



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:52 PM UTC

PDB ID : 7S4G / pdb_00007s4g
Title : Fab fragment bound to the Cter peptide of Ly6G6D
Authors : Rouge, L.; Lupardus, P.
Deposited on : 2021-09-08
Resolution : 2.20 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

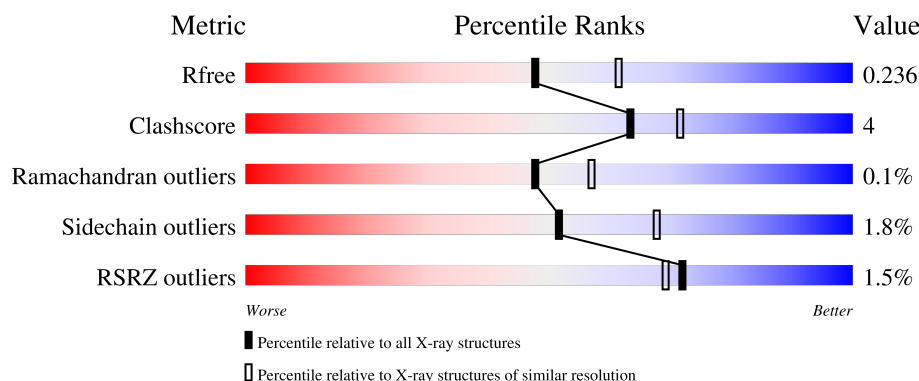
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	223	 2% 80% 12% 7%
1	C	223	 84% 9% 6%
1	E	223	 84% 9% 7%
1	H	223	 83% 11% 6%
2	B	220	 2% 90% 9%

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Mol	Chain	Length	Quality of chain
2	D	220	% 88%11%.
2	F	220	2% 84%14%..
2	L	220	% 88%11%.
3	G	9	11% 67%33%
3	I	9	11% 100%
3	J	9	11% 56%44%
3	K	9	11% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14394 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 heavy chain Fab 1G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1584	1003	267	306	8			
1	C	210	Total	C	N	O	S	0	0	0
			1592	1007	269	308	8			
1	E	208	Total	C	N	O	S	0	0	0
			1583	1002	267	306	8			
1	H	210	Total	C	N	O	S	0	0	0
			1592	1007	269	308	8			

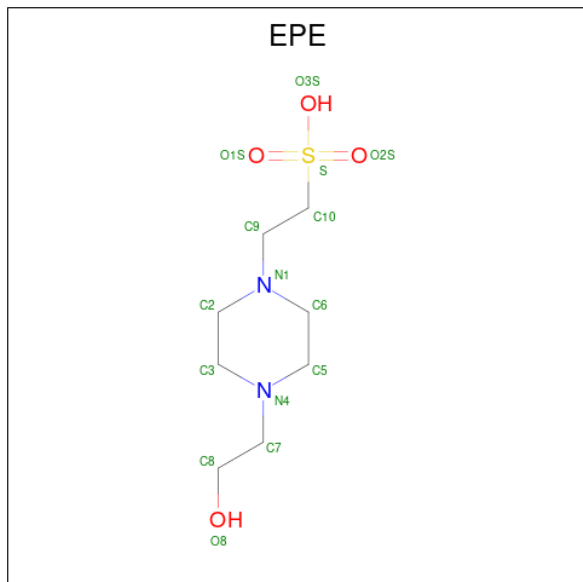
- Molecule 2 is a protein called light chain Fab 1G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	1	0
			1667	1041	281	340	5			
2	D	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			
2	F	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			
2	L	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			

- Molecule 3 is a protein called Lymphocyte antigen 6 complex locus protein G6d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	I	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	J	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	K	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	5
			112	112		
6	B	138	Total	O	0	5
			143	143		
6	C	148	Total	O	0	3
			151	151		
6	D	130	Total	O	0	7
			137	137		
6	E	96	Total	O	0	2
			98	98		
6	F	124	Total	O	0	3
			127	127		
6	G	5	Total	O	0	0
			5	5		
6	I	5	Total	O	0	1
			6	6		
6	J	6	Total	O	0	0
			6	6		
6	K	6	Total	O	0	0
			6	6		

