



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:25 AM UTC

PDB ID : 3TF7 / pdb_00003tf7
Title : 42F3 QL9/H2-Ld complex
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Deposited on : 2011-08-15
Resolution : 2.75 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

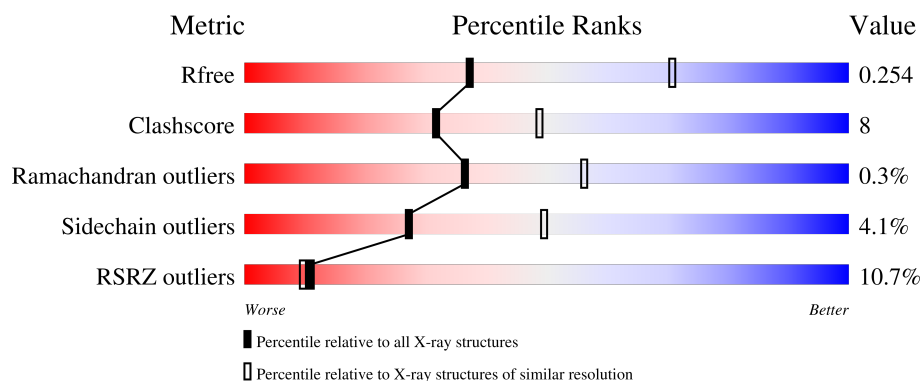
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	180	9% 74% 19% • • •
1	E	180	7% 81% 14% • •
2	B	9	67% 33%
2	F	9	44% 56%
3	C	256	3% 76% 13% • 9%

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Mol	Chain	Length	Quality of chain
3	G	256	2% 75% 12% • 12%
3	I	256	7% 74% 14% • 11%
3	K	256	29% 75% 11% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10138 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 H2-Ld SBM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	175	Total	C	N	O	S	0	0	0
			1452	910	258	277	7			
1	A	175	Total	C	N	O	S	0	0	0
			1448	908	257	276	7			

- Molecule 2 is a protein called QL9 peptide (QLSPFPFDL).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	9	Total	C	N	O	0	0	0
			75	52	10	13			
2	B	9	Total	C	N	O	0	0	0
			75	52	10	13			

- Molecule 3 is a protein called 42F3 Mut7 scFv (42F3 alpha chain, linker, 42F3 beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	232	Total	C	N	O	S	0	0	0
			1823	1150	315	352	6			
3	G	224	Total	C	N	O	S	0	0	0
			1751	1106	295	344	6			
3	I	228	Total	C	N	O	S	0	0	0
			1787	1128	306	347	6			
3	K	220	Total	C	N	O	S	0	0	0
			1715	1085	287	337	6			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

