



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:43 PM UTC

PDB ID : 8GYE / pdb_00008gye
Title : Crystal Structure of the 4-1BB in complex with ZG033 Fab
Authors : Zhu, M.; Cheng, L.S.; Gao, Y.
Deposited on : 2022-09-22
Resolution : 2.30 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 : 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

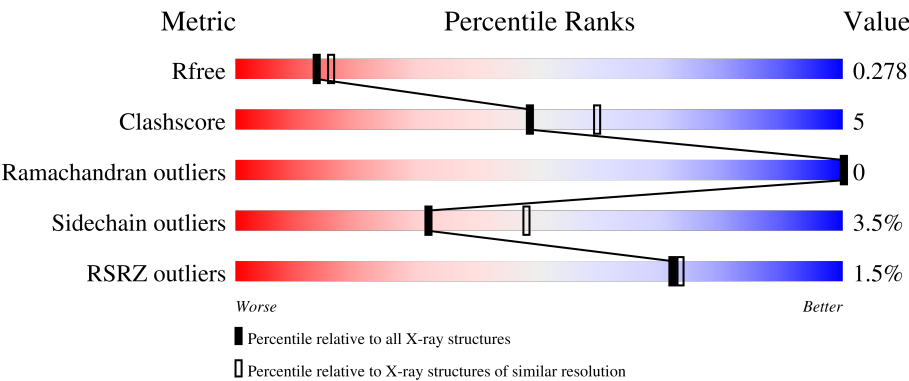
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	174	
1	D	174	
2	B	220	
2	E	220	
3	C	214	

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Mol	Chain	Length	Quality of chain
3	F	214	% 89% 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8661 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 Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1012	597	190	203	22			
1	D	138	Total	C	N	O	S	0	0	0
			1019	602	191	204	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	LEU	-	expression tag	UNP Q07011
A	188	GLU	-	expression tag	UNP Q07011
A	189	GLY	-	expression tag	UNP Q07011
A	190	GLY	-	expression tag	UNP Q07011
A	191	GLY	-	expression tag	UNP Q07011
A	192	HIS	-	expression tag	UNP Q07011
A	193	HIS	-	expression tag	UNP Q07011
A	194	HIS	-	expression tag	UNP Q07011
A	195	HIS	-	expression tag	UNP Q07011
A	196	HIS	-	expression tag	UNP Q07011
A	197	HIS	-	expression tag	UNP Q07011
D	187	LEU	-	expression tag	UNP Q07011
D	188	GLU	-	expression tag	UNP Q07011
D	189	GLY	-	expression tag	UNP Q07011
D	190	GLY	-	expression tag	UNP Q07011
D	191	GLY	-	expression tag	UNP Q07011
D	192	HIS	-	expression tag	UNP Q07011
D	193	HIS	-	expression tag	UNP Q07011
D	194	HIS	-	expression tag	UNP Q07011
D	195	HIS	-	expression tag	UNP Q07011
D	196	HIS	-	expression tag	UNP Q07011
D	197	HIS	-	expression tag	UNP Q07011

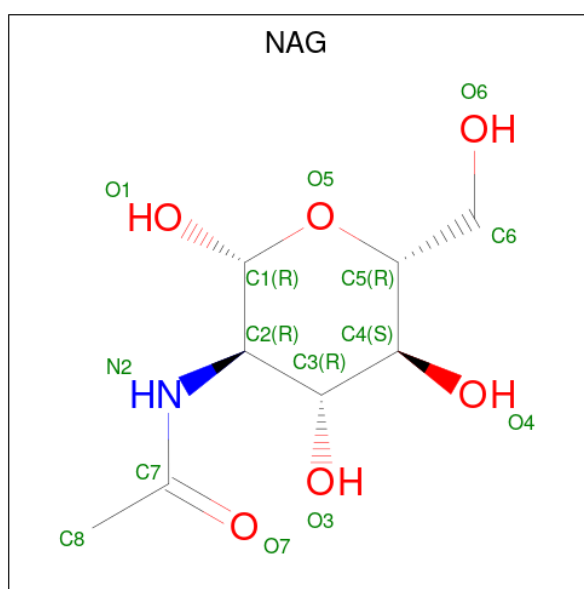
- Molecule 2 is a protein called ZG033 Fab H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1593	999	266	321	7			
2	E	216	Total	C	N	O	S	0	0	0
			1593	999	266	321	7			

- Molecule 3 is a protein called ZG033 Fab L chain.

