



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:45 pm BST

PDB ID : 3TF7  
Title : 42F3 QL9/H2-Ld complex  
Authors : Adams, J.J.; Kranz, D.M.; Garcia, K.C.  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

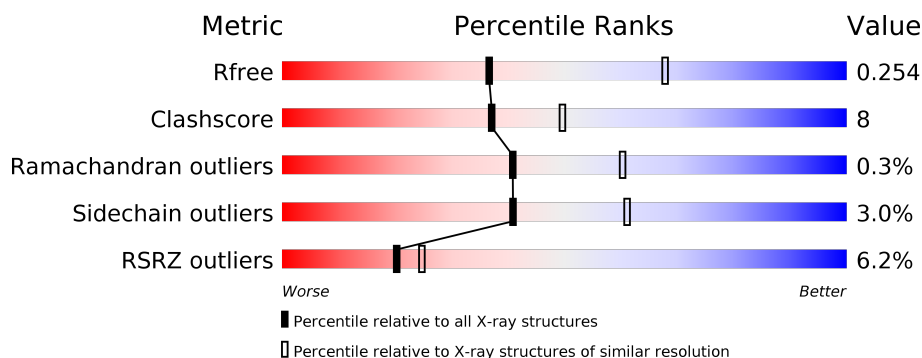
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	E	180	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
2	B	9	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	F	9	<div> <div></div> <div> <div>44%</div> <div>56%</div> </div> </div>
3	C	256	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 9%</div> </div> </div>
3	G	256	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	I	256	<div><div></div><div>3%</div><div>78%</div><div>11%</div><div>11%</div></div>
3	K	256	<div><div></div><div>16%</div><div>75%</div><div>10%</div><div>14%</div></div>

## 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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

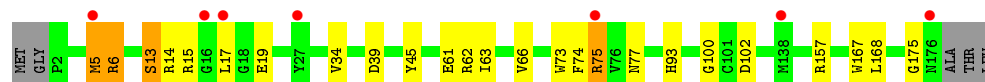
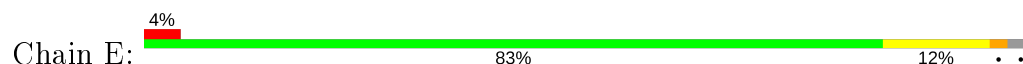


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

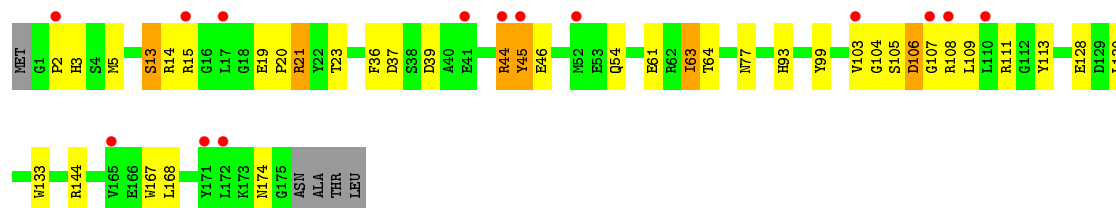
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



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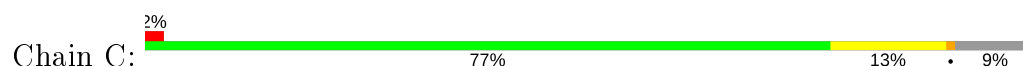
- Molecule 2: QL9 peptide (QLSPFPFDL)



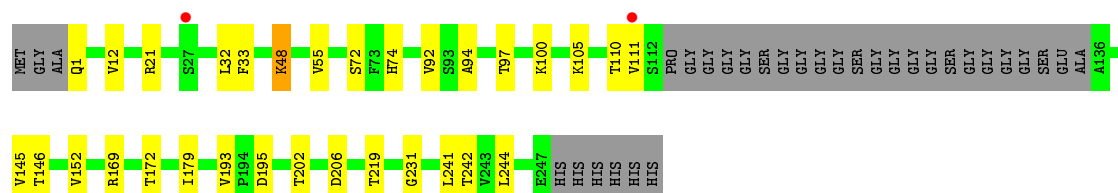
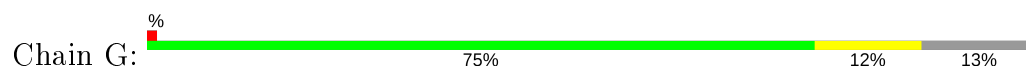
- Molecule 2: QL9 peptide (QLSPFPFDL)



