



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 02:49 AM EDT

PDB ID : 8FYM  
Title : Crystal structure of Fab235 in complex with MPER peptide  
Authors : Tan, K.; Kim, M.; Reinherz, E.L.  
Deposited on : 2023-01-26  
Resolution : 2.45 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

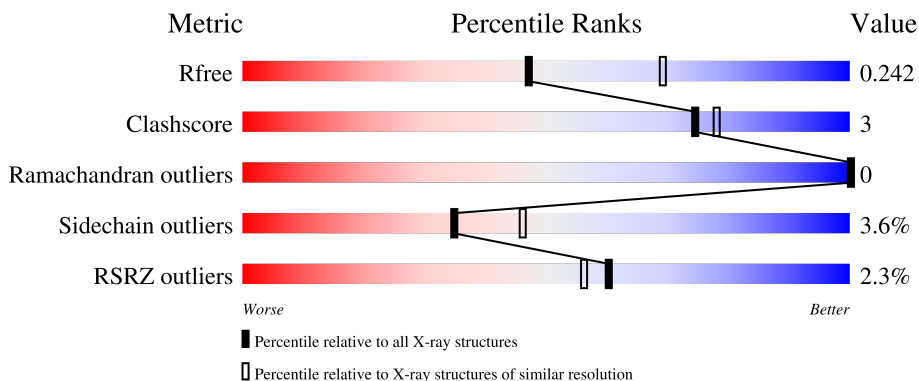
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	220	 92% 8%
1	D	220	 89% 10%
1	G	220	 45% 6% 48%
1	L	220	 87% 13%
2	B	228	 89% 7%

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Mol	Chain	Length	Quality of chain
2	E	228	<p>8% 87% 9%</p>
2	H	228	<p>86% 13%</p>
2	I	228	<p>3% 48% 7% 45%</p>
3	C	20	<p>5% 90% 5% 5%</p>
3	F	20	<p>5% 85% 10% 5%</p>
3	J	20	<p>85% 10% 5%</p>
3	P	20	<p>75% 15% 10%</p>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13145 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 Fab235, L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	220	Total 1708	C 1072	N 282	O 346	S 8	0	1	0
1	A	220	Total 1699	C 1067	N 280	O 344	S 8	0	0	0
1	D	219	Total 1693	C 1064	N 279	O 343	S 7	0	0	0
1	G	114	Total 878	C 557	N 141	O 175	S 5	0	0	0

- Molecule 2 is a protein called Fab235, H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	225	Total 1686	C 1074	N 273	O 334	S 5	0	0	0
2	B	221	Total 1658	C 1059	N 268	O 326	S 5	0	0	0
2	E	220	Total 1654	C 1056	N 267	O 326	S 5	0	0	0
2	I	126	Total 968	C 619	N 155	O 191	S 3	0	0	0

- Molecule 3 is a protein called ALA-SER-LEU-TRP-ASN-TRP-PHE-ASN-ILE-THR-ASN-TRP-LEU-TRP-TYR-ILE-LYS-LYS-LYS.

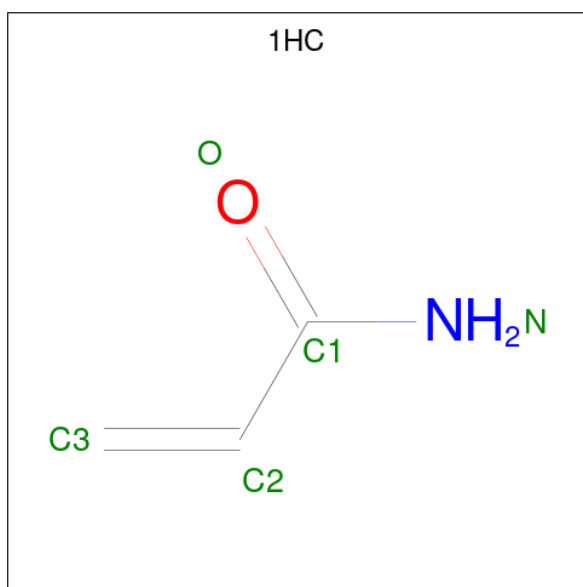
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	18	Total 176	C 123	N 28	O 25	0	0	0
3	C	19	Total 181	C 126	N 29	O 26	0	0	0
3	F	19	Total 181	C 126	N 29	O 26	0	0	0
3	J	19	Total 181	C 126	N 29	O 26	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0