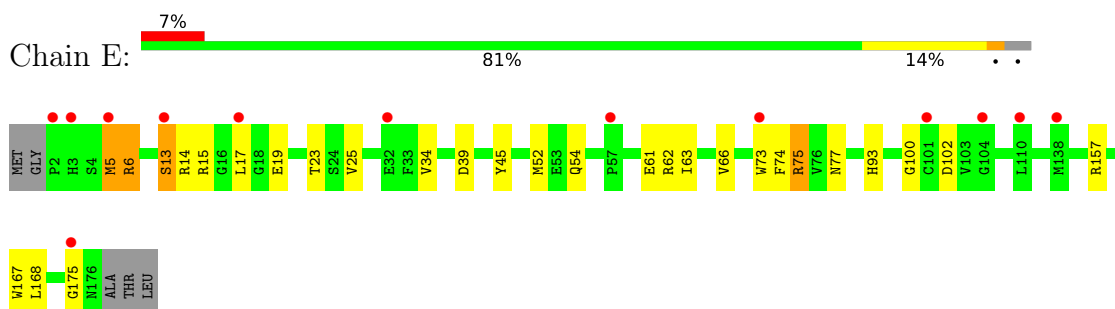


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

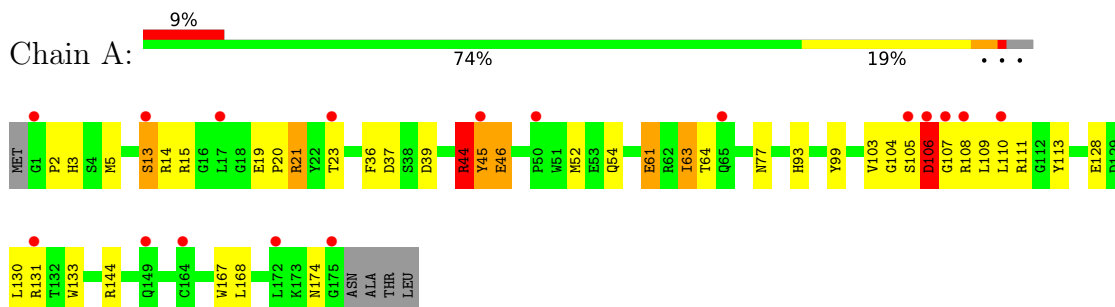
3 Residue-property plots

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: H2-Ld SBM2



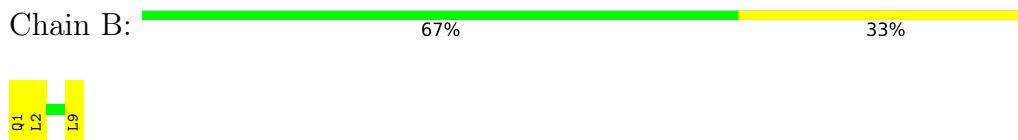
- Molecule 1: H2-Ld SBM2



- Molecule 2: QL9 peptide (QLSPFPFDL)



- Molecule 2: QL9 peptide (QLSPFPFDL)



- Molecule 3: 42F3 Mut7 scFv (42F3 alpha chain, linker, 42F3 beta chain)

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.49Å 109.79Å 213.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.45 – 2.75 37.45 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.45-2.75) 97.2 (37.45-2.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.237 , 0.261 0.236 , 0.254	Depositor DCC
R_{free} test set	3120 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10138	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	1/1488 (0.1%)	0.87	4/2015 (0.2%)
1	E	0.43	0/1492	0.75	0/2020
2	B	0.40	0/78	0.60	0/106
2	F	0.45	0/78	0.91	0/106
3	C	0.51	0/1872	0.72	1/2539 (0.0%)
3	G	0.47	0/1793	0.73	0/2430
3	I	0.41	0/1833	0.74	4/2485 (0.2%)
3	K	0.44	0/1755	0.72	1/2377 (0.0%)
All	All	0.46	1/10389 (0.0%)	0.75	10/14078 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	LEU	C-N	-6.82	1.23	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLU	N-CA-C	10.73	117.88	108.22
3	K	203	THR	N-CA-C	-7.08	99.07	108.34
1	A	44	ARG	CB-CA-C	-5.89	109.76	116.54
3	I	245	GLU	CB-CA-C	5.64	119.84	109.46
3	I	247	GLU	N-CA-C	-5.57	105.69	112.88
3	I	245	GLU	N-CA-C	-5.54	102.28	110.48
1	A	106	ASP	N-CA-C	-5.43	106.24	112.92
3	C	228	ASP	N-CA-C	-5.37	107.38	114.31
1	A	131	ARG	N-CA-C	-5.03	108.88	114.62
3	I	203	THR	N-CA-C	-5.03	100.09	110.80

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	1448	0	1337	55	0
1	E	1452	0	1338	21	0
2	B	75	0	73	3	0
2	F	75	0	73	6	0
3	C	1823	0	1732	27	0
3	G	1751	0	1678	27	0
3	I	1787	0	1700	20	0
3	K	1715	0	1640	14	0
4	C	6	0	8	0	0
4	G	6	0	8	0	0
All	All	10138	0	9587	159	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 8.

