



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:39 AM UTC

PDB ID : 9LUX / pdb_00009lux
Title : Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein
Authors : Hanazono, Y.; Yabuno, S.; Hayashi, T.; Numoto, N.; Ito, N.; Oda, M.
Deposited on : 2025-02-10
Resolution : 1.85 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

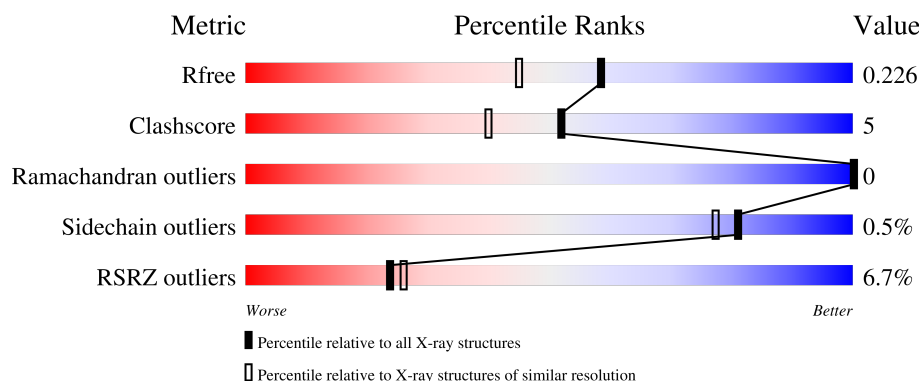
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	271	5% 84% 10% 6%
1	B	271	6% 84% 10% 6%
1	C	271	5% 87% 6% 7%
1	D	271	8% 85% 8% 7%
1	E	271	7% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
1	F	271	6% 85% 9% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12729 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.

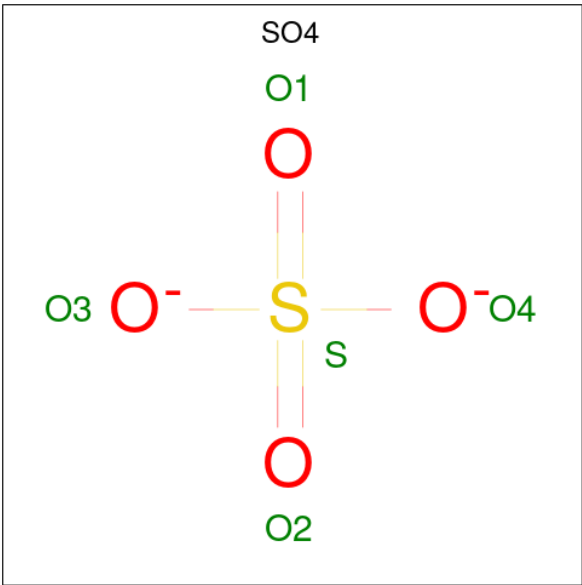
- Molecule 1 is a protein called Major prion protein homolog, Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	3	0
			1965	1234	326	394	11			
1	B	255	Total	C	N	O	S	0	1	0
			1951	1226	324	390	11			
1	C	252	Total	C	N	O	S	0	1	0
			1927	1211	321	385	10			
1	D	252	Total	C	N	O	S	0	1	0
			1927	1211	321	385	10			
1	E	254	Total	C	N	O	S	0	0	0
			1939	1219	323	387	10			
1	F	254	Total	C	N	O	S	0	0	0
			1939	1219	323	387	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P27177
A	2	GLY	-	expression tag	UNP P27177
B	1	MET	-	initiating methionine	UNP P27177
B	2	GLY	-	expression tag	UNP P27177
C	1	MET	-	initiating methionine	UNP P27177
C	2	GLY	-	expression tag	UNP P27177
D	1	MET	-	initiating methionine	UNP P27177
D	2	GLY	-	expression tag	UNP P27177
E	1	MET	-	initiating methionine	UNP P27177
E	2	GLY	-	expression tag	UNP P27177
F	1	MET	-	initiating methionine	UNP P27177
F	2	GLY	-	expression tag	UNP P27177