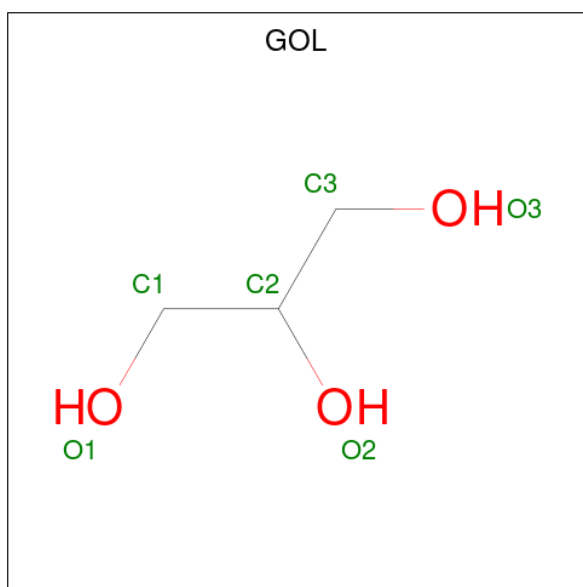
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1641	1028	271	337	5			
3	F	213	Total	C	N	O	S	0	0	0
			1641	1028	271	337	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		

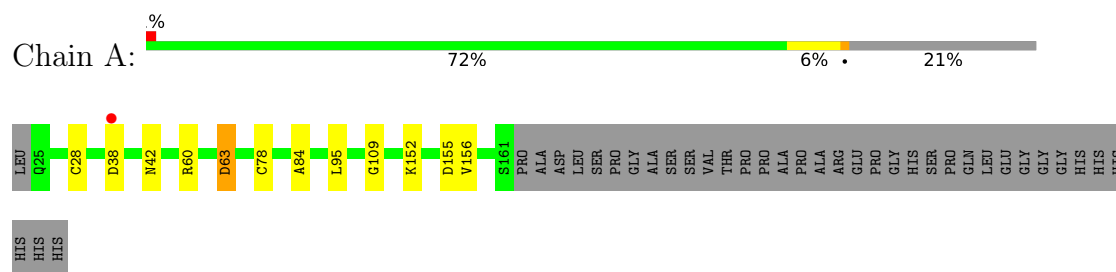
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	D	8	Total	O	0	0
			8	8		
6	B	30	Total	O	0	0
			30	30		
6	C	30	Total	O	0	0
			30	30		
6	E	28	Total	O	0	0
			28	28		
6	F	19	Total	O	0	0
			19	19		

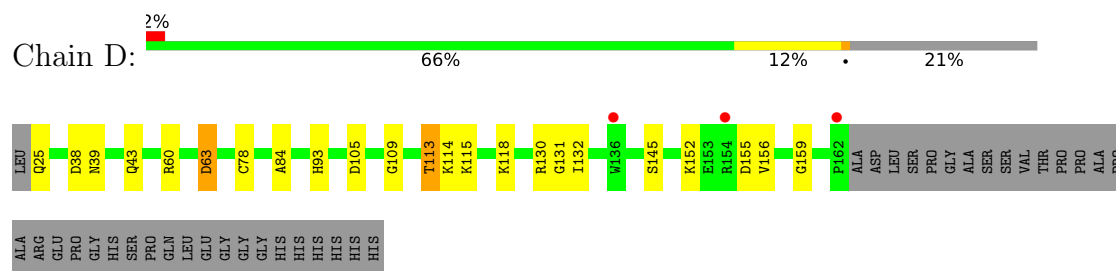
3 Residue-property plots

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.