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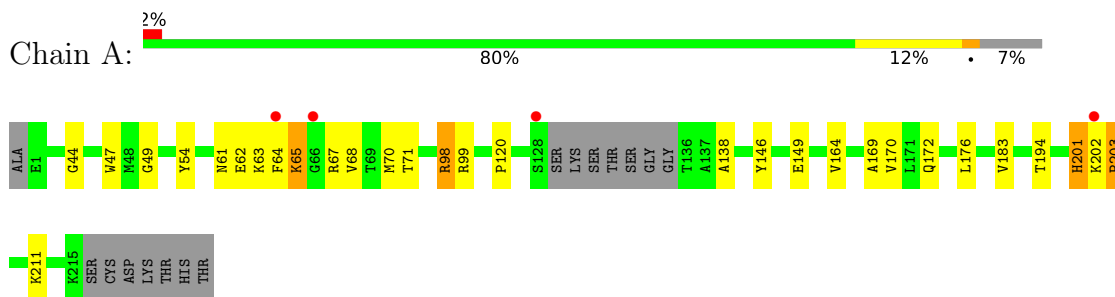
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	113	Total 116	O 116	0	3
6	L	125	Total 127	O 127	0	2

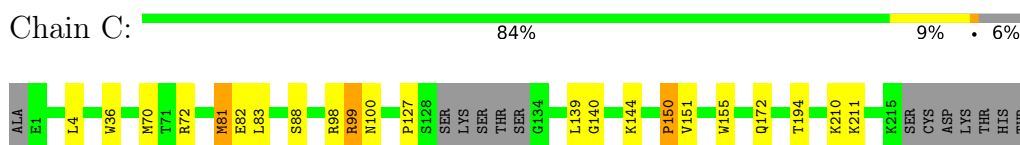
3 Residue-property plots

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.

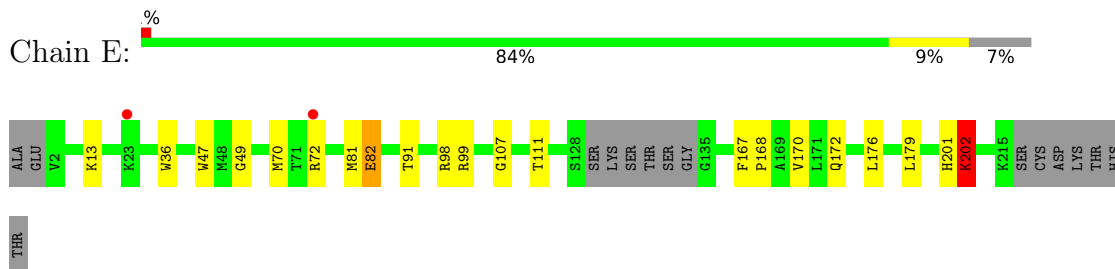
- Molecule 1: heavy chain Fab 1G4



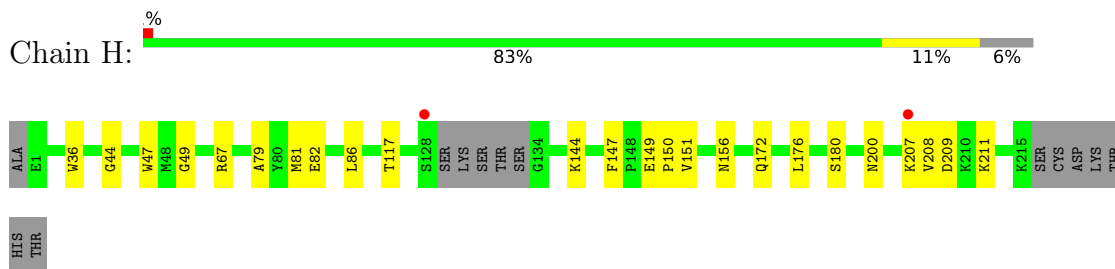
- Molecule 1: heavy chain Fab 1G4



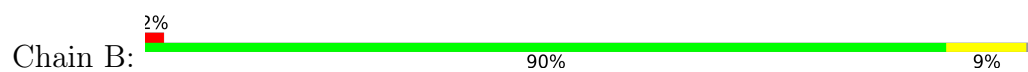
- Molecule 1: heavy chain Fab 1G4



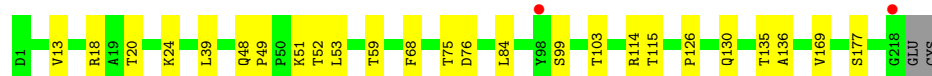
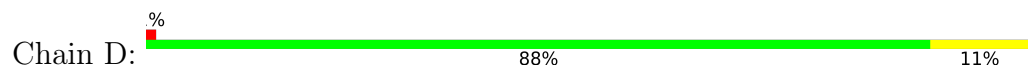
- Molecule 1: heavy chain Fab 1G4