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



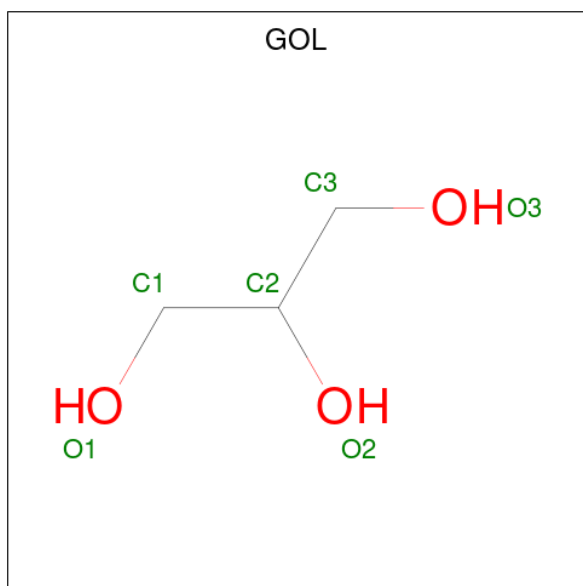
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	154	Total	O	0	0
			154	154		
4	C	182	Total	O	0	0
			182	182		
4	D	171	Total	O	0	0
			171	171		

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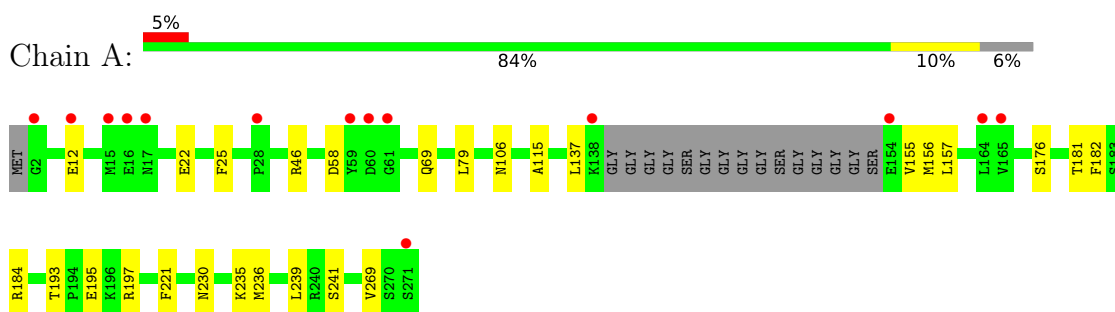
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	115	Total 115	O 115	0	0
4	F	156	Total 156	O 156	0	0

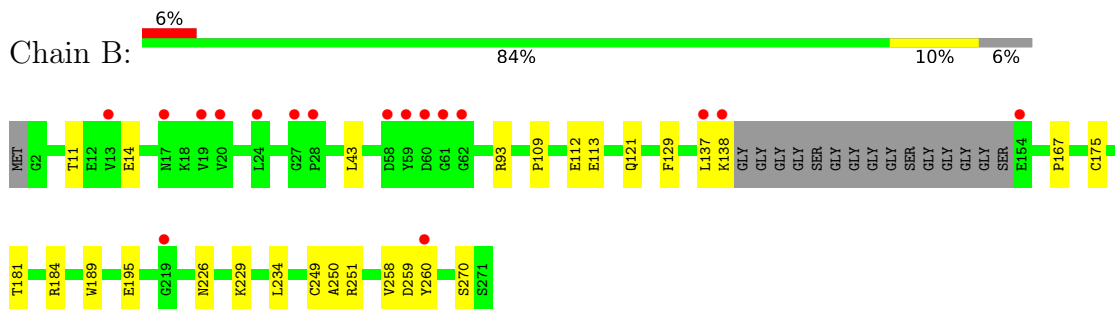
3 Residue-property plots [i](#)

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.

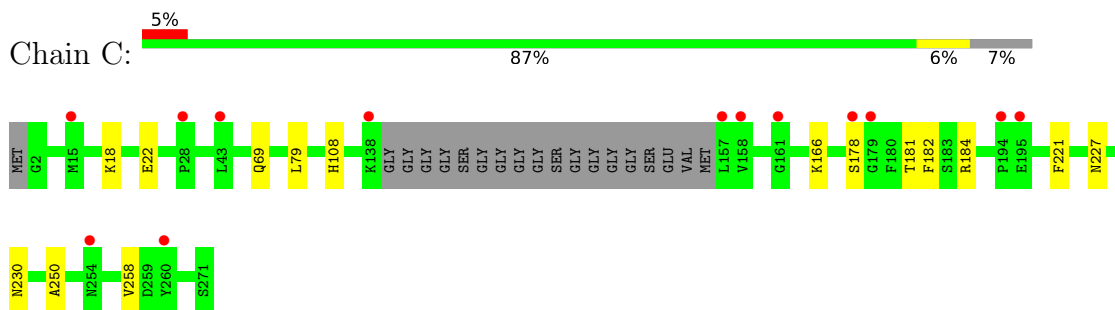
- Molecule 1: Major prion protein homolog,Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