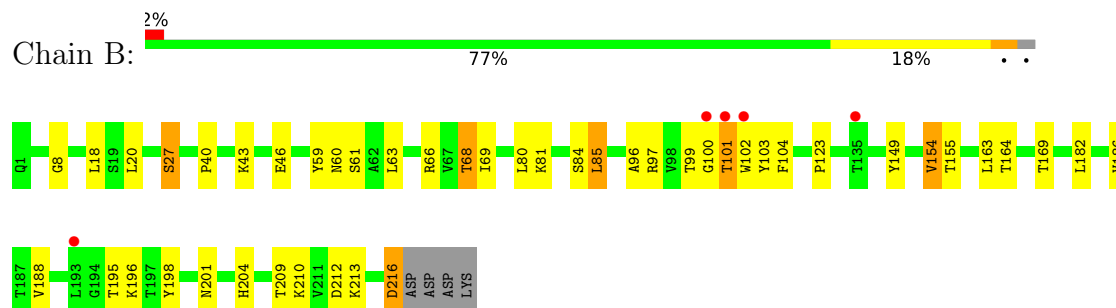
- Molecule 1: Tumor necrosis factor receptor superfamily member 9



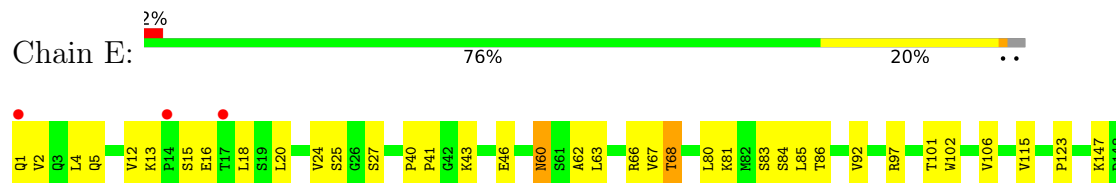
- Molecule 1: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: ZG033 Fab H chain

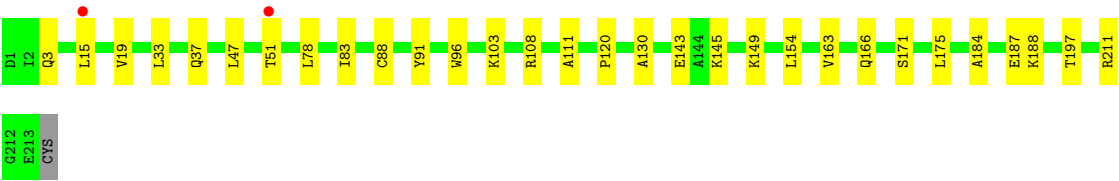
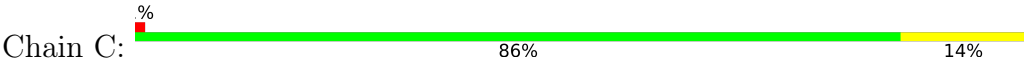


- Molecule 2: ZG033 Fab H chain

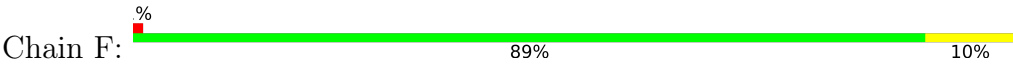




● Molecule 3: ZG033 Fab L chain



● Molecule 3: ZG033 Fab L chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.02Å 65.91Å 83.64Å 90.00° 82.50° 74.82°	Depositor
Resolution (Å)	19.91 – 2.30 19.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.91-2.30) 97.2 (19.91-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.222 , 0.277 0.222 , 0.278	Depositor DCC
R_{free} test set	2594 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.4	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	0.95	EDS
Total number of atoms	8661	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% 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](#)

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

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	0.09	0/1028	0.30	0/1381
1	D	0.10	0/1036	0.32	0/1393
2	B	0.10	0/1630	0.29	0/2229
2	E	0.10	0/1630	0.34	0/2229
3	C	0.09	0/1677	0.29	0/2279
3	F	0.10	0/1677	0.30	0/2279
All	All	0.10	0/8678	0.31	0/11790