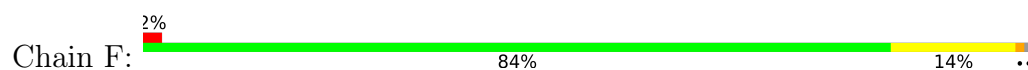
- Molecule 2: light chain Fab 1G4



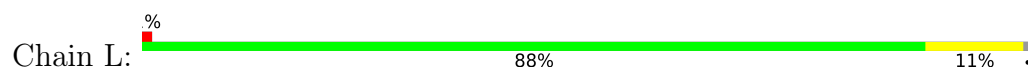
- Molecule 2: light chain Fab 1G4



- Molecule 2: light chain Fab 1G4



- Molecule 2: light chain Fab 1G4



- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d



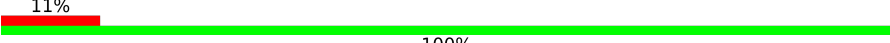
- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d



- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d



- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d

Chain K:  11% 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.29Å 133.39Å 100.04Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	35.05 – 2.20 35.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.05-2.20) 96.9 (35.05-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.192 , 0.235 0.193 , 0.236	Depositor DCC
R_{free} test set	4246 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14394	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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, EPE

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	0.70	5/1623 (0.3%)	0.64	0/2210
1	C	0.55	5/1631 (0.3%)	0.58	0/2220
1	E	0.72	4/1622 (0.2%)	0.63	1/2208 (0.0%)
1	H	0.91	8/1631 (0.5%)	0.68	1/2220 (0.0%)
2	B	0.74	5/1705 (0.3%)	0.70	1/2318 (0.0%)
2	D	0.68	6/1701 (0.4%)	0.71	5/2312 (0.2%)
2	F	0.55	2/1701 (0.1%)	0.61	2/2312 (0.1%)
2	L	0.69	2/1701 (0.1%)	0.70	1/2312 (0.0%)
3	G	0.54	0/68	0.66	0/91
3	I	0.82	0/68	1.35	0/91
3	J	1.52	2/68 (2.9%)	1.45	3/91 (3.3%)
3	K	0.41	0/68	0.61	0/91
All	All	0.70	39/13587 (0.3%)	0.67	14/18476 (0.1%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	202	LYS	C-O	-8.98	1.16	1.24
1	A	202	LYS	C-O	-7.73	1.17	1.24
2	B	144	ASN	C-O	-7.19	1.15	1.24
1	A	138	ALA	C-N	-7.17	1.24	1.33
2	D	48	GLN	C-O	-7.02	1.17	1.24
2	B	153	GLN	C-O	-6.92	1.16	1.24
2	D	49	PRO	C-O	-6.71	1.17	1.24
1	C	83	LEU	C-O	-6.61	1.16	1.24
1	C	82	GLU	C-O	-6.53	1.16	1.24
3	J	99	GLY	C-O	-6.32	1.15	1.23
1	H	156	ASN	C-N	-6.25	1.25	1.33
2	D	52	THR	C-O	-6.14	1.16	1.24
1	C	81	MET	C-O	-6.09	1.17	1.24
2	B	61	ILE	C-O	-5.96	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	99	ARG	C-N	-5.84	1.26	1.33
1	C	98	ARG	C-N	-5.80	1.25	1.33
2	L	217	ARG	C-O	-5.79	1.16	1.24
1	A	71	THR	C-O	-5.67	1.16	1.23
1	H	67	ARG	C-O	-5.65	1.16	1.24
1	H	208	VAL	C-O	-5.63	1.18	1.24
2	F	149	GLU	C-O	-5.61	1.17	1.23
1	H	82	GLU	C-O	-5.60	1.17	1.24
3	J	97	TYR	C-O	-5.52	1.16	1.24
1	A	203	PRO	C-O	-5.44	1.17	1.24
2	F	151	LYS	C-O	-5.43	1.17	1.24
1	H	209	ASP	C-O	-5.37	1.18	1.24
2	D	59	THR	C-O	-5.35	1.17	1.24
1	E	201	HIS	C-O	-5.31	1.17	1.23
1	H	86	LEU	C-O	-5.28	1.17	1.23
1	E	82	GLU	CA-C	-5.26	1.46	1.52
1	H	211	LYS	N-CA	-5.21	1.39	1.46
2	L	42	HIS	C-O	-5.21	1.17	1.24
1	A	201	HIS	C-O	-5.19	1.16	1.23
2	D	53	LEU	C-O	-5.18	1.16	1.23
2	D	169	VAL	C-O	-5.16	1.19	1.24
2	B	151	LYS	C-O	-5.13	1.17	1.24
1	H	79	ALA	C-O	-5.08	1.17	1.24
2	B	214	SER	C-O	-5.02	1.18	1.23
1	E	70	MET	C-O	-5.00	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	97	TYR	N-CA-C	7.20	122.06	113.28
2	D	103	THR	N-CA-C	7.06	120.46	110.50
3	J	102	CYS	N-CA-C	6.27	118.92	108.20
2	D	49	PRO	CA-C-N	-6.02	114.07	120.03
2	D	49	PRO	C-N-CA	-6.02	114.07	120.03
2	B	214	SER	N-CA-C	5.79	116.20	108.38
2	F	148	ARG	N-CA-C	5.65	118.17	111.33
2	D	48	GLN	CA-C-N	-5.40	114.82	120.38
2	D	48	GLN	C-N-CA	-5.40	114.82	120.38
2	L	44	GLN	N-CA-C	5.39	117.20	108.26
2	F	146	TYR	C-N-CD	5.33	132.31	120.60
3	J	98	LEU	N-CA-C	-5.25	100.83	109.40
1	E	107	GLY	N-CA-C	5.05	118.59	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	86	LEU	N-CA-C	5.05	117.36	110.24