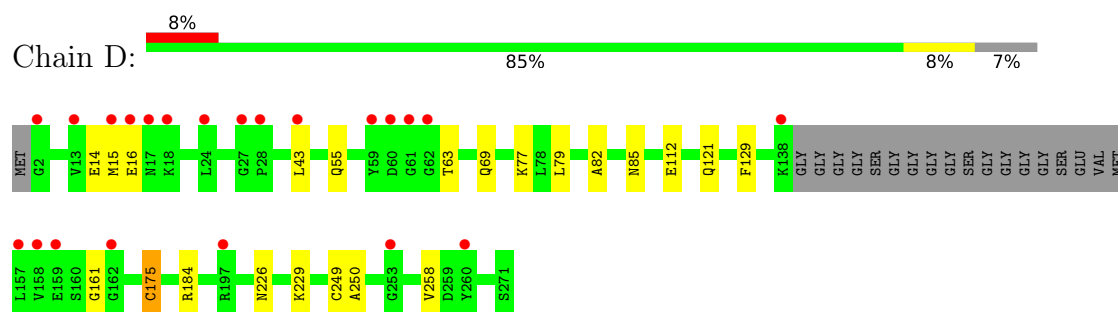
- Molecule 1: Major prion protein homolog,Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



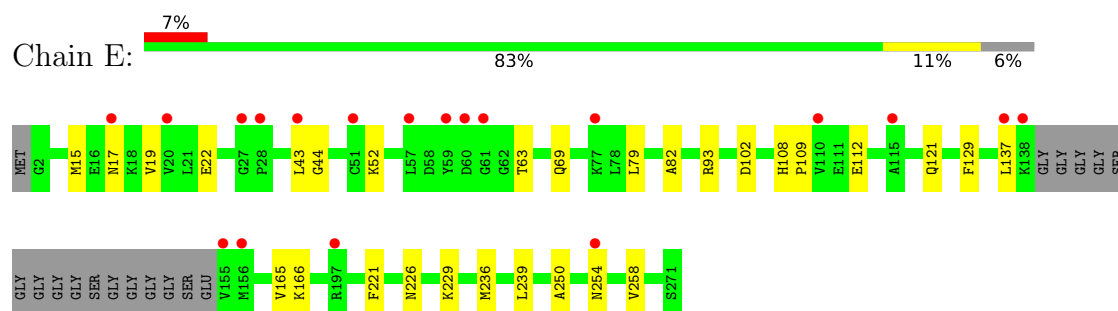
- Molecule 1: Major prion protein homolog,Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



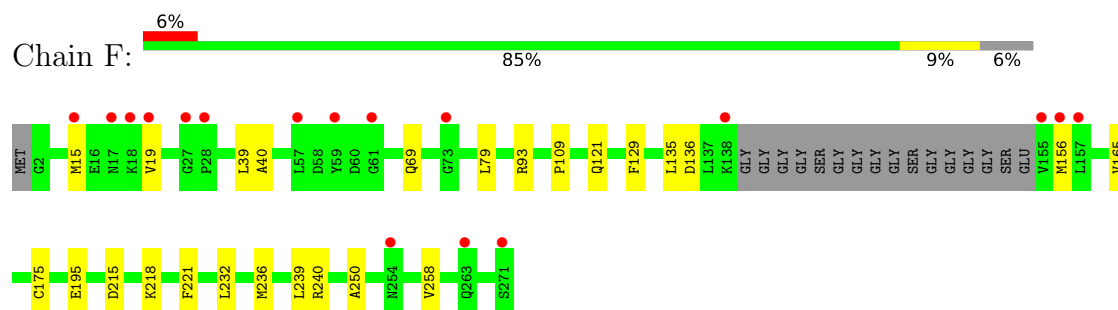
- Molecule 1: Major prion protein homolog,Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