- Molecule 5 is prop-2-enamide (three-letter code: 1HC) (formula:  $C_3H_5NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	I	1	Total	C	N	O	0	0
			5	3	1	1		
5	J	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total	Cl	0	0
			2	2		
6	G	1	Total	Cl	0	0
			1	1		
6	I	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	76	Total	O	0	0
			76	76		
7	H	91	Total	O	0	0
			91	91		
7	P	4	Total	O	0	0
			4	4		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
7	A	71	Total O 71 71	0	0
7	B	78	Total O 78 78	0	0
7	C	4	Total O 4 4	0	0
7	D	24	Total O 24 24	0	0
7	E	29	Total O 29 29	0	0
7	F	8	Total O 8 8	0	0
7	G	21	Total O 21 21	0	0
7	I	22	Total O 22 22	0	0
7	J	5	Total O 5 5	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: Fab235, L chain

Chain L: 



- Molecule 1: Fab235, L chain

Chain A: 



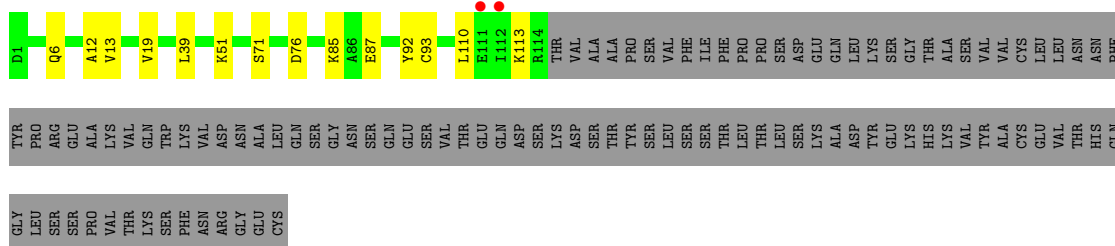
- Molecule 1: Fab235, L chain

Chain D: 




- Molecule 1: Fab235, L chain

Chain G: 



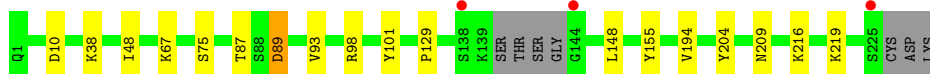
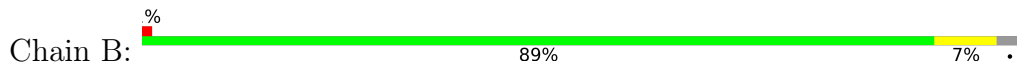
- Molecule 2: Fab235, H chain

Chain H: 

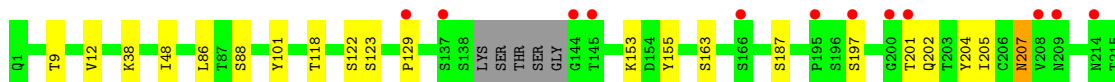
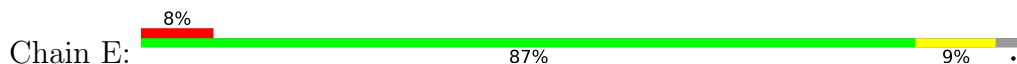




• Molecule 2: Fab235, H chain



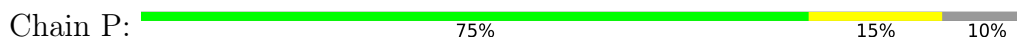
• Molecule 2: Fab235, H chain



• Molecule 2: Fab235, H chain




• Molecule 3: ALA-SER-LEU-TRP-ASN-TRP-PHE-ASN-ILE-THR-ASN-TRP-LEU-TRP-TYR-ILE-LYS-LYS-LYS

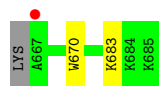


• Molecule 3: ALA-SER-LEU-TRP-ASN-TRP-PHE-ASN-ILE-THR-ASN-TRP-LEU-TRP-TYR-ILE-LYS-LYS-LYS




- Molecule 3: ALA-SER-LEU-TRP-ASN-TRP-PHE-ASN-ILE-THR-ASN-TRP-LEU-TRP-TYR-ILE-LYS-LYS-LYS

Chain F: 