All (159) 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:A:14:ARG:NH2	1:A:39:ASP:OD2	1.97	0.97
3:G:219:THR:HG23	3:G:242:THR:HA	1.46	0.94
3:C:140:SER:HB3	3:C:141:PRO:HD3	1.50	0.90
1:E:14:ARG:NH2	1:E:39:ASP:OD2	2.08	0.85
1:A:36:PHE:CE2	1:A:44:ARG:O	2.29	0.85
1:A:13:SER:OG	1:A:93:HIS:N	2.11	0.84
3:K:32:LEU:HD23	3:K:92:VAL:HG12	1.60	0.83
1:A:2:PRO:HA	1:A:104:GLY:HA2	1.61	0.82
1:A:44:ARG:CG	1:A:45:TYR:H	1.92	0.82
1:E:13:SER:OG	1:E:93:HIS:N	2.13	0.81
1:A:111:ARG:HD3	1:A:113:TYR:OH	1.81	0.81
1:A:103:VAL:HG12	1:A:109:LEU:HA	1.64	0.80
1:A:21:ARG:HH21	1:A:37:ASP:CG	1.91	0.77
1:A:21:ARG:NH2	1:A:37:ASP:OD1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:97:THR:HG22	3:G:100:LYS:HB3	1.66	0.76
3:C:219:THR:HG23	3:C:242:THR:HA	1.66	0.75
1:A:44:ARG:HH22	1:A:61:GLU:HG2	1.51	0.75
1:E:19:GLU:OE1	1:E:75:ARG:HG3	1.87	0.75
1:A:54:GLN:NE2	1:A:174:ASN:HD21	1.85	0.75
1:A:36:PHE:CD2	1:A:44:ARG:O	2.39	0.74
3:C:31:TYR:HB2	3:C:93:SER:HB3	1.71	0.73
1:E:6:ARG:NH2	1:E:102:ASP:OD1	2.23	0.72
3:C:1:GLN:O	3:C:2:SER:HB3	1.90	0.71
3:C:1:GLN:HB3	3:C:26:TYR:CE1	2.26	0.70
1:A:111:ARG:NH1	1:A:128:GLU:HG3	2.05	0.70
1:A:54:GLN:HE21	1:A:174:ASN:HD21	1.39	0.70
1:A:167:TRP:CZ2	2:B:1:GLN:HG2	2.27	0.70
3:G:219:THR:CG2	3:G:242:THR:HA	2.20	0.70
1:A:45:TYR:HB2	1:A:64:THR:OG1	1.92	0.69
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.27	0.67
1:A:2:PRO:HA	1:A:104:GLY:CA	2.24	0.67
1:A:21:ARG:NH2	1:A:37:ASP:CG	2.51	0.67
3:K:219:THR:HG22	3:K:243:VAL:H	1.61	0.66
3:G:193:VAL:CG1	3:G:193:VAL:O	2.43	0.65
3:G:219:THR:HG23	3:G:241:LEU:O	1.96	0.65
1:A:103:VAL:HG12	1:A:108:ARG:O	1.97	0.65
1:E:5:MET:HB2	1:E:168:LEU:HD13	1.79	0.65
1:A:44:ARG:HH22	1:A:61:GLU:CG	2.11	0.64
1:A:103:VAL:CG1	1:A:108:ARG:O	2.46	0.63
1:A:45:TYR:C	1:A:46:GLU:HG2	2.21	0.63
3:C:214:ALA:HB1	3:C:243:VAL:HG21	1.81	0.63
1:A:44:ARG:CG	1:A:45:TYR:N	2.61	0.63
1:E:6:ARG:HD3	1:E:100:GLY:HA3	1.82	0.62
3:C:1:GLN:HB3	3:C:26:TYR:CZ	2.34	0.62
3:I:219:THR:HG22	3:I:243:VAL:H	1.64	0.62
3:C:148:THR:HG21	3:G:172:THR:HG21	1.80	0.62
1:A:111:ARG:HH11	1:A:128:GLU:HG3	1.63	0.61
1:E:73:TRP:CH2	2:F:7:PHE:O	2.53	0.61
3:G:12:VAL:HG23	3:G:111:VAL:HG22	1.82	0.61
1:A:44:ARG:NH2	1:A:61:GLU:HG2	2.15	0.61
3:C:219:THR:CG2	3:C:242:THR:HA	2.31	0.60
3:C:219:THR:HG23	3:C:241:LEU:O	2.01	0.60
1:A:45:TYR:CD2	1:A:63:ILE:HG23	2.36	0.60
1:A:54:GLN:NE2	1:A:174:ASN:OD1	2.34	0.60
1:A:36:PHE:HE2	1:A:44:ARG:O	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:VAL:HG12	3:C:193:VAL:O	2.03	0.59
1:A:52:MET:HA	1:A:52:MET:HE2	1.85	0.58
3:I:32:LEU:HD23	3:I:92:VAL:HG12	1.85	0.58
1:A:54:GLN:NE2	1:A:174:ASN:ND2	2.50	0.57
3:I:81:HIS:O	3:I:111:VAL:HG21	2.04	0.57
3:C:140:SER:HB2	3:C:155:SER:HB2	1.86	0.56
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.86	0.56
1:A:45:TYR:HD2	1:A:64:THR:HA	1.70	0.56
3:K:164:TYR:HB2	3:K:227:SER:HB3	1.86	0.56
1:A:106:ASP:OD1	1:A:106:ASP:N	2.30	0.56
3:G:12:VAL:CG2	3:G:111:VAL:HG22	2.35	0.56
3:C:140:SER:CB	3:C:141:PRO:HD3	2.22	0.56
1:A:44:ARG:HG3	1:A:45:TYR:H	1.67	0.55
3:C:140:SER:CB	3:C:155:SER:HB2	2.36	0.55
3:C:177:ARG:NH2	3:G:195:ASP:OD2	2.38	0.55
3:I:190:ILE:HG23	3:I:194:PRO:HG3	1.88	0.54
1:A:44:ARG:HG3	1:A:45:TYR:N	2.20	0.54
1:E:73:TRP:HH2	2:F:7:PHE:O	1.90	0.54
3:G:97:THR:CG2	3:G:100:LYS:HB3	2.37	0.53
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.43	0.53
1:E:6:ARG:HG2	1:E:6:ARG:NH1	2.24	0.53
1:E:6:ARG:HG2	1:E:6:ARG:HH11	1.74	0.53
1:E:52:MET:HA	1:E:52:MET:HE2	1.91	0.52
3:G:97:THR:HG22	3:G:97:THR:O	2.09	0.52
3:I:219:THR:CG2	3:I:243:VAL:H	2.22	0.52
1:E:14:ARG:HH22	1:E:39:ASP:CG	2.12	0.52
1:A:77:ASN:HB3	2:B:9:LEU:HD12	1.92	0.51
3:C:148:THR:CG2	3:G:172:THR:HG21	2.40	0.51
3:G:193:VAL:O	3:G:193:VAL:HG12	2.11	0.51
3:G:145:VAL:CG1	3:G:244:LEU:HD11	2.40	0.50