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	15	SER	Peptide

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	1012	0	930	7	0
1	D	1019	0	937	12	0
2	B	1593	0	1574	23	0
2	E	1593	0	1574	26	0
3	C	1641	0	1590	16	0
3	F	1641	0	1590	11	0
4	A	14	0	13	0	0
4	D	14	0	13	0	0
5	E	6	0	8	3	0
6	A	13	0	0	0	0
6	B	30	0	0	0	0
6	C	30	0	0	0	0
6	D	8	0	0	0	0
6	E	28	0	0	1	0
6	F	19	0	0	1	0
All	All	8661	0	8229	92	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 (92) 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:16:GLU:HB3	2:E:85:LEU:H	1.32	0.94
2:E:66:ARG:HD2	2:E:84:SER:HB2	1.60	0.82
3:C:33:LEU:HB3	3:C:51:THR:HG22	1.74	0.67
1:D:115:LYS:HB2	1:D:118:LYS:HE3	1.77	0.67
2:B:27:SER:HB3	2:B:97:ARG:HH11	1.61	0.66
3:F:33:LEU:HB3	3:F:51:THR:HG22	1.77	0.66
2:E:205:LYS:HG3	2:E:206:PRO:HD3	1.76	0.65
2:E:60:ASN:HD22	2:E:62:ALA:H	1.43	0.65
2:E:123:PRO:HB3	2:E:149:TYR:HB3	1.78	0.64
2:E:27:SER:HB3	2:E:97:ARG:HH11	1.63	0.64
2:E:201:ASN:ND2	2:E:212:ASP:OD1	2.32	0.63
1:D:25:GLN:HG3	2:E:41:PRO:HB3	1.80	0.62
2:B:18:LEU:HB2	2:B:85:LEU:HD21	1.82	0.62
2:B:201:ASN:ND2	2:B:212:ASP:OD1	2.28	0.61
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.82	0.61
2:E:68:THR:HG23	2:E:81:LYS:HB2	1.83	0.60
2:E:5:GLN:NE2	6:E:401:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:LEU:HB2	2:E:85:LEU:HD21	1.85	0.59
2:E:101:THR:HA	2:E:102:TRP:CG	2.38	0.58
2:B:60:ASN:HB3	2:B:63:LEU:HD23	1.86	0.58
2:E:147:LYS:HA	2:E:181:SER:HB2	1.86	0.57
1:D:155:ASP:OD1	1:D:156:VAL:N	2.39	0.56
2:E:46:GLU:HA	5:E:301:GOL:H31	1.90	0.54
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.89	0.54
1:D:145:SER:O	1:D:159:GLY:N	2.40	0.54
2:B:68:THR:HG23	2:B:81:LYS:HB2	1.90	0.53
1:D:113:THR:OG1	1:D:114:LYS:N	2.39	0.53
1:D:63:ASP:N	1:D:63:ASP:OD1	2.42	0.52
5:E:301:GOL:H2	3:F:97:THR:HG22	1.91	0.52
3:F:45:LYS:NZ	6:F:302:HOH:O	2.41	0.51
2:B:195:THR:HG23	2:B:196:LYS:HG3	1.93	0.51
3:F:132:VAL:HG13	3:F:179:LEU:HB3	1.93	0.51
1:D:38:ASP:OD1	1:D:39:ASN:N	2.44	0.50
1:A:78:CYS:HB3	1:A:84:ALA:HB2	1.94	0.50
5:E:301:GOL:H2	3:F:97:THR:HA	1.93	0.50
1:A:28:CYS:SG	1:A:60:ARG:NH1	2.85	0.49
1:A:63:ASP:OD1	1:A:63:ASP:N	2.45	0.49
3:C:3:GLN:NE2	2:E:25:SER:OG	2.42	0.49
2:B:99:THR:HG22	2:B:100:GLY:H	1.79	0.48
2:E:123:PRO:HD2	2:E:209:THR:HG21	1.96	0.48
3:C:19:VAL:HG21	3:C:78:LEU:HD22	1.95	0.48
3:F:21:ILE:HD11	3:F:73:LEU:HD23	1.96	0.47
1:D:78:CYS:HB3	1:D:84:ALA:HB2	1.96	0.47
2:B:66:ARG:HD2	2:B:84:SER:HB2	1.96	0.47
2:B:154:VAL:HG12	2:B:182:LEU:HD13	1.97	0.47
2:B:204:HIS:HB3	2:B:209:THR:HB	1.97	0.47
2:B:101:THR:O	2:B:102:TRP:CG	2.68	0.47
2:E:63:LEU:HD13	2:E:67:VAL:HG21	1.96	0.46