- Molecule 3: ALA-SER-LEU-TRP-ASN-TRP-PHE-ASN-ILE-THR-ASN-TRP-LEU-TRP-TYR-ILE-LYS-LYS-LYS

Chain J: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.48Å 108.30Å 121.21Å 85.63° 82.95° 85.59°	Depositor
Resolution (Å)	47.95 – 2.45 47.95 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.95-2.45) 95.7 (47.95-2.45)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.200 , 0.243 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	3808 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: 1HC, GOL, CL

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	0.25	0/1736	0.48	0/2355
1	D	0.25	0/1730	0.45	0/2347
1	G	0.26	0/898	0.46	0/1217
1	L	0.25	0/1745	0.45	0/2367
2	B	0.26	0/1703	0.49	0/2326
2	E	0.25	0/1699	0.48	0/2320
2	H	0.26	0/1732	0.48	0/2365
2	I	0.26	0/995	0.49	0/1356
3	C	0.22	0/190	0.30	0/258
3	F	0.22	0/190	0.36	0/258
3	J	0.21	0/190	0.32	0/258
3	P	0.23	0/185	0.28	0/251
All	All	0.25	0/12993	0.47	0/17678

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	1699	0	1651	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1693	0	1646	11	0
1	G	878	0	854	7	0
1	L	1708	0	1658	11	0
2	B	1658	0	1609	8	0
2	E	1654	0	1610	9	0
2	H	1686	0	1644	13	0
2	I	968	0	922	7	0
3	C	181	0	175	0	0
3	F	181	0	175	1	0
3	J	181	0	175	1	0
3	P	176	0	170	2	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	D	6	0	8	0	0
4	G	6	0	8	0	0
4	L	6	0	8	0	0
5	B	5	0	5	0	0
5	I	5	0	5	1	0
5	J	5	0	5	0	0
6	E	2	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	1	0
7	A	71	0	0	0	0
7	B	78	0	0	0	0
7	C	4	0	0	0	0
7	D	24	0	0	0	0
7	E	29	0	0	0	0
7	F	8	0	0	1	0
7	G	21	0	0	0	0
7	H	91	0	0	0	0
7	I	22	0	0	0	0
7	J	5	0	0	0	0
7	L	76	0	0	1	0
7	P	4	0	0	0	0
All	All	13145	0	12344	79	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 3.