3:K:222:TYR:HB2	3:K:239:SER:HB2	1.93	0.50
1:E:73:TRP:HD1	1:E:74:PHE:CD2	2.29	0.50
3:C:12:VAL:HG23	3:C:111:VAL:HG12	1.93	0.50
3:C:3:VAL:HG23	3:C:104:GLY:HA2	1.94	0.49
1:A:106:ASP:O	1:A:108:ARG:HG3	2.11	0.49
3:I:164:TYR:HB2	3:I:227:SER:HB3	1.93	0.49
3:C:55:VAL:HG12	3:K:230:PRO:HG2	1.95	0.49
1:A:103:VAL:HB	1:A:108:ARG:O	2.13	0.49
3:I:33:PHE:HD2	3:I:45:MET:HE2	1.77	0.48
1:E:167:TRP:CZ2	2:F:1:GLN:HG2	2.48	0.48
1:A:104:GLY:O	1:A:105:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HB2	1:A:15:ARG:NH1	2.29	0.47
1:A:44:ARG:HH22	1:A:61:GLU:HA	1.79	0.47
1:E:34:VAL:HG22	1:E:45:TYR:HD1	1.80	0.47
3:C:81:HIS:O	3:C:111:VAL:HG21	2.14	0.47
3:G:55:VAL:HG12	3:I:230:PRO:HG2	1.95	0.47
3:I:216:PRO:O	3:I:219:THR:HG23	2.14	0.47
1:A:128:GLU:O	1:A:130:LEU:HD12	2.15	0.47
3:C:82:ARG:HH11	3:C:113:PRO:HD3	1.80	0.47
3:I:45:MET:HE1	3:I:232:GLN:HG2	1.96	0.47
3:K:72:SER:HB2	3:K:74:HIS:CE1	2.49	0.47
3:K:48:LYS:HE2	3:K:232:GLN:NE2	2.30	0.47
3:C:92:VAL:HG22	3:C:93:SER:N	2.30	0.46
3:I:211:LEU:HD23	3:I:218:GLN:OE1	2.15	0.46
3:G:72:SER:HB2	3:G:74:HIS:CE1	2.51	0.46
3:C:47:LEU:C	3:C:47:LEU:HD12	2.41	0.46
1:E:73:TRP:CZ3	2:F:8:ASP:HA	2.51	0.46
3:I:29:THR:HA	3:I:30:PRO:HD3	1.84	0.45
1:A:106:ASP:OD2	1:A:108:ARG:HB2	2.16	0.45
3:G:32:LEU:HD23	3:G:92:VAL:HG23	1.99	0.45
3:I:228:ASP:HB2	3:I:234:TYR:HE2	1.81	0.45
3:K:12:VAL:HG22	3:K:109:LEU:HD11	1.99	0.45
3:G:169:ARG:HB3	3:G:179:ILE:HD11	1.98	0.45
1:A:54:GLN:NE2	1:A:174:ASN:CG	2.75	0.45
3:K:91:ALA:HB1	3:K:101:LEU:HD22	1.99	0.44
3:C:33:PHE:CZ	3:C:231:GLY:HA3	2.52	0.44
3:C:34:TRP:CE2	3:C:75:LEU:HB2	2.51	0.44
3:G:202:THR:OG1	3:G:206:ASP:HB2	2.17	0.44
3:G:33:PHE:CZ	3:G:231:GLY:HA3	2.52	0.44
1:E:62:ARG:O	1:E:66:VAL:HG23	2.17	0.44
3:G:172:THR:C	3:G:174:HIS:H	2.26	0.43
1:A:133:TRP:HB2	1:A:144:ARG:HG2	2.00	0.43
1:A:3:HIS:N	1:A:103:VAL:O	2.43	0.43
3:G:33:PHE:CD2	3:G:48:LYS:HB2	2.54	0.42
1:A:19:GLU:HA	1:A:20:PRO:HD3	1.88	0.42
1:E:77:ASN:HB3	2:F:9:LEU:HD12	2.02	0.42
1:A:44:ARG:HG2	1:A:45:TYR:H	1.82	0.42
3:I:138:THR:O	3:I:138:THR:HG23	2.20	0.42
1:A:103:VAL:CB	1:A:108:ARG:O	2.68	0.42
3:I:34:TRP:CE2	3:I:75:LEU:HB2	2.54	0.42
3:G:146:THR:HG21	3:G:152:VAL:HG21	2.01	0.42
3:I:72:SER:HB2	3:I:74:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:NH2	1:A:61:GLU:HA	2.35	0.42
1:E:167:TRP:CE2	2:F:1:GLN:HG2	2.55	0.42
3:I:179:ILE:HG22	3:I:180:TYR:HD2	1.84	0.42
3:G:94:ALA:HB3	3:G:97:THR:HB	2.02	0.41
3:I:219:THR:HG22	3:I:243:VAL:HB	2.02	0.41
3:K:85:SER:OG	3:K:111:VAL:HG22	2.21	0.41
1:E:15:ARG:O	1:E:17:LEU:N	2.50	0.41
3:G:110:THR:HG23	3:G:110:THR:O	2.21	0.41
3:G:193:VAL:O	3:G:193:VAL:HG13	2.18	0.41
1:A:45:TYR:C	1:A:46:GLU:CG	2.92	0.41
1:A:99:TYR:OH	2:B:2:LEU:HD22	2.21	0.41
3:I:33:PHE:CD2	3:I:45:MET:HE2	2.56	0.41
3:K:34:TRP:CE2	3:K:75:LEU:HB2	2.56	0.41
3:K:219:THR:CG2	3:K:243:VAL:H	2.31	0.41
3:K:182:SER:HB3	3:K:201:ARG:HH11	1.86	0.40
1:E:6:ARG:HD3	1:E:6:ARG:HA	1.59	0.40
1:A:15:ARG:HB2	1:A:15:ARG:HH11	1.85	0.40
3:G:21:ARG:HG2	3:G:74:HIS:CE1	2.56	0.40
3:I:166:TYR:HE1	3:I:227:SER:HB2	1.86	0.40
3:K:164:TYR:HA	3:K:182:SER:O	2.21	0.40
3:C:140:SER:HB3	3:C:155:SER:HB2	2.04	0.40
3:C:93:SER:OG	3:C:98:GLY:HA2	2.21	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	A	173/180 (96%)	159 (92%)	13 (8%)	1 (1%)	21	38
1	E	173/180 (96%)	164 (95%)	8 (5%)	1 (1%)	21	38
2	B	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	7/9 (78%)	7 (100%)	0	0	100	100
3	C	228/256 (89%)	216 (95%)	10 (4%)	2 (1%)	14	28
3	G	220/256 (86%)	213 (97%)	7 (3%)	0	100	100
3	I	224/256 (88%)	215 (96%)	9 (4%)	0	100	100
3	K	214/256 (84%)	209 (98%)	5 (2%)	0	100	100
All	All	1246/1402 (89%)	1190 (96%)	52 (4%)	4 (0%)	36	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	175	GLY
3	C	2	SER
3	C	141	PRO
1	A	107	GLY

