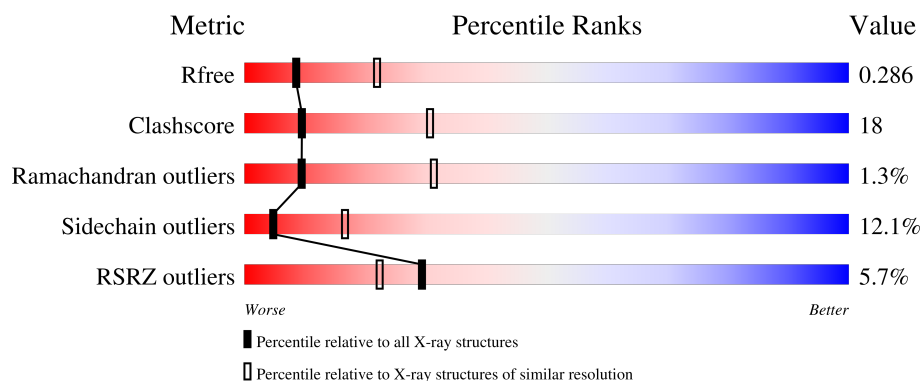
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	B	228	3% 59% 33% • •
2	D	215	2% 56% 36% 6% •
3	A	161	9% 51% 42% • 5%
4	C	65	15% 43% 34% • • 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4822 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 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	S	0	0	0
			1622	1029	268	320	5			

- Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	209	Total	C	N	O	S	0	0	0
			1597	999	269	324	5			

- Molecule 3 is a protein called Histone chaperone ASF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	153	Total	C	N	O	S	0	0	0
			1222	785	198	237	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P32447
A	160	LEU	-	expression tag	UNP P32447
A	161	GLU	-	expression tag	UNP P32447

- Molecule 4 is a protein called Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	53	Total	C	N	O	0	0	0
			367	228	57	82			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	15	ARG	LYS	conflict	UNP P19909

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	SER	LYS	conflict	UNP P19909
C	20	TYR	GLU	conflict	UNP P19909
C	24	THR	GLU	conflict	UNP P19909
C	40	PHE	ASN	conflict	UNP P19909
C	41	GLY	ASP	conflict	UNP P19909
C	65	LYS	-	expression tag	UNP P19909
C	66	LEU	-	expression tag	UNP P19909

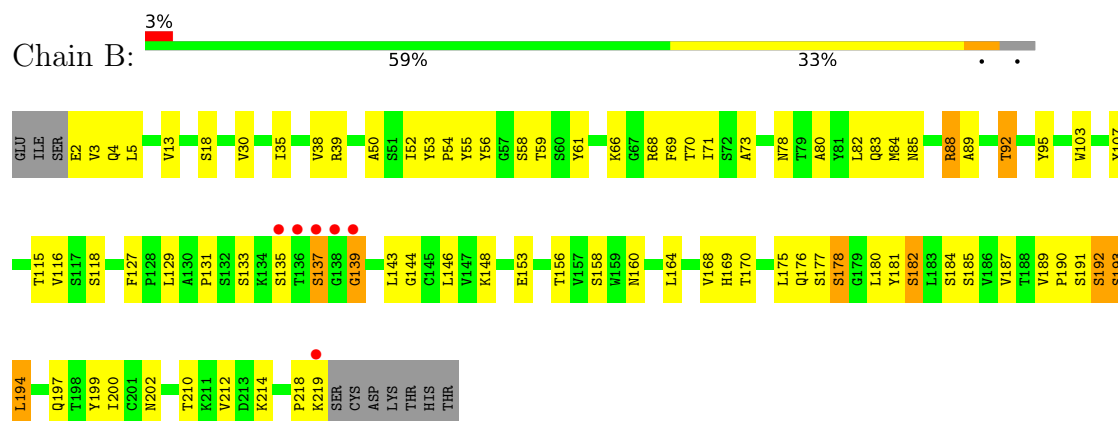
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total O 2 2	0	0
5	D	10	Total O 10 10	0	0
5	C	2	Total O 2 2	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.