1:D:93:HIS:ND1	1:D:105:ASP:OD1	2.30	0.46
2:E:16:GLU:O	2:E:83:SER:HA	2.16	0.46
2:B:40:PRO:HB2	2:B:43:LYS:HD2	1.99	0.46
1:A:42:ASN:OD1	1:A:42:ASN:N	2.48	0.45
2:B:46:GLU:HG3	2:E:1:GLN:HE21	1.81	0.45
3:C:149:LYS:HG2	3:C:154:LEU:HD23	1.98	0.45
1:A:38:ASP:N	1:A:38:ASP:OD1	2.48	0.45
3:C:143:GLU:N	3:C:143:GLU:OE1	2.50	0.44
3:C:145:LYS:HB2	3:C:197:THR:HB	1.98	0.44
2:E:2:VAL:HG21	2:E:106:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:PRO:HB2	2:E:43:LYS:HD2	2.00	0.44
3:F:193:ALA:HB2	3:F:208:SER:HB3	2.00	0.44
2:B:8:GLY:HA3	2:B:20:LEU:HD23	2.00	0.44
2:B:188:VAL:HG11	2:B:198:TYR:CE1	2.53	0.44
1:D:93:HIS:NE2	1:D:130:ARG:HG3	2.32	0.43
2:E:60:ASN:ND2	2:E:62:ALA:H	2.12	0.43
1:D:109:GLY:HA2	1:D:152:LYS:O	2.18	0.43
2:B:100:GLY:HA3	2:B:103:TYR:CE2	2.52	0.43
3:C:163:VAL:HG22	3:C:175:LEU:HD12	2.01	0.43
1:D:130:ARG:HG2	1:D:131:GLY:N	2.33	0.43
1:A:155:ASP:OD1	1:A:156:VAL:N	2.51	0.43
3:C:120:PRO:HG3	3:C:130:ALA:HB1	2.01	0.43
3:C:108:ARG:NH1	3:C:111:ALA:HB2	2.35	0.42
3:C:15:LEU:HD12	3:C:15:LEU:H	1.83	0.42
3:C:184:ALA:O	3:C:188:LYS:HG3	2.19	0.42
2:E:157:SER:OG	2:E:201:ASN:HB2	2.19	0.42
1:A:109:GLY:HA2	1:A:152:LYS:O	2.20	0.42
2:B:59:TYR:HE1	2:B:69:ILE:HG13	1.84	0.42
3:C:91:TYR:HA	3:C:96:TRP:CD1	2.54	0.42
2:E:20:LEU:HD12	2:E:80:LEU:HD23	2.02	0.42
3:C:187:GLU:O	3:C:211:ARG:NH2	2.53	0.41
2:B:163:LEU:HD21	2:B:186:VAL:HG21	2.02	0.41
2:B:216:ASP:OD1	2:B:216:ASP:N	2.53	0.41
2:E:4:LEU:HG	2:E:24:VAL:HG12	2.02	0.41
3:F:18:ARG:NH2	3:F:74:THR:HG21	2.35	0.41
3:C:33:LEU:HD11	3:C:88:CYS:HB2	2.02	0.41
2:E:12:VAL:O	2:E:115:VAL:HA	2.20	0.41
2:B:169:THR:HG23	2:B:182:LEU:HD21	2.03	0.41
3:C:166:GLN:HG2	3:C:171:SER:HA	2.03	0.41
3:F:37:GLN:HB2	3:F:47:LEU:HD11	2.03	0.41
3:F:207:LYS:HA	3:F:207:LYS:HE2	2.03	0.40
2:B:99:THR:HG22	2:B:100:GLY:N	2.37	0.40
3:F:6:GLN:NE2	3:F:102:THR:HG23	2.36	0.40
2:B:96:ALA:HB1	2:B:104:PHE:HB3	2.03	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	135/174 (78%)	135 (100%)	0	0	100	100
1	D	136/174 (78%)	133 (98%)	3 (2%)	0	100	100
2	B	214/220 (97%)	211 (99%)	3 (1%)	0	100	100
2	E	214/220 (97%)	210 (98%)	4 (2%)	0	100	100
3	C	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
3	F	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	1121/1216 (92%)	1104 (98%)	17 (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	119/147 (81%)	117 (98%)	2 (2%)	53	72
1	D	120/147 (82%)	115 (96%)	5 (4%)	26	40
2	B	186/190 (98%)	174 (94%)	12 (6%)	15	22
2	E	186/190 (98%)	177 (95%)	9 (5%)	23	35
3	C	189/190 (100%)	187 (99%)	2 (1%)	65	81
3	F	189/190 (100%)	184 (97%)	5 (3%)	40	59
All	All	989/1054 (94%)	954 (96%)	35 (4%)	32	48