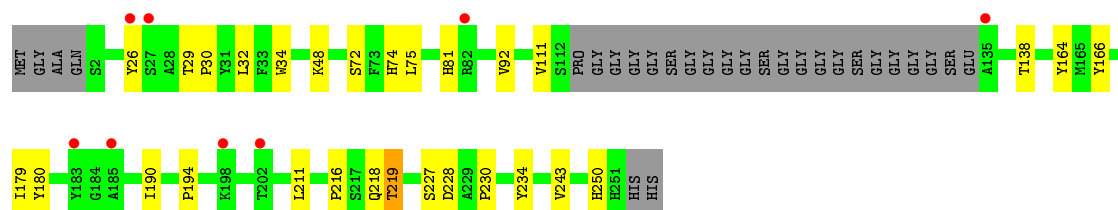
- Molecule 3: 42F3 Mut7 scFv (42F3 alpha chain, linker, 42F3 beta chain)



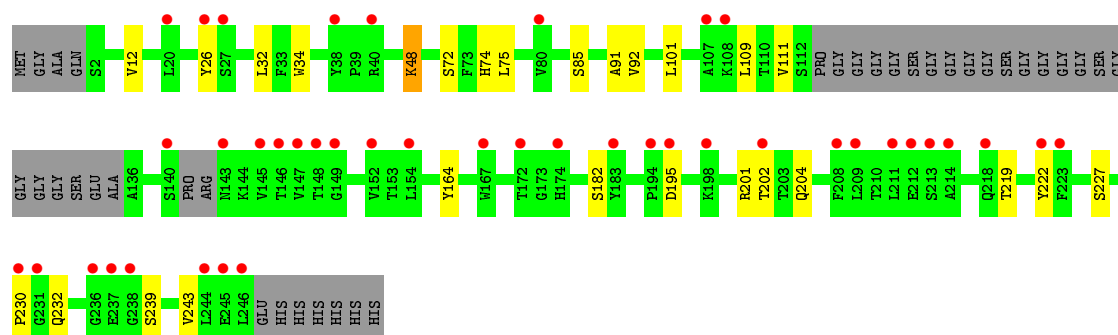
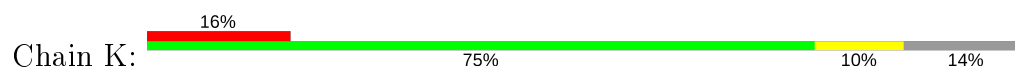
- Molecule 3: 42F3 Mut7 scFv (42F3 alpha chain, linker, 42F3 beta chain)



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



- 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, $\alpha$ , $\beta$ , $\gamma$	102.49Å 109.79Å 213.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.45 – 2.75 37.46 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.45-2.75) 97.1 (37.46-2.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.36	0/1488	0.51	0/2015
1	E	0.36	0/1492	0.47	0/2020
2	B	0.45	0/78	0.56	0/106
2	F	0.45	0/78	0.63	0/106
3	C	0.41	0/1872	0.52	0/2539
3	G	0.40	0/1793	0.53	0/2430
3	I	0.34	0/1833	0.54	0/2485
3	K	0.35	0/1755	0.51	0/2377
All	All	0.37	0/10389	0.52	0/14078