- Molecule 1: Major prion protein homolog, Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



- Molecule 1: Major prion protein homolog, Single-chain Fv antibody of G2 fused with antigen peptide from chicken prion protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.36Å 86.72Å 86.58Å 105.13° 107.91° 100.88°	Depositor
Resolution (Å)	49.32 – 1.85 49.32 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.32-1.85) 91.5 (49.32-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.194 , 0.226 0.194 , 0.226	Depositor DCC
R_{free} test set	9155 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12729	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, SO4

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	0.41	0/2011	0.62	0/2722
1	B	0.38	0/1994	0.60	0/2699
1	C	0.40	0/1970	0.60	0/2667
1	D	0.39	0/1970	0.59	0/2667
1	E	0.35	0/1979	0.54	0/2679
1	F	0.36	0/1979	0.57	0/2679
All	All	0.38	0/11903	0.59	0/16113

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	A	1965	0	1895	16	0
1	B	1951	0	1885	15	0
1	C	1927	0	1860	20	0
1	D	1927	0	1861	25	0
1	E	1939	0	1874	25	0
1	F	1939	0	1874	19	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	20	0	0	0	0
2	D	15	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	12	0	16	5	0
4	A	204	0	0	3	0
4	B	154	0	0	0	0
4	C	182	0	0	3	0
4	D	171	0	0	3	0
4	E	115	0	0	1	0
4	F	156	0	0	0	0
All	All	12729	0	11281	117	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 (117) 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)
1:E:15:MET:HE2	1:E:19:VAL:HG11	1.17	1.10
1:E:15:MET:HE2	1:E:19:VAL:CG1	1.97	0.95
1:F:240:ARG:HH11	1:F:240:ARG:HG2	1.42	0.85
1:C:181:THR:HB	1:C:184:ARG:HD2	1.60	0.84
1:D:43:LEU:HD21	1:D:112:GLU:HG2	1.60	0.84
1:D:14:GLU:O	1:D:15:MET:HE2	1.80	0.81
1:E:15:MET:CE	1:E:19:VAL:HG11	2.09	0.76
1:D:15:MET:HE2	1:D:15:MET:HA	1.66	0.76
1:C:227:ASN:H	3:C:305:GOL:H2	1.51	0.75
1:F:215:ASP:O	1:F:218:LYS:HG2	1.88	0.73
1:E:226:ASN:CG	1:E:229:LYS:HD2	2.16	0.70
1:E:165:VAL:HG11	1:E:239:LEU:HD13	1.74	0.69
1:E:226:ASN:ND2	1:E:229:LYS:HD2	2.10	0.67
1:D:16:GLU:HB2	1:E:108:HIS:CD2	2.30	0.66
1:D:82:ALA:HB3	1:D:85:ASN:HD22	1.61	0.66
1:D:226:ASN:HD21	1:D:229:LYS:NZ	1.95	0.65
1:F:165:VAL:HG11	1:F:239:LEU:HD13	1.79	0.64
1:B:43:LEU:HD11	1:B:112:GLU:HG2	1.80	0.63
1:C:166:LYS:HD3	4:C:424:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:PHE:O	3:C:306:GOL:H32	2.00	0.61
1:D:82:ALA:HB3	1:D:85:ASN:ND2	2.16	0.60
1:B:260:TYR:OH	1:F:156:MET:HE3	2.02	0.59
1:D:226:ASN:HD21	1:D:229:LYS:HZ2	1.50	0.59