There are no chirality outliers.

There are no planarity outliers.

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	1584	0	1551	17	0
1	C	1592	0	1557	9	0
1	E	1583	0	1549	18	0
1	H	1592	0	1557	10	0
2	B	1667	0	1623	10	0
2	D	1666	0	1620	9	0
2	F	1666	0	1620	31	0
2	L	1666	0	1620	13	0
3	G	68	0	55	2	0
3	I	68	0	55	0	0
3	J	68	0	55	0	0
3	K	68	0	55	0	0
4	B	15	0	17	0	0
4	D	15	0	17	0	0
4	F	15	0	17	1	0
4	L	15	0	18	1	0
5	D	6	0	8	1	0
5	L	6	0	8	2	0
6	A	112	0	0	1	0
6	B	143	0	0	3	0
6	C	151	0	0	1	0
6	D	137	0	0	1	0
6	E	98	0	0	1	0
6	F	127	0	0	1	0
6	G	5	0	0	0	0
6	H	116	0	0	1	0
6	I	6	0	0	0	0
6	J	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	6	0	0	0	0
6	L	127	0	0	1	0
All	All	14394	0	13002	106	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 4.

All (106) 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:164:ASN:O	2:F:185:LEU:HD12	1.68	0.93
2:B:194:LYS:HE2	6:B:488:HOH:O	1.68	0.93
2:F:167:GLU:OE1	6:F:401[B]:HOH:O	1.90	0.87
1:A:64:PHE:O	1:A:68:VAL:HG12	1.74	0.86
1:E:170:VAL:CG1	2:F:166:GLN:NE2	2.40	0.84
2:F:167:GLU:OE2	2:F:181:LEU:HD11	1.80	0.81
2:L:197:VAL:HG22	2:L:216:ASN:OD1	1.86	0.76
2:F:165:SER:HA	2:F:184:THR:O	1.88	0.74
2:L:65:PRO:HG2	5:L:302:GOL:H32	1.72	0.70
2:F:167:GLU:HA	2:F:182:SER:O	1.93	0.69
1:H:200:ASN:OD1	1:H:207:LYS:HE3	1.93	0.67
2:B:130:GLN:O	2:B:133:SER:HB3	1.95	0.67
1:E:170:VAL:HG11	2:F:166:GLN:CD	2.23	0.63
1:E:170:VAL:HG11	2:F:166:GLN:NE2	2.15	0.61
1:E:170:VAL:HG12	2:F:166:GLN:NE2	2.14	0.61
2:D:114:ARG:NH1	2:D:115:THR:O	2.34	0.60
1:E:172:GLN:HG2	1:E:176:LEU:O	2.01	0.60
2:F:164:ASN:O	2:F:165:SER:HB3	2.00	0.60
1:A:65:LYS:NZ	6:A:304:HOH:O	2.36	0.59
1:A:201:HIS:CD2	1:A:203:PRO:HD2	2.38	0.59
3:G:98:LEU:HB2	3:G:101:LEU:HB2	1.86	0.57
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.41	0.56
1:E:170:VAL:CG1	2:F:166:GLN:CD	2.79	0.56
2:L:164:ASN:OD1	2:L:185:LEU:HD12	2.08	0.54
2:D:13:VAL:HG23	2:D:84:LEU:HD22	1.90	0.54
1:A:65:LYS:HG2	1:C:88:SER:OG	2.07	0.54
2:F:187:LEU:HD23	2:F:191:ASP:HB3	1.90	0.54
2:F:164:ASN:O	2:F:185:LEU:CD1	2.50	0.53
