



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 05:11 AM EDT

PDB ID : 5VJQ  
Title : Complex between HyHEL10 Fab fragment heavy chain mutant (I29F, S52T, Y53F) and Pekin duck egg lysozyme isoform I (DEL-I)  
Authors : Langley, D.B.; Christ, D.  
Deposited on : 2017-04-19  
Resolution : 1.90 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)  
Xtriage (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

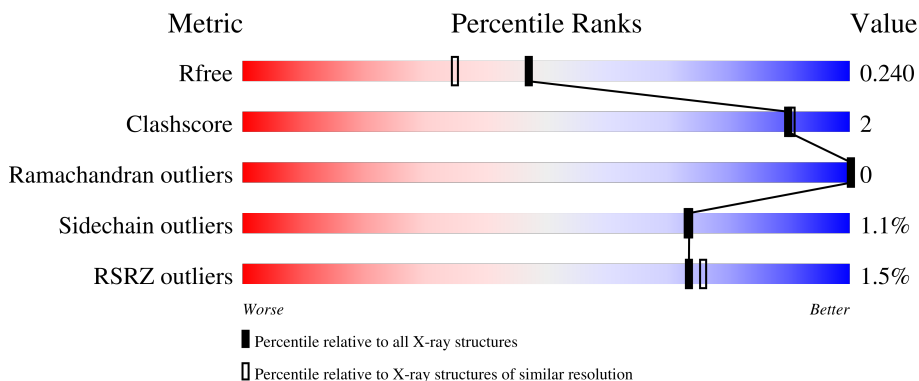
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.



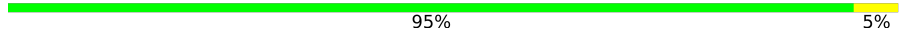
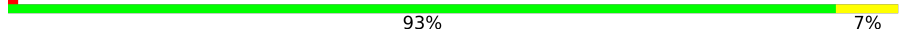
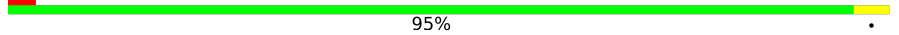
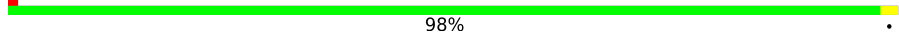
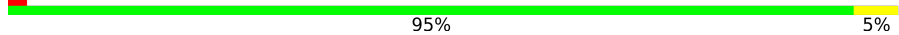


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	213	 93% 5% .
1	C	213	 91% 6% .
1	E	213	 93% . .
1	G	213	 93% . .
2	B	213	 95% 5%

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Mol	Chain	Length	Quality of chain
2	D	213	 95% 5%
2	F	213	 93% 7%
2	H	213	 95% . 3%
3	I	129	 98% . 2%
3	J	129	 95% 5%
3	K	129	 86% 10% . . 11%
3	L	129	 91% 7% . 2%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17903 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 HyHEL10 heavy chain Fab fragment carrying three mutations; I29F, S52T, Y53F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total	C	N	O	S	0	3	0
			1598	1014	255	321	8			
1	C	207	Total	C	N	O	S	0	3	0
			1599	1015	258	318	8			
1	E	207	Total	C	N	O	S	0	0	0
			1576	1002	249	319	6			
1	G	206	Total	C	N	O	S	0	0	0
			1566	996	248	316	6			

- Molecule 2 is a protein called HyHEL10 light chain Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	Total	C	N	O	S	0	4	0
			1658	1029	283	338	8			
2	D	213	Total	C	N	O	S	0	1	0
			1636	1016	277	337	6			
2	F	212	Total	C	N	O	S	0	2	0
			1635	1018	277	334	6			
2	H	212	Total	C	N	O	S	0	4	0
			1653	1028	280	339	6			

- Molecule 3 is a protein called Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	129	Total	C	N	O	S	0	1	0
			998	615	185	188	10			
3	J	129	Total	C	N	O	S	0	1	0
			1002	616	188	188	10			
3	K	125	Total	C	N	O	S	0	3	0
			981	599	189	183	10			
3	L	126	Total	C	N	O	S	0	0	0
			967	593	182	182	10			