1:D:250:ALA:HB1	1:D:258:VAL:CG1	2.32	0.59
1:F:236:MET:HE2	1:F:239:LEU:HD21	1.85	0.57
1:E:226:ASN:HD21	1:E:229:LYS:NZ	2.02	0.57
1:E:236:MET:HE2	1:E:239:LEU:HD21	1.86	0.57
1:C:181:THR:CB	1:C:184:ARG:HD2	2.34	0.57
1:E:69:GLN:HB2	1:E:79:LEU:HD11	1.87	0.57
1:C:166:LYS:H	1:C:166:LYS:HE2	1.71	0.56
1:A:197:ARG:HD3	4:A:406:HOH:O	2.06	0.56
1:D:184:ARG:NH1	4:D:402:HOH:O	2.38	0.55
1:D:14:GLU:C	1:D:15:MET:HE2	2.32	0.55
1:A:181:THR:HB	1:A:184:ARG:HD2	1.89	0.54
1:E:22:GLU:HG2	4:E:405:HOH:O	2.07	0.54
1:C:227:ASN:HB2	3:C:305:GOL:H11	1.88	0.53
1:C:108:HIS:HE1	4:C:549:HOH:O	1.89	0.53
1:C:166:LYS:HD3	1:C:166:LYS:N	2.24	0.53
1:F:240:ARG:HH11	1:F:240:ARG:CG	2.18	0.53
1:C:166:LYS:H	1:C:166:LYS:CE	2.22	0.53
1:F:240:ARG:HG2	1:F:240:ARG:NH1	2.19	0.53
1:E:112:GLU:HA	1:E:137:LEU:HD13	1.90	0.52
1:D:175[A]:CYS:HB2	1:D:249:CYS:SG	2.49	0.52
1:E:15:MET:HE3	1:E:17:ASN:HB2	1.91	0.52
1:A:236:MET:HB3	1:A:239:LEU:HD21	1.93	0.50
1:B:121:GLN:HG3	1:B:129:PHE:CE2	2.47	0.50
1:F:175:CYS:HB3	1:F:232:LEU:HB3	1.93	0.50
1:C:166:LYS:H	1:C:166:LYS:CD	2.24	0.50
1:E:93:ARG:HD2	1:E:109:PRO:O	2.12	0.50
1:C:22:GLU:OE1	3:C:306:GOL:H31	2.12	0.49
1:D:226:ASN:CG	1:D:229:LYS:HD2	2.38	0.49
1:F:221:PHE:CZ	1:F:236:MET:HE3	2.47	0.49
1:C:166:LYS:N	1:C:166:LYS:CD	2.76	0.49
1:F:250:ALA:HB1	1:F:258:VAL:CG1	2.43	0.49
1:D:226:ASN:OD1	1:D:229:LYS:HD2	2.13	0.48
1:B:251:ARG:NH2	1:B:259:ASP:OD2	2.40	0.48
1:D:161:GLY:O	4:D:401:HOH:O	2.20	0.48
1:B:181:THR:HG21	1:B:184:ARG:HE	1.78	0.48
1:D:15:MET:HE2	1:D:15:MET:CA	2.39	0.47
1:D:16:GLU:CB	1:E:108:HIS:CD2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:LEU:HD21	1:F:135:LEU:HD13	1.96	0.47
1:F:15:MET:SD	1:F:19:VAL:HG11	2.54	0.47
1:E:52:LYS:HD3	1:E:102:ASP:OD1	2.14	0.47
1:B:167:PRO:HD3	1:B:270:SER:O	2.14	0.47
1:E:254:ASN:OD1	1:E:254:ASN:N	2.48	0.47
1:F:69:GLN:HB2	1:F:79:LEU:HD11	1.97	0.47
1:A:46:ARG:NH1	1:A:106[B]:ASN:OD1	2.48	0.47
1:B:250:ALA:HB1	1:B:258:VAL:CG1	2.45	0.47
1:D:15:MET:HA	1:D:15:MET:CE	2.31	0.47
1:A:221:PHE:CE1	1:A:236:MET:HG2	2.50	0.46
1:E:63:THR:O	1:E:82:ALA:HA	2.15	0.46
1:D:250:ALA:HB1	1:D:258:VAL:HG13	1.96	0.46
1:B:189:TRP:CE2	1:B:234:LEU:HB2	2.50	0.46
1:B:226:ASN:ND2	1:B:229:LYS:HG3	2.31	0.46
1:E:250:ALA:HB1	1:E:258:VAL:CG1	2.46	0.46
1:E:112:GLU:HA	1:E:137:LEU:CD1	2.47	0.45
1:A:195[B]:GLU:H	1:A:195[B]:GLU:CD	2.24	0.45
1:C:250:ALA:HB1	1:C:258:VAL:CG1	2.46	0.45
1:D:63:THR:O	1:D:82:ALA:HA	2.17	0.45
1:E:221:PHE:CZ	1:E:236:MET:HE3	2.51	0.45
1:A:58:ASP:OD2	4:A:401:HOH:O	2.21	0.45