2:F:166:GLN:O	2:F:184:THR:N	2.30	0.53
2:D:68:PHE:CE2	5:D:302:GOL:H31	2.44	0.52
1:E:168:PRO:HB2	2:F:168:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:119:PRO:HB3	2:L:145:PHE:HB3	1.92	0.52
1:C:144:LYS:NZ	1:C:172:GLN:OE1	2.42	0.52
1:E:36:TRP:CE2	1:E:81:MET:HB2	2.45	0.51
2:F:31:LEU:HD11	3:G:103:ASN:C	2.36	0.51
2:L:151:LYS:HB3	2:L:203:THR:OG1	2.11	0.51
1:A:172:GLN:HG2	1:A:176:LEU:O	2.11	0.50
2:F:190:ALA:O	2:F:194:LYS:HG3	2.11	0.50
2:B:111:GLU:OE1	2:B:179:TYR:OH	2.21	0.50
2:L:164:ASN:OD1	2:L:185:LEU:CD1	2.59	0.50
1:E:98:ARG:HG2	1:E:99:ARG:HB2	1.94	0.50
1:A:98:ARG:HG2	1:A:99:ARG:HB2	1.94	0.50
2:F:155:LYS:HE2	2:F:160:LEU:HD21	1.94	0.49
1:A:61:ASN:C	1:A:63:LYS:H	2.19	0.49
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.47	0.49
1:A:149:GLU:OE2	1:A:169:ALA:HB3	2.12	0.49
2:F:167:GLU:CA	2:F:182:SER:O	2.60	0.49
1:C:194:THR:HG23	1:C:211:LYS:HE2	1.93	0.49
2:B:205:GLN:HG2	6:B:416:HOH:O	2.13	0.48
1:E:167:PHE:CD2	2:F:170:THR:HG23	2.49	0.48
2:D:51:LYS:HD2	6:D:427[B]:HOH:O	2.14	0.48
2:F:114:ARG:HG2	2:F:115:THR:N	2.29	0.48
1:H:172:GLN:HG2	1:H:176:LEU:O	2.14	0.48
1:E:47:TRP:CE3	2:F:101:PRO:HA	2.48	0.48
1:A:62:GLU:O	1:A:62:GLU:HG3	2.12	0.48
2:B:60:ARG:HG2	2:B:64:VAL:HB	1.95	0.48
1:H:117:THR:HA	1:H:147:PHE:O	2.15	0.47
1:C:150:PRO:HB3	6:C:436:HOH:O	2.13	0.47
1:C:99:ARG:HG2	1:C:100:ASN:H	1.80	0.47
2:B:194:LYS:O	2:B:194:LYS:HG2	2.15	0.46
1:E:170:VAL:HG12	2:F:166:GLN:HE22	1.79	0.46
1:H:200:ASN:OD1	1:H:207:LYS:CE	2.63	0.46
2:B:11:LEU:HG	2:B:13:VAL:HG23	1.97	0.45
2:L:175:LYS:HE3	6:L:446:HOH:O	2.15	0.45
2:D:24:LYS:HD2	2:D:75:THR:O	2.17	0.45
2:F:4:MET:HE3	2:F:23:CYS:SG	2.57	0.45
1:A:44:GLY:HA3	6:B:454:HOH:O	2.17	0.45
1:H:44:GLY:HA3	6:H:319:HOH:O	2.16	0.45
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.52	0.45
2:L:65:PRO:CG	5:L:302:GOL:H32	2.43	0.45
2:F:13:VAL:HB	2:F:84:LEU:HD22	1.98	0.44
2:D:130:GLN:HG2	2:D:135:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:59:THR:HG21	4:L:301:EPE:H102	1.99	0.44
2:B:131:LEU:C	2:B:133:SER:H	2.26	0.44