All (79) 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:B:87:THR:HG22	2:B:89:ASP:H	1.49	0.76
1:L:43:GLN:HB2	1:L:53:LEU:HD11	1.72	0.71
1:L:129:GLU:OE2	2:H:219:LYS:NZ	2.24	0.69
1:L:45:LYS:NZ	1:L:87:GLU:O	2.26	0.68
1:A:43:GLN:HB2	1:A:53:LEU:HD11	1.79	0.63
1:G:12:ALA:HB1	1:G:113:LYS:HG2	1.83	0.60
1:D:151:LYS:HB3	1:D:203:THR:HB	1.83	0.60
2:E:38:LYS:HB2	2:E:48:ILE:HD11	1.84	0.59
1:L:151:LYS:HB3	1:L:203:THR:HB	1.85	0.59
2:E:12:VAL:HG21	2:E:86:LEU:HD13	1.86	0.58
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.86	0.58
1:L:196:LYS:NZ	7:L:401:HOH:O	2.37	0.57
1:D:128:ASP:HA	1:D:131:LEU:HD12	1.87	0.57
3:F:683:LYS:NZ	7:F:701:HOH:O	2.37	0.57
2:E:9:THR:HG23	2:E:118:THR:HB	1.88	0.55
2:H:30:THR:HA	2:H:53:PRO:HG2	1.92	0.52
2:B:209:ASN:HD22	2:B:216:LYS:HG3	1.75	0.52
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.92	0.52
2:E:201:THR:OG1	2:E:202:GLN:N	2.44	0.51
1:D:126:PRO:HG3	1:D:136:ALA:HB1	1.92	0.51
2:I:32:TYR:HB3	2:I:98:ARG:HG3	1.92	0.51
2:H:178:ALA:HB2	2:H:188:LEU:HD23	1.93	0.51
2:I:9:THR:HG23	2:I:118:THR:HB	1.93	0.50
1:A:39:LEU:HD21	1:A:94:CYS:HB2	1.93	0.50
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.93	0.50
2:E:163:SER:OG	2:E:207:ASN:OD1	2.27	0.49
1:A:126:PRO:HD3	1:A:138:VAL:HG22	1.95	0.49
1:A:192:TYR:CZ	1:A:217:ARG:HG3	2.47	0.49
2:B:209:ASN:ND2	2:B:216:LYS:HG3	2.27	0.49
1:A:60:ARG:HG3	1:A:64:VAL:HB	1.95	0.49
1:G:6:GLN:HE22	1:G:93:CYS:HA	1.78	0.49
3:P:684:LYS:HD2	3:P:684:LYS:HA	1.61	0.48
2:B:129:PRO:HB3	2:B:155:TYR:HB3	1.95	0.48
1:A:188:SER:OG	1:A:191:ASP:OD1	2.31	0.48
1:G:92:TYR:HE2	1:G:110:LEU:HD22	1.77	0.48
1:L:38:TYR:HB2	1:L:98:TYR:HB2	1.96	0.47
1:A:32:SER:O	1:A:35:GLN:NE2	2.45	0.47
2:E:129:PRO:HB3	2:E:155:TYR:HB3	1.96	0.47
1:A:53:LEU:HA	1:A:64:VAL:HG21	1.96	0.47
1:D:142:LEU:HB2	1:D:181:LEU:HB3	1.97	0.47
1:L:21:MET:HG2	1:L:108:THR:HG21	1.97	0.46
1:L:53:LEU:HA	1:L:64:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.99	0.45
1:A:114:ARG:HG2	1:A:115:THR:N	2.31	0.45
1:D:6:GLN:HE22	1:D:93:CYS:HA	1.82	0.45
1:L:89:LEU:HD11	1:L:112:ILE:HG12	1.99	0.44
1:A:66:ASP:N	1:A:66:ASP:OD1	2.49	0.44
1:G:85:LYS:HZ2	1:G:87:GLU:H	1.66	0.44
2:H:207:ASN:ND2	2:H:218:ASP:OD1	2.31	0.44
2:I:1:GLN:O	2:I:3:GLN:HG2	2.18	0.43
1:G:13:VAL:HG21	1:G:19:VAL:HG13	2.01	0.43
2:B:93:VAL:HG21	4:B:302:GOL:H12	2.01	0.43
2:H:67:LYS:HB2	2:H:67:LYS:HE2	1.79	0.42
2:I:14:PRO:HD3	2:I:121:VAL:HG12	2.01	0.42