1:C:181:THR:HB	1:C:184:ARG:CD	2.39	0.44
1:D:69:GLN:HB2	1:D:79:LEU:HD11	1.98	0.44
1:B:195:GLU:H	1:B:195:GLU:CD	2.26	0.44
1:F:240:ARG:CG	1:F:240:ARG:NH1	2.79	0.44
1:A:69:GLN:HB2	1:A:79:LEU:HD11	2.00	0.44
1:E:166:LYS:HB3	1:E:166:LYS:HE3	1.55	0.43
1:A:182:PHE:CD2	1:A:230:ASN:HA	2.53	0.43
1:D:77:LYS:HE2	2:D:303:SO4:S	2.57	0.43
1:E:43:LEU:C	1:E:43:LEU:HD13	2.43	0.43
1:F:40:ALA:HA	1:F:136:ASP:O	2.18	0.43
1:F:250:ALA:HB1	1:F:258:VAL:HG11	2.00	0.43
1:D:55:GLN:HG3	4:D:440:HOH:O	2.18	0.43
1:A:22:GLU:HG2	4:A:408:HOH:O	2.19	0.43
1:A:221:PHE:CD1	1:A:236:MET:HG2	2.54	0.42
1:B:93:ARG:HD2	1:B:109:PRO:O	2.19	0.42
1:C:69:GLN:HB2	1:C:79:LEU:HD11	2.00	0.42
1:C:182:PHE:CD2	1:C:230:ASN:HA	2.54	0.42
1:A:115:ALA:HB2	1:A:137:LEU:HD23	2.01	0.42
1:C:166:LYS:CD	4:C:424:HOH:O	2.64	0.42
1:A:193:THR:OG1	1:A:195[A]:GLU:CD	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:THR:O	1:B:14:GLU:HG3	2.20	0.42
1:D:175[A]:CYS:SG	1:D:249:CYS:SG	3.17	0.42
1:C:22:GLU:OE1	3:C:306:GOL:C3	2.68	0.42
1:C:18:LYS:H	1:C:18:LYS:HD2	1.85	0.42
1:A:241:SER:HA	1:A:269:VAL:HB	2.02	0.41
1:E:43:LEU:HD13	1:E:44:GLY:N	2.34	0.41
1:F:93:ARG:HD2	1:F:109:PRO:O	2.21	0.41
1:F:195:GLU:H	1:F:195:GLU:CD	2.29	0.41
1:B:112:GLU:HA	1:B:137:LEU:CD1	2.50	0.41
1:B:113:GLU:OE1	1:B:113:GLU:N	2.34	0.41
1:D:121:GLN:HG3	1:D:129:PHE:CE2	2.56	0.41
1:A:156:MET:HG3	1:A:157:LEU:N	2.35	0.40
1:F:121:GLN:HG3	1:F:129:PHE:CE2	2.56	0.40
1:A:12:GLU:OE2	1:A:25:PHE:HE2	2.04	0.40
1:E:121:GLN:HG3	1:E:129:PHE:CE2	2.56	0.40
1:B:175[B]:CYS:CB	1:B:249:CYS:SG	3.09	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	254/271 (94%)	246 (97%)	8 (3%)	0	100	100
1	B	252/271 (93%)	244 (97%)	8 (3%)	0	100	100
1	C	249/271 (92%)	241 (97%)	8 (3%)	0	100	100
1	D	249/271 (92%)	239 (96%)	10 (4%)	0	100	100
1	E	250/271 (92%)	239 (96%)	11 (4%)	0	100	100
1	F	250/271 (92%)	239 (96%)	11 (4%)	0	100	100
All	All	1504/1626 (92%)	1448 (96%)	56 (4%)	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	214/215 (100%)	211 (99%)	3 (1%)	59	49
1	B	212/215 (99%)	211 (100%)	1 (0%)	81	77
1	C	209/215 (97%)	208 (100%)	1 (0%)	81	77
1	D	209/215 (97%)	207 (99%)	2 (1%)	68	60
1	E	210/215 (98%)	210 (100%)	0	100	100
1	F	210/215 (98%)	210 (100%)	0	100	100
All	All	1264/1290 (98%)	1257 (99%)	7 (1%)	81	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	176	SER
1	A	235	LYS
1	B	138	LYS
1	C	178	SER
1	D	175[A]	CYS
1	D	175[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	192	GLN
1	A	254	ASN
1	C	17	ASN
1	C	55	GLN
1	D	26	GLN
1	D	70	GLN