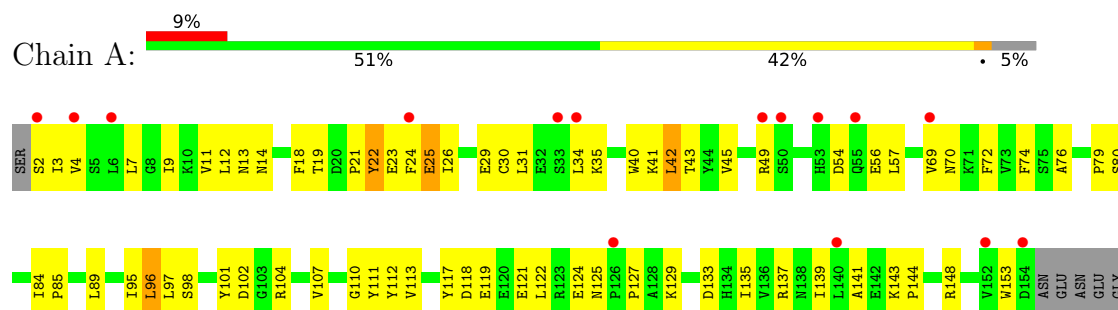
• Molecule 1: Fab Heavy Chain



• Molecule 2: Fab Light Chain

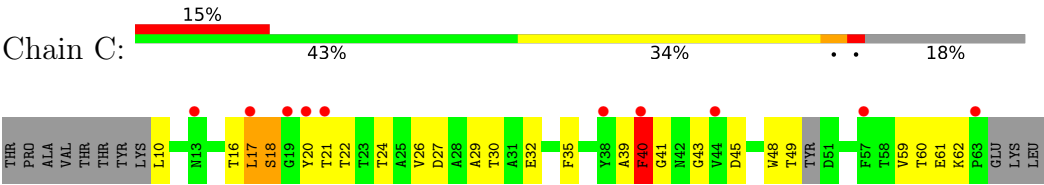


• Molecule 3: Histone chaperone ASF1



LEU
GLU

● Molecule 4: Immunoglobulin G-binding protein G



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.87Å 85.66Å 180.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.05 – 2.80 90.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (90.05-2.80) 95.5 (90.05-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.250 , 0.293 0.246 , 0.286	Depositor DCC
R_{free} test set	1095 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.4	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	0.92	EDS
Total number of atoms	4822	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/1665	0.65	0/2275
2	D	0.41	0/1631	0.67	0/2214
3	A	0.45	0/1251	0.70	0/1708
4	C	0.39	0/372	0.66	0/513
All	All	0.41	0/4919	0.67	0/6710

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	1622	0	1569	53	0
2	D	1597	0	1557	60	0
3	A	1222	0	1196	47	0
4	C	367	0	311	19	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	10	0	0	0	0
All	All	4822	0	4633	169	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 18.