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	144/148 (97%)	136 (94%)	8 (6%)	19	36
1	E	145/148 (98%)	135 (93%)	10 (7%)	14	26
2	B	9/9 (100%)	9 (100%)	0	100	100
2	F	9/9 (100%)	8 (89%)	1 (11%)	6	11
3	C	198/204 (97%)	192 (97%)	6 (3%)	36	60
3	G	191/204 (94%)	186 (97%)	5 (3%)	40	63
3	I	194/204 (95%)	185 (95%)	9 (5%)	24	45
3	K	187/204 (92%)	182 (97%)	5 (3%)	39	62
All	All	1077/1130 (95%)	1033 (96%)	44 (4%)	27	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	MET
1	E	6	ARG
1	E	13	SER
1	E	23	THR
1	E	25	VAL
1	E	54	GLN
1	E	61	GLU
1	E	63	ILE
1	E	75	ARG
1	E	157	ARG
2	F	2	LEU
3	C	1	GLN
3	C	48	LYS
3	C	139	GLN
3	C	198	LYS
3	C	200	THR
3	C	205	GLU
1	A	13	SER
1	A	21	ARG
1	A	23	THR
1	A	44	ARG
1	A	45	TYR
1	A	61	GLU
1	A	63	ILE
1	A	106	ASP
3	G	48	LYS
3	G	105	LYS
3	G	188	LEU
3	G	193	VAL
3	G	205	GLU
3	I	3	VAL
3	I	26	TYR
3	I	48	LYS
3	I	92	VAL
3	I	198	LYS
3	I	200	THR
3	I	205	GLU
3	I	219	THR
3	I	250	HIS
3	K	48	LYS
3	K	59	VAL
3	K	198	LYS
3	K	202	THR