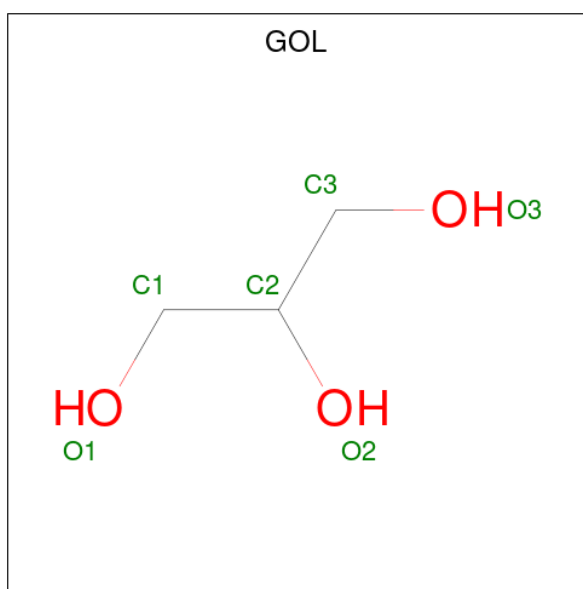
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	37	SER	GLY	conflict	UNP U3J0P1
I	71	GLY	ARG	conflict	UNP U3J0P1
J	37	SER	GLY	conflict	UNP U3J0P1
J	71	GLY	ARG	conflict	UNP U3J0P1
K	37	SER	GLY	conflict	UNP U3J0P1
K	71	GLY	ARG	conflict	UNP U3J0P1
L	37	SER	GLY	conflict	UNP U3J0P1
L	71	GLY	ARG	conflict	UNP U3J0P1

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 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
5	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

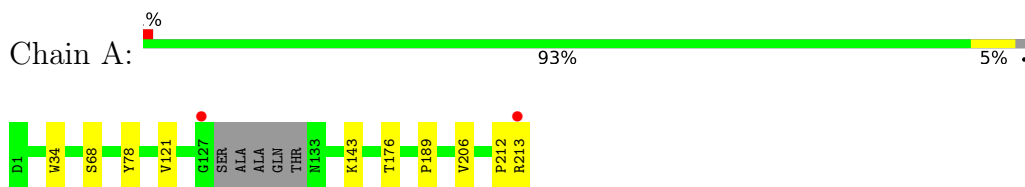
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	108	Total O 108 108	0	0
6	B	159	Total O 159 159	0	0
6	I	51	Total O 51 51	0	0
6	C	104	Total O 104 104	0	0
6	D	130	Total O 130 130	0	0
6	J	71	Total O 71 71	0	0
6	E	74	Total O 74 74	0	0
6	F	92	Total O 92 92	0	0
6	K	39	Total O 39 39	0	0
6	G	71	Total O 71 71	0	0
6	H	65	Total O 65 65	0	0
6	L	30	Total O 30 30	0	0

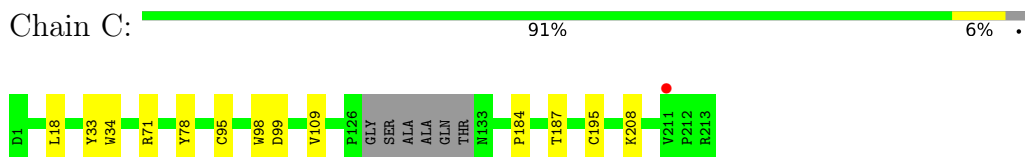
### 3 Residue-property plots [i](#)

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.

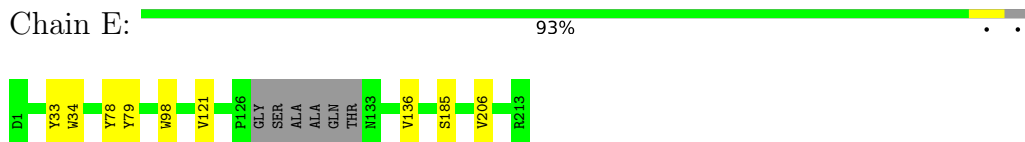
- Molecule 1: HyHEL10 heavy chain Fab fragment carrying three mutations; I29F, S52T, Y53F



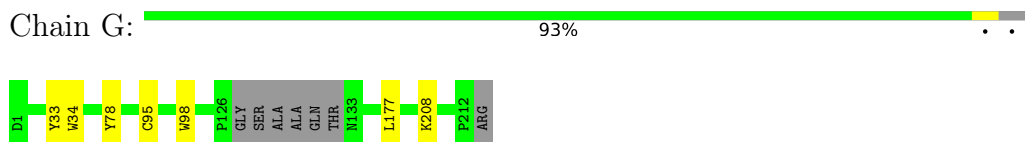
- Molecule 1: HyHEL10 heavy chain Fab fragment carrying three mutations; I29F, S52T, Y53F