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	1448	0	1337	53	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1751	0	1678	26	0
3	I	1787	0	1700	17	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	153	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 (153) 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:NH2	1:A:37:ASP:OD1	2.18	0.76
3:G:97:THR:HG22	3:G:100:LYS:HB3	1.66	0.76
1:A:44:ARG:HH22	1:A:61:GLU:HG2	1.51	0.75
3:C:219:THR:HG23	3:C:242:THR:HA	1.66	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:A:21:ARG:HH21	1:A:37:ASP:CG	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:A:21:ARG:NH2	1:A:37:ASP:CG	2.51	0.62
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
1:A:54:GLN:NE2	1:A:174:ASN:OD1	2.34	0.60
1:A:45:TYR:CD2	1:A:63:ILE:HG23	2.36	0.60
3:C:219:THR:HG23	3:C:241:LEU:O	2.01	0.60
1:A:36:PHE:HE2	1:A:44:ARG:O	1.84	0.59
3:C:193:VAL:O	3:C:193:VAL:HG12	2.03	0.59
1:A:45:TYR:C	1:A:46:GLU:HG2	2.21	0.59
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
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:C:140:SER:HB2	3:C:155:SER:HB2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1.74	0.53
1:E:6:ARG:HG2	1:E:6:ARG:NH1	2.24	0.53
1:A:111:ARG:HD3	1:A:113:TYR:HH	1.73	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: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:HG12	3:G:193:VAL:O	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
1:A:106:ASP:O	1:A:108:ARG:HG3	2.11	0.49
3:C:3:VAL:HG23	3:C:104:GLY:HA2	1.94	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
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
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:I:216:PRO:O	3:I:219:THR:HG23	2.14	0.47
3:G:55:VAL:HG12	3:I:230:PRO:HG2	1.95	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:13:SER:HG	1:E:93:HIS:H	1.52	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
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:A:44:ARG:HG2	1:A:45:TYR:H	1.82	0.42
1:E:77:ASN:HB3	2:F:9:LEU:HD12	2.02	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
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:HG13	3:G:193:VAL:O	2.18	0.41
1:A:99:TYR:OH	2:B:2:LEU:HD22	2.21	0.41
3:C:47:LEU:HD12	3:C:47:LEU:C	2.41	0.41
3:K:219:THR:CG2	3:K:243:VAL:H	2.31	0.41
3:K:34:TRP:CE2	3:K:75:LEU:HB2	2.56	0.41
3:K:182:SER:HB3	3:K:201:ARG:HH11	1.86	0.40
1:A:15:ARG:HH11	1:A:15:ARG:HB2	1.85	0.40
1:E:6:ARG:HD3	1:E:6:ARG:HA	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:SER:OG	3:C:98:GLY:HA2	2.21	0.40
1:E:14:ARG:HH22	1:E:39:ASP:CG	2.12	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%)	25	42
1	E	173/180 (96%)	164 (95%)	8 (5%)	1 (1%)	25	42
2	B	7/9 (78%)	7 (100%)	0	0	100	100
2	F	7/9 (78%)	7 (100%)	0	0	100	100
3	C	228/256 (89%)	216 (95%)	10 (4%)	2 (1%)	17	31
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%)	41	60

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%)	137 (95%)	7 (5%)	25	43
1	E	145/148 (98%)	138 (95%)	7 (5%)	25	44
2	B	9/9 (100%)	9 (100%)	0	100	100
2	F	9/9 (100%)	8 (89%)	1 (11%)	6	10
3	C	198/204 (97%)	193 (98%)	5 (2%)	47	67
3	G	191/204 (94%)	188 (98%)	3 (2%)	62	77
3	I	194/204 (95%)	190 (98%)	4 (2%)	53	71
3	K	187/204 (92%)	182 (97%)	5 (3%)	44	65
All	All	1077/1130 (95%)	1045 (97%)	32 (3%)	41	61

All (32) 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	61	GLU
1	E	63	ILE
1	E	75	ARG
1	E	157	ARG
2	F	2	LEU
3	C	1	GLN
3	C	9	ARG
3	C	48	LYS
3	C	139	GLN
3	C	181	TYR
1	A	13	SER
1	A	21	ARG
1	A	23	THR
1	A	44	ARG
1	A	45	TYR
1	A	63	ILE