2:D:114:ARG:HD2	2:D:177:SER:O	2.18	0.43
1:E:167:PHE:CD2	2:F:170:THR:CG2	3.01	0.43
1:A:54:TYR:CZ	2:L:35:GLN:HG2	2.53	0.43
1:C:140:GLY:HA2	1:C:155:TRP:CZ2	2.53	0.43
1:E:91:THR:HG23	1:E:111:THR:HA	2.01	0.43
1:A:61:ASN:OD1	1:A:63:LYS:HB2	2.17	0.43
2:D:24:LYS:HD3	2:D:76:ASP:OD1	2.18	0.43
2:F:39:LEU:HD13	2:F:77:PHE:CD2	2.53	0.43
4:F:301:EPE:H102	4:F:301:EPE:H22	1.70	0.43
1:H:207:LYS:HE3	1:H:207:LYS:HB2	1.68	0.43
2:B:131:LEU:C	2:B:133:SER:N	2.77	0.43
1:E:167:PHE:CE2	2:F:170:THR:HG23	2.54	0.42
1:A:98:ARG:HG2	1:A:99:ARG:CB	2.48	0.42
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.54	0.42
1:H:149:GLU:HG2	1:H:150:PRO:HA	2.01	0.42
1:A:194:THR:HB	1:A:211:LYS:HE3	2.02	0.42
2:B:15:LEU:HD12	2:B:15:LEU:HA	1.83	0.42
1:E:202:LYS:H	1:E:202:LYS:HG3	1.64	0.42
2:D:126:PRO:HG3	2:D:136:ALA:HB1	2.02	0.41
2:L:130:GLN:O	2:L:133:SER:OG	2.32	0.41
1:C:127:PRO:HG3	1:C:139:LEU:HB3	2.01	0.41
2:F:132:LYS:HA	2:F:132:LYS:HD3	1.76	0.41
2:F:155:LYS:HG2	2:F:160:LEU:HD23	2.03	0.41
1:C:36:TRP:CE2	1:C:81:MET:HB2	2.56	0.41
1:C:36:TRP:HB2	1:C:70:MET:HE2	2.03	0.41
2:L:54:ILE:HD13	2:L:60:ARG:HA	2.03	0.41
1:E:47:TRP:CZ2	1:E:49:GLY:HA2	2.55	0.41
1:A:120:PRO:HB3	1:A:146:TYR:HB3	2.03	0.40
1:A:164:VAL:HG22	1:A:183:VAL:HB	2.04	0.40
2:F:146:TYR:HA	2:F:147:PRO:HA	1.82	0.40
1:E:13:LYS:NZ	6:E:301:HOH:O	2.22	0.40
2:L:11:LEU:HG	2:L:13:VAL:HG23	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	204/223 (92%)	192 (94%)	11 (5%)	1 (0%)	24	27
1	C	206/223 (92%)	201 (98%)	5 (2%)	0	100	100
1	E	204/223 (92%)	201 (98%)	3 (2%)	0	100	100
1	H	206/223 (92%)	200 (97%)	6 (3%)	0	100	100
2	B	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
2	D	216/220 (98%)	210 (97%)	6 (3%)	0	100	100
2	F	216/220 (98%)	208 (96%)	7 (3%)	1 (0%)	24	27
2	L	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
3	G	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
3	K	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1712/1808 (95%)	1655 (97%)	55 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
2	F	165	SER