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Mol	Chain	Res	Type
3	K	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	87	GLN
1	E	96	GLN
1	E	149	GLN
3	C	143	ASN
3	C	189	GLN
1	A	42	ASN
1	A	54	GLN
1	A	115	GLN
3	G	37	GLN
3	G	41	GLN
3	G	44	GLN
3	G	151	ASN
3	G	170	GLN
3	G	189	GLN
3	I	151	ASN
3	I	160	ASN
3	K	204	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 ⓘ

2 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	GOL	G	254	-	5,5,5	0.38	0	5,5,5	0.27	0
4	GOL	C	254	-	5,5,5	0.39	0	5,5,5	0.24	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	GOL	G	254	-	-	2/4/4/4	-
4	GOL	C	254	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	254	GOL	C1-C2-C3-O3
4	C	254	GOL	O2-C2-C3-O3
4	G	254	GOL	O1-C1-C2-O2
4	C	254	GOL	O1-C1-C2-C3
4	G	254	GOL	O1-C1-C2-C3
4	C	254	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	175/180 (97%)	0.74	17 (9%)	13	13	62, 92, 151, 174	0
1	E	175/180 (97%)	0.68	13 (7%)	20	20	67, 92, 144, 166	0
2	B	9/9 (100%)	0.51	0	100	100	62, 67, 84, 94	0
2	F	9/9 (100%)	0.58	0	100	100	64, 72, 91, 101	0
3	C	232/256 (90%)	0.15	8 (3%)	48	46	33, 68, 101, 122	0
3	G	224/256 (87%)	0.18	6 (2%)	56	54	53, 71, 99, 112	0
3	I	228/256 (89%)	0.52	19 (8%)	17	18	55, 81, 107, 122	0
3	K	220/256 (85%)	1.62	73 (33%)	1	0	70, 112, 163, 192	0
All	All	1272/1402 (90%)	0.63	136 (10%)	11	10	33, 83, 141, 192	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	246	LEU	9.2
3	K	140	SER	8.5
1	A	175	GLY	7.7
3	K	147	VAL	6.2
1	E	2	PRO	6.2
3	C	1	GLN	6.0
3	K	244	LEU	5.6
3	K	172	THR	5.5
3	K	167	TRP	5.4
3	K	154	LEU	5.3
1	A	1	GLY	5.2
3	K	143	ASN	5.2
3	K	236	GLY	5.2
3	K	136	ALA	5.0
3	I	183	TYR	4.9
3	K	146	THR	4.7