All (169) 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)
3:A:12:LEU:HD11	3:A:25:GLU:HB2	1.49	0.92
1:B:92:THR:HG22	1:B:116:VAL:HG22	1.59	0.83
3:A:18:PHE:HD1	3:A:135:ILE:HG21	1.46	0.80
4:C:17:LEU:HD12	4:C:18:SER:H	1.46	0.80
1:B:30:VAL:HG23	1:B:35:ILE:HG13	1.64	0.79
4:C:48:TRP:HD1	4:C:59:VAL:HG22	1.49	0.77
1:B:178:SER:HB2	1:B:180:LEU:HD23	1.67	0.77
3:A:40:TRP:HZ3	3:A:97:LEU:HD21	1.50	0.74
3:A:14:ASN:ND2	3:A:139:ILE:HB	2.06	0.71
2:D:122:ASP:HA	2:D:125:LEU:HD12	1.72	0.71
2:D:140:TYR:CD1	2:D:141:PRO:HA	2.28	0.69
2:D:158:ASN:HD22	2:D:179:LEU:HD21	1.59	0.68
2:D:132:VAL:HG13	2:D:179:LEU:HB3	1.76	0.68
4:C:48:TRP:CD1	4:C:59:VAL:HG22	2.27	0.68
3:A:18:PHE:HE2	3:A:79:PRO:HB2	1.60	0.67
2:D:158:ASN:ND2	2:D:179:LEU:HD21	2.09	0.67
3:A:40:TRP:CZ3	3:A:97:LEU:HD21	2.29	0.67
2:D:164:THR:HG22	2:D:174:SER:H	1.59	0.67
1:B:82:LEU:HD23	1:B:84:MET:HE2	1.75	0.67
2:D:164:THR:HG23	2:D:165:GLU:O	1.95	0.67
1:B:2:GLU:OE2	1:B:4:GLN:NE2	2.28	0.67
2:D:146:VAL:HG12	2:D:196:VAL:HG22	1.76	0.66
3:A:107:VAL:HG22	3:A:148:ARG:HG2	1.77	0.66
4:C:29:ALA:HA	4:C:32:GLU:HG2	1.77	0.66
3:A:122:LEU:HG	3:A:127:PRO:HD3	1.78	0.65
2:D:183:LYS:HD3	2:D:184:ALA:H	1.64	0.63
2:D:31:SER:HA	2:D:50:SER:OG	1.97	0.63
2:D:170:ASP:HB2	2:D:172:THR:OG1	1.99	0.63
2:D:20:THR:HB	2:D:74:THR:HG22	1.80	0.62
2:D:181:LEU:HD22	2:D:185:ASP:HB2	1.81	0.61
2:D:47:LEU:HA	2:D:58:VAL:HG21	1.83	0.61
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.81	0.61
2:D:108:ARG:HG3	2:D:140:TYR:CD2	2.36	0.60
3:A:95:ILE:HD13	3:A:113:VAL:HG21	1.81	0.60
2:D:110:VAL:HG21	2:D:199:GLN:NE2	2.16	0.60
3:A:119:GLU:HB3	3:A:122:LEU:HB2	1.84	0.60
2:D:155:GLN:HB3	2:D:158:ASN:HD21	1.67	0.60
4:C:17:LEU:HD12	4:C:18:SER:N	2.15	0.59
3:A:18:PHE:CD1	3:A:135:ILE:HG21	2.34	0.59
3:A:41:LYS:HD3	3:A:56:GLU:OE1	2.03	0.58
4:C:39:ALA:HB1	4:C:43:GLY:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:18:PHE:HE1	3:A:89:LEU:HA	1.69	0.57
1:B:52:ILE:HD12	1:B:59:THR:HG22	1.85	0.57
3:A:133:ASP:OD2	3:A:133:ASP:N	2.37	0.57
1:B:153:GLU:HG2	1:B:181:TYR:CD2	2.40	0.56
1:B:148:LYS:HA	1:B:182:SER:HB3	1.86	0.56
1:B:61:TYR:CE1	1:B:71:ILE:HG22	2.41	0.56
3:A:14:ASN:HD21	3:A:139:ILE:HB	1.70	0.55
3:A:18:PHE:CE1	3:A:89:LEU:HD13	2.41	0.55
1:B:53:TYR:CD2	3:A:143:LYS:HG2	2.41	0.54
1:B:131:PRO:HD3	1:B:143:LEU:HB3	1.89	0.54
1:B:54:PRO:HD2	3:A:144:PRO:HG2	1.88	0.54
3:A:2:SER:N	3:A:153:TRP:HE1	2.05	0.54
3:A:42:LEU:HD23	3:A:57:LEU:HB2	1.88	0.54
2:D:183:LYS:HD3	2:D:184:ALA:N	2.21	0.54
2:D:193:ALA:HB2	2:D:208:SER:HB3	1.88	0.54
1:B:89:ALA:O	1:B:92:THR:HG23	2.08	0.53
1:B:197:GLN:HG2	1:B:199:TYR:CE2	2.44	0.53