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	177/191 (93%)	173 (98%)	4 (2%)	44	59
1	C	177/191 (93%)	172 (97%)	5 (3%)	38	52
1	E	177/191 (93%)	173 (98%)	4 (2%)	44	59
1	H	177/191 (93%)	174 (98%)	3 (2%)	53	69
2	B	191/192 (100%)	189 (99%)	2 (1%)	68	81
2	D	190/192 (99%)	186 (98%)	4 (2%)	47	63
2	F	190/192 (99%)	189 (100%)	1 (0%)	81	90
2	L	190/192 (99%)	186 (98%)	4 (2%)	47	63
3	G	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	8 (100%)	0	100	100
3	J	8/8 (100%)	8 (100%)	0	100	100
3	K	8/8 (100%)	8 (100%)	0	100	100
All	All	1501/1564 (96%)	1474 (98%)	27 (2%)	51	68

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	70	MET
1	A	98	ARG
1	A	170	VAL
2	B	39	LEU
2	B	45	LYS
1	C	4	LEU
1	C	72	ARG
1	C	150	PRO
1	C	151	VAL
1	C	210	LYS
2	D	18	ARG
2	D	20	THR
2	D	39	LEU
2	D	99	SER
1	E	72	ARG
1	E	82	GLU
1	E	179	LEU
1	E	202	LYS
2	F	208	SER
1	H	144	LYS
1	H	151	VAL

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Mol	Chain	Res	Type
1	H	180	SER
2	L	99	SER
2	L	111	GLU
2	L	114	ARG
2	L	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	205	GLN
1	C	43	GLN
1	C	193	GLN
2	D	143	ASN
1	E	193	GLN
2	F	85	GLN
2	F	153	GLN
2	F	161	GLN
2	F	166	GLN
2	F	195	HIS
1	H	193	GLN
2	L	35	GLN
2	L	48	GLN
2	L	153	GLN
2	L	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	EPE	F	301	-	15,15,15	2.26	1 (6%)	19,20,20	2.09	6 (31%)
5	GOL	D	302	-	5,5,5	0.21	0	5,5,5	0.99	1 (20%)
5	GOL	L	302	-	5,5,5	1.11	1 (20%)	5,5,5	0.57	0
4	EPE	L	301	-	15,15,15	0.52	0	19,20,20	0.78	1 (5%)
4	EPE	B	301	-	15,15,15	1.75	1 (6%)	19,20,20	1.99	4 (21%)
4	EPE	D	301	-	15,15,15	0.89	1 (6%)	19,20,20	0.88	1 (5%)

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	EPE	F	301	-	-	3/9/19/19	0/1/1/1
5	GOL	D	302	-	-	0/4/4/4	-
5	GOL	L	302	-	-	4/4/4/4	-
4	EPE	L	301	-	-	5/9/19/19	0/1/1/1
4	EPE	B	301	-	-	9/9/19/19	0/1/1/1
4	EPE	D	301	-	-	6/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	EPE	C10-S	-8.57	1.65	1.77
4	B	301	EPE	C10-S	-6.42	1.68	1.77
4	D	301	EPE	O2S-S	3.19	1.54	1.45
5	L	302	GOL	O2-C2	-2.23	1.36	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	301	EPE	O3S-S-C10	6.11	117.96	106.00
4	B	301	EPE	O3S-S-C10	5.51	116.78	106.00
4	B	301	EPE	O2S-S-O1S	-4.39	99.55	113.82
4	B	301	EPE	O1S-S-C10	3.75	112.40	106.73
4	F	301	EPE	O1S-S-C10	3.23	111.61	106.73
4	F	301	EPE	O2S-S-C10	-3.09	102.06	106.73
4	D	301	EPE	O3S-S-O1S	2.91	118.68	111.40
4	F	301	EPE	O2S-S-O1S	-2.71	105.00	113.82
4	F	301	EPE	C7-N4-C5	2.42	117.69	111.24
4	L	301	EPE	O3S-S-C10	-2.39	101.32	106.00
4	B	301	EPE	C5-N4-C3	2.32	113.84	108.84
4	F	301	EPE	C5-N4-C3	2.29	113.76	108.84
5	D	302	GOL	O3-C3-C2	2.10	119.83	110.38