6:I:301:CL:CL	3:J:674:ASN:ND2	2.89	0.42
2:H:162:VAL:HG22	2:H:208:VAL:HG22	2.01	0.42
2:B:219:LYS:HB2	2:B:219:LYS:HE2	1.80	0.42
2:H:102:TYR:HB2	2:H:108:TYR:OH	2.20	0.42
1:D:138:VAL:HB	1:D:185:LEU:HB3	2.02	0.42
2:H:178:ALA:HA	2:H:188:LEU:HB3	2.00	0.42
2:I:14:PRO:HA	2:I:86:LEU:O	2.19	0.42
1:D:172:GLN:HG3	1:D:179:TYR:CZ	2.55	0.42
2:I:38:LYS:NZ	5:I:302:1HC:O	2.41	0.42
1:L:12:ALA:HA	1:L:111:GLU:HG2	2.02	0.42
3:P:670:TRP:CD1	3:P:670:TRP:N	2.88	0.42
2:H:38:LYS:HB2	2:H:48:ILE:HD11	2.01	0.41
1:D:13:VAL:HG21	1:D:19:VAL:HB	2.02	0.41
1:D:142:LEU:HD13	1:D:181:LEU:HD22	2.02	0.41
2:E:205:ILE:HG13	2:E:220:LYS:HG3	2.03	0.41
2:B:194:VAL:HG11	2:B:204:TYR:CE1	2.56	0.41
1:L:112:ILE:HD13	1:L:112:ILE:HA	1.85	0.41
1:G:6:GLN:NE2	1:G:92:TYR:O	2.51	0.41
2:I:69:THR:HB	2:I:82:HIS:HB3	2.03	0.41
2:E:204:TYR:C	2:E:205:ILE:HD12	2.42	0.40
1:D:164:ASN:OD1	1:D:164:ASN:N	2.51	0.40
1:D:31:TYR:CE2	1:D:33:SER:HB3	2.56	0.40
1:G:92:TYR:CE2	1:G:110:LEU:HD22	2.55	0.40
2:E:153:LYS:HG3	2:E:187:SER:HB2	2.04	0.40
2:H:210:HIS:HB3	2:H:215:THR:HB	2.03	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	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
1	D	217/220 (99%)	211 (97%)	6 (3%)	0	100	100
1	G	112/220 (51%)	107 (96%)	5 (4%)	0	100	100
1	L	219/220 (100%)	215 (98%)	4 (2%)	0	100	100
2	B	217/228 (95%)	212 (98%)	5 (2%)	0	100	100
2	E	216/228 (95%)	208 (96%)	8 (4%)	0	100	100
2	H	223/228 (98%)	219 (98%)	4 (2%)	0	100	100
2	I	124/228 (54%)	120 (97%)	4 (3%)	0	100	100
3	C	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
3	F	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
3	J	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
3	P	16/20 (80%)	15 (94%)	1 (6%)	0	100	100
All	All	1613/1872 (86%)	1567 (97%)	46 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	195/195 (100%)	194 (100%)	1 (0%)	88	93
1	D	194/195 (100%)	190 (98%)	4 (2%)	53	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	99/195 (51%)	95 (96%)	4 (4%)	31	41
1	L	196/195 (100%)	185 (94%)	11 (6%)	21	27
2	B	185/193 (96%)	178 (96%)	7 (4%)	33	43
2	E	186/193 (96%)	180 (97%)	6 (3%)	39	50
2	H	190/193 (98%)	182 (96%)	8 (4%)	30	39
2	I	104/193 (54%)	98 (94%)	6 (6%)	20	25
3	C	18/19 (95%)	17 (94%)	1 (6%)	21	27
3	F	18/19 (95%)	17 (94%)	1 (6%)	21	27
3	J	18/19 (95%)	17 (94%)	1 (6%)	21	27
3	P	18/19 (95%)	17 (94%)	1 (6%)	21	27
All	All	1421/1628 (87%)	1370 (96%)	51 (4%)	35	46