2:D:113:PRO:HB3	2:D:139:PHE:HB3	1.91	0.53
2:D:148:TRP:CD1	2:D:159:SER:HG	2.27	0.53
1:B:169:HIS:CE1	2:D:137:ASN:HD21	2.28	0.52
2:D:161:GLU:OE1	2:D:175:LEU:HD11	2.10	0.52
3:A:111:TYR:CD1	3:A:141:ALA:HA	2.44	0.52
2:D:182:SER:OG	2:D:185:ASP:OD1	2.28	0.51
1:B:88:ARG:O	1:B:116:VAL:HG21	2.11	0.51
1:B:214:LYS:HE3	4:C:16:THR:OG1	2.10	0.51
3:A:3:ILE:HG22	3:A:4:VAL:HG23	1.92	0.51
1:B:127:PHE:CE2	2:D:124:GLN:HG3	2.46	0.51
2:D:108:ARG:NH2	2:D:111:ALA:HB2	2.25	0.51
2:D:61:ARG:CZ	2:D:79:GLN:HG3	2.41	0.51
1:B:175:LEU:HD12	1:B:181:TYR:CE1	2.45	0.51
2:D:135:LEU:HD21	2:D:137:ASN:HB2	1.93	0.50
4:C:45:ASP:O	4:C:61:GLU:HG2	2.10	0.50
1:B:189:VAL:HG22	1:B:190:PRO:HD2	1.93	0.50
3:A:22:TYR:HB2	3:A:76:ALA:HB3	1.93	0.50
2:D:17:ASP:O	2:D:77:SER:HA	2.11	0.50
3:A:24:PHE:CD2	3:A:97:LEU:HD12	2.46	0.50
1:B:3:VAL:HG13	1:B:107:TYR:CE2	2.46	0.50
2:D:135:LEU:CD2	2:D:137:ASN:HB2	2.42	0.50
3:A:45:VAL:HG21	3:A:96:LEU:HD22	1.93	0.50
1:B:212:VAL:HB	4:C:17:LEU:HD11	1.94	0.49
2:D:118:PHE:O	2:D:132:VAL:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:VAL:HA	2:D:89:GLN:O	2.13	0.49
2:D:192:TYR:HB2	2:D:209:PHE:CE2	2.48	0.49
4:C:39:ALA:O	4:C:41:GLY:N	2.43	0.49
3:A:7:LEU:HD22	3:A:29:GLU:HG2	1.93	0.49
4:C:21:THR:HG22	4:C:22:THR:H	1.76	0.48
1:B:103:TRP:NE1	3:A:112:TYR:HE2	2.11	0.48
1:B:192:SER:OG	1:B:193:SER:N	2.44	0.48
3:A:3:ILE:HB	3:A:153:TRP:CD2	2.48	0.48
3:A:26:ILE:HG21	3:A:40:TRP:CH2	2.49	0.48
2:D:49:TYR:HE1	2:D:55:TYR:HA	1.78	0.48
3:A:113:VAL:HG22	3:A:139:ILE:HG12	1.96	0.48
1:B:103:TRP:HB3	2:D:91:ASP:HB3	1.95	0.47
2:D:132:VAL:HG22	2:D:148:TRP:CH2	2.48	0.47
1:B:210:THR:OG1	4:C:21:THR:HG23	2.14	0.47
2:D:83:PHE:CE1	2:D:106:ILE:HG12	2.49	0.47
3:A:34:LEU:HD23	3:A:101:TYR:OH	2.14	0.47
1:B:54:PRO:O	1:B:56:TYR:N	2.44	0.47
2:D:197:THR:O	2:D:197:THR:OG1	2.24	0.47
3:A:102:ASP:HB3	3:A:104:ARG:NH1	2.30	0.47
2:D:206:THR:O	2:D:207:LYS:HD3	2.14	0.46
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.51	0.46
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.82	0.46
2:D:190:LYS:HB2	2:D:190:LYS:HE2	1.65	0.46
2:D:117:ILE:HG13	2:D:118:PHE:N	2.31	0.46
3:A:11:VAL:HG13	3:A:11:VAL:O	2.16	0.46
3:A:84:ILE:HG22	3:A:85:PRO:O	2.16	0.46
2:D:132:VAL:HG22	2:D:148:TRP:HH2	1.81	0.45
3:A:9:ILE:HD12	3:A:111:TYR:OH	2.16	0.45
1:B:69:PHE:CE2	1:B:84:MET:HG2	2.52	0.45
1:B:129:LEU:HB2	1:B:144:GLY:O	2.15	0.45
1:B:30:VAL:CG2	1:B:35:ILE:HG13	2.43	0.45
2:D:77:SER:O	2:D:77:SER:OG	2.34	0.45
1:B:69:PHE:HA	1:B:83:GLN:O	2.17	0.45
1:B:176:GLN:OE1	1:B:182:SER:OG	2.35	0.44
1:B:30:VAL:HG12	1:B:78:ASN:OD1	2.18	0.44
1:B:160:ASN:HA	1:B:200:ILE:HG13	1.99	0.44
3:A:11:VAL:HG11	3:A:14:ASN:HD22	1.82	0.44