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Mol	Chain	Res	Type
1	D	74	GLN
1	D	85	ASN
1	D	192	GLN
1	D	226	ASN
1	E	17	ASN
1	E	55	GLN
1	E	70	GLN
1	E	108	HIS
1	E	192	GLN
1	E	226	ASN
1	F	69	GLN
1	F	230	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](#)

19 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	$\# Z > 2$
2	SO4	D	303	-	4,4,4	0.81	0	6,6,6	0.66	0
2	SO4	C	303	-	4,4,4	0.80	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	301	-	4,4,4	0.71	0	6,6,6	0.24	0
2	SO4	B	302	-	4,4,4	0.68	0	6,6,6	0.41	0
3	GOL	A	305	-	5,5,5	0.33	0	5,5,5	0.43	0
2	SO4	C	302	-	4,4,4	0.66	0	6,6,6	0.40	0
3	GOL	B	303	-	5,5,5	0.24	0	5,5,5	0.71	0
3	GOL	C	306	-	5,5,5	0.56	0	5,5,5	0.85	0
2	SO4	A	302	-	4,4,4	0.87	0	6,6,6	0.36	0
2	SO4	E	301	-	4,4,4	0.66	0	6,6,6	0.47	0
2	SO4	C	304	-	4,4,4	0.76	0	6,6,6	0.43	0
3	GOL	C	305	-	5,5,5	0.66	0	5,5,5	0.60	0
2	SO4	A	304	-	4,4,4	0.77	0	6,6,6	0.51	0
2	SO4	F	301	-	4,4,4	0.65	0	6,6,6	0.62	0
2	SO4	B	301	-	4,4,4	0.70	0	6,6,6	0.41	0
2	SO4	C	301	-	4,4,4	0.72	0	6,6,6	0.23	0
2	SO4	A	303	-	4,4,4	0.74	0	6,6,6	0.44	0
2	SO4	A	301	-	4,4,4	0.90	0	6,6,6	0.57	0
2	SO4	D	302	-	4,4,4	0.76	0	6,6,6	0.49	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	A	305	-	-	4/4/4/4	-
3	GOL	C	306	-	-	1/4/4/4	-
3	GOL	B	303	-	-	4/4/4/4	-
3	GOL	C	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	305	GOL	O1-C1-C2-O2
3	A	305	GOL	O1-C1-C2-C3
3	B	303	GOL	O1-C1-C2-C3
3	B	303	GOL	C1-C2-C3-O3
3	B	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	305	GOL	C1-C2-C3-O3
3	A	305	GOL	C1-C2-C3-O3
3	C	305	GOL	O2-C2-C3-O3
3	A	305	GOL	O2-C2-C3-O3
3	C	306	GOL	O1-C1-C2-C3
3	B	303	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	303	SO4	1	0
3	C	306	GOL	3	0
3	C	305	GOL	2	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	255/271 (94%)	0.34	14 (5%)	30	33	14, 32, 53, 101	3 (1%)
1	B	255/271 (94%)	0.57	17 (6%)	24	26	24, 35, 58, 91	1 (0%)
1	C	252/271 (92%)	0.53	13 (5%)	33	35	24, 35, 54, 70	1 (0%)
1	D	252/271 (92%)	0.55	22 (8%)	16	16	23, 35, 62, 91	1 (0%)
1	E	254/271 (93%)	0.70	19 (7%)	20	22	27, 40, 63, 95	0
1	F	254/271 (93%)	0.62	17 (6%)	24	26	28, 37, 62, 98	0
All	All	1522/1626 (93%)	0.55	102 (6%)	24	26	14, 36, 59, 101	6 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	LEU	6.1
1	E	155	VAL	5.8
1	D	61	GLY	5.5
1	F	155	VAL	5.3
1	B	154	GLU	5.3
1	D	157	LEU	4.7
1	F	59	TYR	4.3
1	D	138	LYS	4.3
1	E	61	GLY	4.3
1	B	62	GLY	4.1
1	D	59	TYR	4.0
1	B	19	VAL	4.0
1	F	28	PRO	3.9
1	A	2	GLY	3.9
1	D	15	MET	3.6
1	C	260	TYR	3.6
1	C	28	PRO	3.6
1	F	17	ASN	3.5
1	A	16	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	138	LYS	3.5
1	D	260	TYR	3.4
1	E	59	TYR	3.4
1	A	15	MET	3.3
1	B	60	ASP	3.3
1	A	61	GLY	3.3
1	B	61	GLY	3.2
1	D	2	GLY	3.2
1	D	62	GLY	3.2
1	F	138	LYS	3.2
1	B	59	TYR	3.2
1	C	254	ASN	3.2
1	B	260	TYR	3.2
1	E	43	LEU	3.1
1	F	157	LEU	3.1
1	F	271	SER	3.1
1	D	60	ASP	3.1
1	D	28	PRO	3.1
1	D	16	GLU	3.0
1	A	60	ASP	3.0
1	C	195	GLU	3.0
1	B	27	GLY	3.0
1	F	61	GLY	3.0
1	F	73	GLY	2.9
1	A	271	SER	2.9
1	D	27	GLY	2.9
1	D	158	VAL	2.8
1	D	24	LEU	2.8
1	D	18	LYS	2.6
1	A	164	LEU	2.6
1	E	156	MET	2.6
1	B	20	VAL	2.6
1	F	19	VAL	2.6
1	D	17	ASN	2.6
1	A	28	PRO	2.5
1	E	137	LEU	2.5
1	E	254	ASN	2.5
1	E	17	ASN	2.5
1	B	13	VAL	2.5
1	C	158	VAL	2.5
1	E	60	ASP	2.5
1	B	138	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	17	ASN	2.4
1	D	197	ARG	2.4
1	D	13	VAL	2.4
1	D	162	GLY	2.4
1	C	138	LYS	2.4
1	E	115	ALA	2.4
1	A	12	GLU	2.4
1	B	28	PRO	2.4
1	F	263	GLN	2.3
1	E	28	PRO	2.3
1	B	219	GLY	2.3
1	B	24	LEU	2.3
1	A	59	TYR	2.3
1	F	18	LYS	2.3
1	F	57	LEU	2.3
1	A	154	GLU	2.2
1	C	161	GLY	2.2
1	A	165	VAL	2.2
1	E	20	VAL	2.2
1	E	27	GLY	2.2
1	B	58	ASP	2.2
1	E	110	VAL	2.2
1	E	51	CYS	2.2
1	D	43	LEU	2.2
1	E	197	ARG	2.2
1	C	15	MET	2.1
1	F	15	MET	2.1
1	F	156	MET	2.1
1	C	179	GLY	2.1
1	C	43	LEU	2.1
1	C	194	PRO	2.1
1	E	57	LEU	2.1
1	D	159	GLU	2.1
1	B	17	ASN	2.1
1	B	137	LEU	2.1
1	A	138	LYS	2.0
1	D	253	GLY	2.0
1	E	77	LYS	2.0
1	C	178	SER	2.0
1	F	27	GLY	2.0
1	F	254	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](#)