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Mol	Chain	Res	Type	RSRZ
3	K	223	PHE	4.7
1	E	17	LEU	4.7
3	I	135	ALA	4.7
3	K	222	TYR	4.6
3	K	183	TYR	4.5
3	K	174	HIS	4.5
1	A	45	TYR	4.4
3	C	140	SER	4.4
3	K	193	VAL	4.1
3	K	241	LEU	4.0
3	G	247	GLU	3.8
3	I	204	GLN	3.8
3	K	209	LEU	3.7
3	K	152	VAL	3.6
3	K	237	GLU	3.6
3	C	135	ALA	3.5
3	K	145	VAL	3.5
1	A	13	SER	3.5
3	K	28	ALA	3.4
1	E	5	MET	3.4
3	K	137	VAL	3.4
3	K	202	THR	3.3
3	K	112	SER	3.3
3	K	238	GLY	3.3
3	G	111	VAL	3.3
3	K	159	THR	3.3
3	K	2	SER	3.2
3	K	153	THR	3.2
3	K	144	LYS	3.2
3	K	211	LEU	3.1
1	E	175	GLY	3.1
3	K	190	ILE	3.1
3	K	214	ALA	3.1
1	E	13	SER	3.1
3	I	193	VAL	3.1
3	K	95	LYS	3.0
1	A	105	SER	3.0
3	K	26	TYR	3.0
3	K	9	ARG	3.0
1	A	17	LEU	3.0
1	E	73	TRP	2.9
3	I	174	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
3	I	2	SER	2.8
3	K	242	THR	2.8
3	K	216	PRO	2.8
3	K	208	PHE	2.8
3	K	217	SER	2.8
3	K	176	LEU	2.8
3	K	188	LEU	2.8
3	I	172	THR	2.8
3	I	246	LEU	2.7
3	I	164	TYR	2.7
3	K	161	SER	2.7
3	I	136	ALA	2.7
3	C	141	PRO	2.7
3	K	168	TYR	2.7
3	G	112	SER	2.7
3	G	1	GLN	2.6
1	E	138	MET	2.6
3	K	150	GLU	2.6
3	C	82	ARG	2.6
3	K	40	ARG	2.6
1	E	32	GLU	2.6
3	K	235	PHE	2.6
3	I	250	HIS	2.5
3	I	251	HIS	2.5
1	A	23	THR	2.5
3	K	239	SER	2.5
1	A	149	GLN	2.5
3	C	136	ALA	2.5
3	K	170	GLN	2.4
3	K	240	LYS	2.4
1	A	107	GLY	2.4
3	K	105	LYS	2.4
3	K	173	GLY	2.4
3	K	139	GLN	2.4
3	G	202	THR	2.3
3	K	138	THR	2.3
1	A	106	ASP	2.3
3	I	112	SER	2.3
3	K	17	SER	2.3
3	I	97	THR	2.3
3	K	219	THR	2.3
1	E	104	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	108	ARG	2.3
3	K	218	GLN	2.3
3	K	166	TYR	2.3
1	E	110	LEU	2.3
3	K	96	GLY	2.3
3	K	243	VAL	2.3
3	K	175	GLU	2.2
3	I	27	SER	2.2
1	E	101	CYS	2.2
3	C	113	PRO	2.2
1	A	110	LEU	2.2
3	C	243	VAL	2.2
3	K	108	LYS	2.2
1	E	3	HIS	2.2
1	E	57	PRO	2.2
3	K	8	ALA	2.2
1	A	131	ARG	2.2
1	A	50	PRO	2.2
3	I	26	TYR	2.2
3	K	194	PRO	2.2
3	K	221	LEU	2.2
3	K	155	SER	2.2
3	G	237	GLU	2.1
1	A	164	CYS	2.1
1	A	172	LEU	2.1
3	K	224	CYS	2.1
3	K	177	ARG	2.1
3	K	198	LYS	2.1
3	K	200	THR	2.1
1	A	65	GLN	2.1
3	I	173	GLY	2.1
3	K	207	PHE	2.1
3	I	175	GLU	2.0
3	K	100	LYS	2.0
3	I	202	THR	2.0
3	K	156	CYS	2.0

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

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	GOL	G	254	6/6	0.87	0.23	90,90,91,91	0
4	GOL	C	254	6/6	0.88	0.26	105,106,106,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.