1:B:61:TYR:HE1	1:B:71:ILE:H	1.65	0.44
1:B:13:VAL:O	1:B:116:VAL:HA	2.18	0.44
1:B:139:GLY:C	1:B:191:SER:HB2	2.44	0.43
2:D:158:ASN:HD22	2:D:179:LEU:CD2	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LEU:HD23	2:D:55:TYR:CG	2.53	0.43
2:D:103:LYS:HD3	2:D:104:VAL:N	2.32	0.43
3:A:102:ASP:HB3	3:A:104:ARG:HH12	1.82	0.43
1:B:50:ALA:HB1	1:B:71:ILE:HB	2.00	0.43
3:A:118:ASP:OD1	3:A:119:GLU:N	2.52	0.43
1:B:210:THR:HG23	4:C:21:THR:OG1	2.19	0.43
4:C:10:LEU:HD21	4:C:59:VAL:HG23	2.00	0.42
1:B:164:LEU:HD21	1:B:187:VAL:HG21	2.01	0.42
1:B:197:GLN:HG2	1:B:199:TYR:CZ	2.55	0.42
2:D:191:VAL:HG23	2:D:209:PHE:O	2.18	0.42
3:A:24:PHE:HD2	3:A:97:LEU:CD1	2.33	0.42
2:D:108:ARG:NH2	2:D:109:THR:O	2.50	0.42
3:A:42:LEU:HD23	3:A:57:LEU:CB	2.50	0.42
4:C:10:LEU:O	4:C:20:TYR:HA	2.20	0.42
2:D:61:ARG:O	2:D:75:ILE:HA	2.20	0.42
3:A:72:PHE:CE2	3:A:74:PHE:HB2	2.55	0.42
3:A:96:LEU:HD12	3:A:110:GLY:HA2	2.00	0.42
4:C:17:LEU:HD23	4:C:40:PHE:CE1	2.54	0.42
3:A:24:PHE:HD2	3:A:97:LEU:HD12	1.83	0.42
1:B:35:ILE:O	1:B:52:ILE:HG22	2.19	0.42
1:B:73:ALA:HA	1:B:80:ALA:HA	2.02	0.42
3:A:13:ASN:OD1	3:A:23:GLU:HG2	2.20	0.42
1:B:39:ARG:NH1	1:B:95:TYR:OH	2.48	0.41
1:B:170:THR:HG23	1:B:185:SER:HB2	2.01	0.41
2:D:29:VAL:HG12	2:D:31:SER:H	1.85	0.41
2:D:110:VAL:HG21	2:D:199:GLN:HE21	1.84	0.41
2:D:142:ARG:HE	2:D:142:ARG:HB2	1.56	0.41
1:B:158:SER:O	1:B:202:ASN:N	2.36	0.41
1:B:153:GLU:HG2	1:B:181:TYR:CE2	2.55	0.41
2:D:143:GLU:O	2:D:198:HIS:HD2	2.03	0.41
3:A:117:TYR:CE2	3:A:127:PRO:HD2	2.55	0.41
2:D:11:LEU:HD12	2:D:11:LEU:HA	1.49	0.41
3:A:121:GLU:OE1	3:A:125:ASN:HB2	2.21	0.41
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.89	0.41
2:D:103:LYS:HD2	2:D:105:GLU:HG2	2.03	0.41
2:D:135:LEU:HD23	2:D:135:LEU:C	2.46	0.41
1:B:129:LEU:HB2	1:B:144:GLY:C	2.46	0.41
2:D:78:LEU:HD23	2:D:78:LEU:HA	1.82	0.41
1:B:218:PRO:O	1:B:219:LYS:C	2.64	0.41
1:B:68:ARG:HB3	1:B:85:ASN:O	2.20	0.40
4:C:10:LEU:HG	4:C:35:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:CD1	1:B:148:LYS:HB2	2.50	0.40
4:C:49:THR:O	4:C:49:THR:OG1	2.39	0.40
2:D:62:PHE:CE1	2:D:75:ILE:HG12	2.56	0.40
3:A:21:PRO:O	3:A:137:ARG:NH2	2.54	0.40
4:C:26:VAL:HG23	4:C:27:ASP:N	2.37	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	B	216/228 (95%)	202 (94%)	10 (5%)	4 (2%)	6	22
2	D	207/215 (96%)	196 (95%)	10 (5%)	1 (0%)	24	55
3	A	151/161 (94%)	143 (95%)	7 (5%)	1 (1%)	18	47
4	C	49/65 (75%)	40 (82%)	7 (14%)	2 (4%)	2	8
All	All	623/669 (93%)	581 (93%)	34 (6%)	8 (1%)	9	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	SER
4	C	40	PHE
3	A	49	ARG
1	B	139	GLY
2	D	121	SER
1	B	55	TYR
1	B	58	SER
4	C	62	LYS