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
3	GOL	A	305	6/6	0.76	0.22	39,49,57,62	0
3	GOL	C	305	6/6	0.78	0.18	38,54,55,70	0
3	GOL	C	306	6/6	0.81	0.15	44,47,55,58	0
2	SO4	D	303	5/5	0.83	0.12	57,66,66,71	0
2	SO4	A	303	5/5	0.83	0.12	53,70,73,78	0
2	SO4	D	301	5/5	0.84	0.10	59,68,83,91	0
2	SO4	C	303	5/5	0.86	0.09	58,67,74,76	0
2	SO4	B	301	5/5	0.86	0.11	66,73,74,79	0
2	SO4	A	304	5/5	0.87	0.11	64,67,71,75	0
2	SO4	A	302	5/5	0.87	0.10	59,61,68,74	0
2	SO4	B	302	5/5	0.87	0.10	61,68,72,72	0
2	SO4	C	304	5/5	0.88	0.09	64,65,91,94	0
2	SO4	D	302	5/5	0.89	0.09	55,69,75,81	0
3	GOL	B	303	6/6	0.89	0.14	35,52,55,62	0
2	SO4	C	302	5/5	0.91	0.09	68,70,74,76	0
2	SO4	F	301	5/5	0.92	0.10	47,53,75,88	0
2	SO4	E	301	5/5	0.93	0.09	54,62,73,74	0
2	SO4	C	301	5/5	0.94	0.07	51,57,72,72	0
2	SO4	A	301	5/5	0.97	0.07	37,39,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.