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	95	LEU
1	D	43	GLN
1	D	60	ARG
1	D	63	ASP
1	D	113	THR
1	D	132	ILE
2	B	27	SER
2	B	61	SER
2	B	68	THR
2	B	80	LEU
2	B	85	LEU
2	B	101	THR
2	B	154	VAL
2	B	155	THR
2	B	164	THR
2	B	210	LYS
2	B	213	LYS
2	B	216	ASP
3	C	83	ILE
3	C	103	LYS
2	E	13	LYS
2	E	60	ASN
2	E	68	THR
2	E	86	THR
2	E	92	VAL
2	E	154	VAL
2	E	181	SER
2	E	199	THR
2	E	214	ARG
3	F	125	LEU
3	F	126	LYS
3	F	165	GLU
3	F	191	VAL
3	F	201	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	51	ASN

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Mol	Chain	Res	Type
1	D	25	GLN
1	D	42	ASN
1	D	67	GLN
2	B	39	GLN
3	C	31	ASN
3	C	38	GLN
3	C	147	GLN
2	E	39	GLN
3	F	38	GLN
3	F	124	GLN

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](#)

3 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	$\# Z > 2$
4	NAG	A	201	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	D	201	1	14,14,15	0.50	0	17,19,21	0.44	0
5	GOL	E	301	-	5,5,5	0.93	0	5,5,5	1.06	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
4	NAG	A	201	1	-	2/6/23/26	0/1/1/1
4	NAG	D	201	1	-	2/6/23/26	0/1/1/1
5	GOL	E	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	NAG	O5-C5-C6-O6
4	D	201	NAG	C8-C7-N2-C2
4	D	201	NAG	O7-C7-N2-C2
4	A	201	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	301	GOL	3	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	A	137/174 (78%)	0.35	1 (0%) 84 85	41, 64, 91, 99	0
1	D	138/174 (79%)	0.47	3 (2%) 62 64	45, 70, 99, 105	0
2	B	216/220 (98%)	0.31	5 (2%) 61 63	39, 56, 87, 121	0
2	E	216/220 (98%)	0.37	4 (1%) 66 68	41, 61, 99, 122	0
3	C	213/214 (99%)	0.27	2 (0%) 81 82	42, 58, 77, 85	0
3	F	213/214 (99%)	0.35	2 (0%) 81 82	43, 60, 85, 94	0
All	All	1133/1216 (93%)	0.35	17 (1%) 72 73	39, 60, 89, 122	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	100	GLY	4.4
2	B	101	THR	4.3
2	B	102	TRP	3.3
3	C	51	THR	3.1
2	E	14	PRO	2.8
2	E	152	GLU	2.6
1	D	136	TRP	2.3
2	E	1	GLN	2.3
3	F	51	THR	2.3
3	C	15	LEU	2.2
3	F	170	ASP	2.2
2	B	193	LEU	2.1
1	A	38	ASP	2.1
1	D	162	PRO	2.1
2	B	135	THR	2.1
2	E	17	THR	2.0
1	D	154	ARG	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](#)

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($\text{\AA}^2$)	Q<0.9
4	NAG	A	201	14/15	0.51	0.12	63,90,94,99	0
4	NAG	D	201	14/15	0.66	0.13	83,96,105,109	0
5	GOL	E	301	6/6	0.68	0.21	52,59,65,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.