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Mol	Chain	Res	Type
1	A	106	ASP
3	G	1	GLN
3	G	48	LYS
3	G	105	LYS
3	I	26	TYR
3	I	48	LYS
3	I	219	THR
3	I	250	HIS
3	K	26	TYR
3	K	48	LYS
3	K	195	ASP
3	K	202	THR
3	K	204	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	143	ASN
1	A	42	ASN
1	A	54	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	0.24	0
4	GOL	C	254	-	5,5,5	0.38	0	5,5,5	0.22	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	G	254	GOL	O1-C1-C2-C3
4	C	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	175/180 (97%)	0.49	14 (8%) 12 15	62, 92, 151, 174	0
1	E	175/180 (97%)	0.46	7 (4%) 38 45	67, 92, 144, 166	0
2	B	9/9 (100%)	0.47	0 100 100	62, 67, 84, 94	0
2	F	9/9 (100%)	1.02	0 100 100	64, 72, 91, 101	0
3	C	232/256 (90%)	0.14	6 (2%) 56 65	33, 68, 101, 122	0
3	G	224/256 (87%)	0.11	2 (0%) 84 89	53, 71, 99, 112	0
3	I	228/256 (89%)	0.24	8 (3%) 44 52	55, 81, 107, 122	0
3	K	220/256 (85%)	1.12	42 (19%) 1 1	70, 112, 163, 192	0
All	All	1272/1402 (90%)	0.42	79 (6%) 20 25	33, 83, 141, 192	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	140	SER	6.9
3	K	236	GLY	6.6
3	K	40	ARG	5.8
3	K	154	LEU	5.6
3	K	212	GLU	5.6
3	K	202	THR	4.8
3	K	167	TRP	4.8
1	A	17	LEU	4.7
3	I	27	SER	4.7
1	E	17	LEU	4.7
3	K	246	LEU	4.6
3	K	149	GLY	4.6
3	K	146	THR	4.6
3	K	174	HIS	4.4
3	K	27	SER	4.4
3	I	202	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	K	237	GLU	4.2
3	K	222	TYR	4.1
1	A	107	GLY	4.0
3	K	172	THR	3.8
3	C	1	GLN	3.7
3	K	214	ALA	3.6
3	K	208	PHE	3.6
3	K	26	TYR	3.5
3	K	223	PHE	3.5
3	K	194	PRO	3.5
3	K	244	LEU	3.4
3	K	143	ASN	3.4
3	C	135	ALA	3.3
1	E	16	GLY	3.3
3	K	152	VAL	3.2
1	E	138	MET	3.2
3	C	82	ARG	3.2
3	K	218	GLN	3.2
1	E	176	ASN	3.1
3	K	147	VAL	3.0
1	A	103	VAL	3.0
3	K	211	LEU	3.0
3	G	111	VAL	2.9
1	A	44	ARG	2.9
1	A	108	ARG	2.9
3	C	140	SER	2.9
3	I	198	LYS	2.9
3	K	108	LYS	2.9
1	A	110	LEU	2.9
1	A	165	VAL	2.8
3	K	238	GLY	2.8
3	K	213	SER	2.7
1	A	172	LEU	2.7
3	K	198	LYS	2.7
3	K	209	LEU	2.6
3	I	183	TYR	2.6
3	K	148	THR	2.6
1	A	2	PRO	2.6
3	K	245	GLU	2.6
3	K	145	VAL	2.5
3	K	230	PRO	2.5
1	A	52	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	5	MET	2.4
1	A	15	ARG	2.4
3	K	38	TYR	2.3
3	I	82	ARG	2.3
3	K	80	VAL	2.3
3	K	195	ASP	2.3
3	C	113	PRO	2.3
1	A	45	TYR	2.3
3	G	27	SER	2.3
3	K	231	GLY	2.2
1	E	75	ARG	2.2
3	C	111	VAL	2.1
3	I	185	ALA	2.1
3	K	107	ALA	2.1
1	A	171	TYR	2.1
3	I	26	TYR	2.1
3	K	183	TYR	2.1
1	A	41	GLU	2.1
3	I	135	ALA	2.0
1	E	27	TYR	2.0
3	K	20	LEU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	C	254	6/6	0.71	0.40	105,106,106,106	0
4	GOL	G	254	6/6	0.88	0.28	90,90,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.