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	178/189 (94%)	158 (89%)	20 (11%)	6	19
2	D	183/189 (97%)	160 (87%)	23 (13%)	4	15
3	A	140/148 (95%)	124 (89%)	16 (11%)	5	19
4	C	34/53 (64%)	28 (82%)	6 (18%)	2	7
All	All	535/579 (92%)	470 (88%)	65 (12%)	5	16

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	SER
1	B	38	VAL
1	B	66	LYS
1	B	70	THR
1	B	88	ARG
1	B	92	THR
1	B	115	THR
1	B	118	SER
1	B	133	SER
1	B	135	SER
1	B	137	SER
1	B	156	THR
1	B	168	VAL
1	B	177	SER
1	B	178	SER
1	B	182	SER
1	B	184	SER
1	B	192	SER
1	B	193	SER
1	B	194	LEU
2	D	7	SER
2	D	9	SER
2	D	14	SER
2	D	20	THR

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Mol	Chain	Res	Type
2	D	28	SER
2	D	30	SER
2	D	65	SER
2	D	77	SER
2	D	94	SER
2	D	105	GLU
2	D	121	SER
2	D	122	ASP
2	D	125	LEU
2	D	127	SER
2	D	132	VAL
2	D	133	VAL
2	D	158	ASN
2	D	161	GLU
2	D	164	THR
2	D	194	CYS
2	D	202	SER
2	D	206	THR
2	D	208	SER
3	A	19	THR
3	A	22	TYR
3	A	25	GLU
3	A	30	CYS
3	A	31	LEU
3	A	35	LYS
3	A	42	LEU
3	A	43	THR
3	A	54	ASP
3	A	69	VAL
3	A	70	ASN
3	A	80	SER
3	A	96	LEU
3	A	98	SER
3	A	124	GLU
3	A	129	LYS
4	C	17	LEU
4	C	18	SER
4	C	24	THR
4	C	30	THR
4	C	40	PHE
4	C	60	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	204	ASN
2	D	100	GLN
2	D	137	ASN
2	D	158	ASN
3	A	14	ASN
3	A	53	HIS
3	A	115	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	218/228 (95%)	0.32	6 (2%) 55 45	51, 71, 106, 166	0
2	D	209/215 (97%)	0.33	5 (2%) 59 49	39, 66, 106, 120	0
3	A	153/161 (95%)	0.85	15 (9%) 13 9	63, 91, 147, 173	0
4	C	53/65 (81%)	1.31	10 (18%) 3 2	78, 102, 130, 161	0
All	All	633/669 (94%)	0.54	36 (5%) 29 22	39, 78, 124, 173	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	69	VAL	4.4
4	C	19	GLY	3.7
4	C	40	PHE	3.7
4	C	63	PRO	3.5
1	B	136	THR	3.4
4	C	21	THR	3.4
3	A	2	SER	3.3
1	B	137	SER	3.1
3	A	154	ASP	3.0
4	C	57	PHE	3.0
1	B	135	SER	2.9
4	C	44	VAL	2.9
3	A	34	LEU	2.9
3	A	4	VAL	2.8
3	A	33	SER	2.8
3	A	55	GLN	2.7
3	A	152	VAL	2.7
3	A	53	HIS	2.7
2	D	11	LEU	2.6
1	B	219	LYS	2.5
4	C	38	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	49	ARG	2.5
3	A	140	LEU	2.4
2	D	67	SER	2.4
1	B	138	GLY	2.4
3	A	50	SER	2.4
2	D	210	ASN	2.3
1	B	139	GLY	2.3
2	D	21	ILE	2.2
3	A	6	LEU	2.2
2	D	93	TRP	2.2
3	A	126	PRO	2.2
4	C	17	LEU	2.2
4	C	20	TYR	2.1
3	A	24	PHE	2.0
4	C	13	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.