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	EPE	C9-C10-S-O1S
4	B	301	EPE	C9-C10-S-O3S
4	F	301	EPE	C8-C7-N4-C5
4	L	301	EPE	S-C10-C9-N1
5	L	302	GOL	O1-C1-C2-C3
5	L	302	GOL	C1-C2-C3-O3
4	L	301	EPE	N4-C7-C8-O8
5	L	302	GOL	O2-C2-C3-O3
4	D	301	EPE	N4-C7-C8-O8
4	D	301	EPE	C9-C10-S-O3S
4	L	301	EPE	C9-C10-S-O3S
5	L	302	GOL	O1-C1-C2-O2
4	B	301	EPE	N4-C7-C8-O8
4	B	301	EPE	S-C10-C9-N1
4	B	301	EPE	C10-C9-N1-C2
4	B	301	EPE	C10-C9-N1-C6
4	D	301	EPE	C10-C9-N1-C2
4	D	301	EPE	C10-C9-N1-C6
4	B	301	EPE	C8-C7-N4-C3
4	B	301	EPE	C8-C7-N4-C5
4	B	301	EPE	C9-C10-S-O2S
4	D	301	EPE	C9-C10-S-O1S
4	D	301	EPE	C9-C10-S-O2S
4	F	301	EPE	C9-C10-S-O1S
4	L	301	EPE	C9-C10-S-O1S

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Mol	Chain	Res	Type	Atoms
4	L	301	EPE	C9-C10-S-O2S
4	F	301	EPE	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	301	EPE	1	0
5	D	302	GOL	1	0
5	L	302	GOL	2	0
4	L	301	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	208/223 (93%)	-0.18	4 (1%) 66 63	22, 31, 42, 52	0
1	C	210/223 (94%)	-0.43	0 100 100	18, 26, 38, 53	0
1	E	208/223 (93%)	-0.05	2 (0%) 79 77	22, 33, 44, 51	0
1	H	210/223 (94%)	-0.26	2 (0%) 79 77	19, 29, 43, 67	0
2	B	217/220 (98%)	-0.18	5 (2%) 61 58	17, 29, 40, 55	1 (0%)
2	D	218/220 (99%)	-0.30	2 (0%) 81 79	17, 27, 41, 49	0
2	F	218/220 (99%)	-0.16	5 (2%) 61 58	21, 30, 44, 53	0
2	L	218/220 (99%)	-0.20	3 (1%) 73 71	18, 28, 43, 50	0
3	G	9/9 (100%)	-0.01	1 (11%) 10 8	21, 26, 35, 61	0
3	I	9/9 (100%)	0.49	1 (11%) 10 8	27, 30, 43, 60	0
3	J	9/9 (100%)	0.03	1 (11%) 10 8	22, 27, 33, 49	0
3	K	9/9 (100%)	-0.17	1 (11%) 10 8	23, 28, 37, 47	0
All	All	1743/1808 (96%)	-0.21	27 (1%) 72 69	17, 29, 43, 67	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	150	ALA	3.8
2	F	165	SER	3.7
1	A	66	GLY	3.6
1	A	128	SER	3.2
2	B	47	GLY	3.1
3	I	103	ASN	3.1
2	F	164	ASN	3.0
2	B	194	LYS	2.9
1	E	72	ARG	2.9
1	H	128	SER	2.8
2	D	98	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	167	GLU	2.6
3	G	103	ASN	2.6
2	F	166	GLN	2.5
3	K	103	ASN	2.3
1	E	23	LYS	2.3
2	L	218	GLY	2.3
3	J	103	ASN	2.2
2	B	148	ARG	2.2
1	A	64	PHE	2.2
2	D	218	GLY	2.2
1	A	202	LYS	2.1
2	F	168	SER	2.1
2	B	48	GLN	2.1
2	L	109	LYS	2.1
2	L	216	ASN	2.1
1	H	207	LYS	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(Å ²)	Q<0.9
4	EPE	B	301	15/15	0.74	0.16	38,52,61,70	0
4	EPE	L	301	15/15	0.76	0.17	43,53,67,70	0
5	GOL	D	302	6/6	0.79	0.16	29,35,51,51	0
4	EPE	F	301	15/15	0.81	0.14	41,51,65,69	0
4	EPE	D	301	15/15	0.82	0.14	34,51,68,71	0
5	GOL	L	302	6/6	0.89	0.11	32,38,44,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.