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	8	PRO
1	L	10	SER
1	L	17	GLU
1	L	132	LYS
1	L	160	LEU
1	L	171	GLU
1	L	175	LYS
1	L	182	SER
1	L	194	LYS
1	L	208	SER
2	H	23	LYS
2	H	75	SER
2	H	88	SER
2	H	98	ARG
2	H	101	TYR
2	H	171	SER
2	H	189	SER
2	H	211	LYS
3	P	685	LYS
1	A	7	SER
2	B	10	ASP
2	B	67	LYS

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Mol	Chain	Res	Type
2	B	75	SER
2	B	89	ASP
2	B	98	ARG
2	B	101	TYR
2	B	148	LEU
3	C	685	LYS
1	D	9	SER
1	D	14	SER
1	D	39	LEU
1	D	180	SER
2	E	88	SER
2	E	101	TYR
2	E	122	SER
2	E	123	SER
2	E	197	SER
2	E	207	ASN
3	F	670	TRP
1	G	39	LEU
1	G	51	LYS
1	G	71	SER
1	G	76	ASP
2	I	74	LYS
2	I	75	SER
2	I	88	SER
2	I	98	ARG
2	I	101	TYR
2	I	123	SER
3	J	670	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	209	ASN
2	E	174	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
5	1HC	J	701	-	4,4,4	0.33	0	2,4,4	0.38	0
4	GOL	L	301	-	5,5,5	0.93	0	5,5,5	0.97	0
4	GOL	D	301	-	5,5,5	0.93	0	5,5,5	0.91	0
5	1HC	I	302	-	4,4,4	0.33	0	2,4,4	0.39	0
4	GOL	G	302	-	5,5,5	0.92	0	5,5,5	0.99	0
4	GOL	B	302	-	5,5,5	0.88	0	5,5,5	1.03	0
4	GOL	A	301	-	5,5,5	0.91	0	5,5,5	0.95	0
5	1HC	B	301	-	4,4,4	0.33	0	2,4,4	0.44	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
5	1HC	J	701	-	-	0/2/2/2	-
4	GOL	L	301	-	-	0/4/4/4	-
4	GOL	D	301	-	-	3/4/4/4	-
5	1HC	I	302	-	-	0/2/2/2	-
4	GOL	G	302	-	-	2/4/4/4	-
4	GOL	B	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	301	-	-	0/4/4/4	-
5	1HC	B	301	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	GOL	C1-C2-C3-O3
5	B	301	1HC	O-C1-C2-C3
4	B	302	GOL	O2-C2-C3-O3
4	D	301	GOL	C1-C2-C3-O3
4	G	302	GOL	O1-C1-C2-C3
4	G	302	GOL	O1-C1-C2-O2
4	D	301	GOL	O1-C1-C2-C3
5	B	301	1HC	N-C1-C2-C3
4	D	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	302	1HC	1	0
4	B	302	GOL	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, 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	220/220 (100%)	-0.26	1 (0%) 91 92	24, 38, 54, 89	0
1	D	219/220 (99%)	-0.15	1 (0%) 91 92	25, 45, 67, 81	0
1	G	114/220 (51%)	0.01	2 (1%) 68 65	27, 51, 80, 97	0
1	L	220/220 (100%)	-0.35	1 (0%) 91 92	22, 34, 54, 84	0
2	B	221/228 (96%)	-0.28	3 (1%) 75 74	21, 31, 53, 97	0
2	E	220/228 (96%)	0.24	19 (8%) 10 7	23, 54, 90, 108	0
2	H	225/228 (98%)	-0.31	1 (0%) 92 93	19, 30, 44, 79	0
2	I	126/228 (55%)	0.16	7 (5%) 24 21	24, 43, 82, 113	0
3	C	19/20 (95%)	-0.10	1 (5%) 26 23	23, 30, 87, 89	0
3	F	19/20 (95%)	0.05	1 (5%) 26 23	21, 26, 58, 70	0
3	J	19/20 (95%)	-0.22	0 100 100	23, 28, 71, 82	0
3	P	18/20 (90%)	-0.20	0 100 100	23, 31, 64, 91	0
All	All	1640/1872 (87%)	-0.14	37 (2%) 60 56	19, 37, 76, 113	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	126	THR	6.0
1	G	112	ILE	4.8
2	I	122	SER	4.1
2	E	225	SER	3.9
1	L	220	CYS	3.7
2	I	41	PRO	3.6
2	B	144	GLY	3.5
3	C	667	ALA	3.4
3	F	667	ALA	3.1
2	E	144	GLY	3.1
2	E	145	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	214	ASN	3.1
2	E	201	THR	3.0
2	E	197	SER	2.9
1	G	111	GLU	2.8
2	B	138	SER	2.6
2	I	125	SER	2.6
2	E	200	GLY	2.6
2	E	224	LYS	2.6
2	I	120	THR	2.5
2	E	216	LYS	2.5
2	E	129	PRO	2.4
2	B	225	SER	2.4
1	A	220	CYS	2.4
2	E	209	ASN	2.3
2	I	11	LEU	2.3
2	E	221	VAL	2.3
2	I	123	SER	2.3
2	E	218	ASP	2.3
2	E	195	PRO	2.3
2	E	222	GLU	2.3
2	E	137	SER	2.2
2	E	217	VAL	2.1
2	E	166	SER	2.1
1	D	171	GLU	2.0
2	H	225	SER	2.0
2	E	208	VAL	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 monosaccharides 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, 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	B	302	6/6	0.86	0.17	38,39,43,45	0
4	GOL	L	301	6/6	0.90	0.20	43,46,48,48	0
4	GOL	A	301	6/6	0.91	0.24	40,43,49,51	0
5	1HC	I	302	5/5	0.91	0.12	50,56,61,61	0
5	1HC	B	301	5/5	0.92	0.15	34,34,39,40	0
6	CL	G	301	1/1	0.93	0.10	56,56,56,56	0
5	1HC	J	701	5/5	0.94	0.17	43,43,44,46	0
4	GOL	D	301	6/6	0.95	0.14	35,36,45,49	0
4	GOL	G	302	6/6	0.95	0.13	36,39,42,45	0
6	CL	E	302	1/1	0.97	0.21	50,50,50,50	0
6	CL	E	301	1/1	0.99	0.13	27,27,27,27	0
6	CL	I	301	1/1	1.00	0.08	23,23,23,23	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.