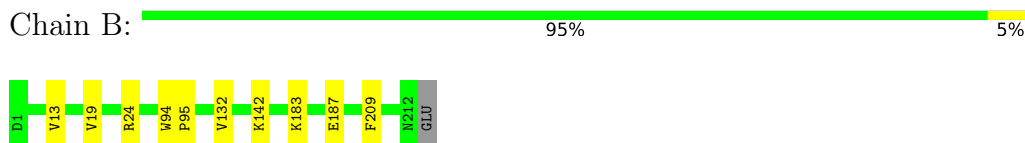
- Molecule 1: HyHEL10 heavy chain Fab fragment carrying three mutations; I29F, S52T, Y53F



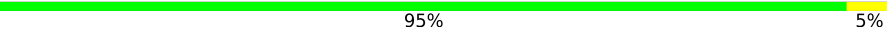
- Molecule 1: HyHEL10 heavy chain Fab fragment carrying three mutations; I29F, S52T, Y53F



- Molecule 2: HyHEL10 light chain Fab fragment

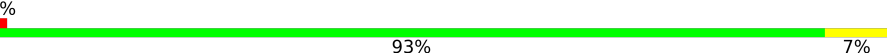


- Molecule 2: HyHEL10 light chain Fab fragment

Chain D:  95% 5%



• Molecule 2: HyHEL10 light chain Fab fragment

Chain F:  93% 7%



• Molecule 2: HyHEL10 light chain Fab fragment

Chain H:  95% 3%

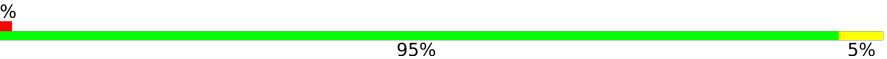


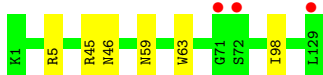
• Molecule 3: Lysozyme

Chain I:  98%




• Molecule 3: Lysozyme

Chain J:  95% 5%




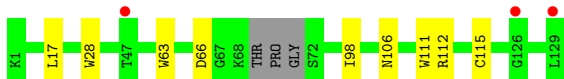
• Molecule 3: Lysozyme

Chain K:  86% 11% 10%



• Molecule 3: Lysozyme

Chain L:  91% 7%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.65Å 132.66Å 199.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 1.90 49.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.32-1.90) 97.8 (49.32-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.193 , 0.235 0.199 , 0.240	Depositor DCC
$R_{free}$ test set	9009 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtrriage
Anisotropy	0.147	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.3	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	0.95	EDS
Total number of atoms	17903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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, 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	0.63	0/1643	0.79	0/2258
1	C	0.63	0/1644	0.80	0/2259
1	E	0.60	0/1621	0.75	0/2230
1	G	0.59	0/1611	0.74	0/2214
2	B	0.66	0/1696	0.81	0/2303
2	D	0.67	0/1674	0.80	1/2278 (0.0%)
2	F	0.59	0/1673	0.75	0/2275
2	H	0.61	0/1690	0.77	0/2298
3	I	0.56	0/1019	0.70	0/1383
3	J	0.62	0/1023	0.83	3/1387 (0.2%)
3	K	0.68	0/998	0.79	0/1349
3	L	0.53	0/984	0.74	1/1332 (0.1%)
All	All	0.62	0/17276	0.77	5/23566 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	45	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	J	45	ARG	NE-CZ-NH2	-6.33	117.13	120.30
2	D	170	ASP	CB-CG-OD1	5.18	122.96	118.30
3	L	66	ASP	CB-CG-OD1	5.11	122.90	118.30
3	J	5	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	1598	0	1513	7	0
1	C	1599	0	1520	9	0
1	E	1576	0	1495	5	0
1	G	1566	0	1487	4	0
2	B	1658	0	1562	4	0
2	D	1636	0	1526	4	0
2	F	1635	0	1530	6	0
2	H	1653	0	1549	4	0
3	I	998	0	936	1	0
3	J	1002	0	940	2	0
3	K	981	0	909	8	0
3	L	967	0	906	5	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	C	18	0	24	4	0
5	E	6	0	8	0	0
5	H	6	0	8	1	0
5	J	6	0	8	0	0
6	A	108	0	0	2	0
6	B	159	0	0	0	0
6	C	104	0	0	1	0
6	D	130	0	0	1	0
6	E	74	0	0	0	0
6	F	92	0	0	0	0
6	G	71	0	0	0	0
6	H	65	0	0	0	0
6	I	51	0	0	0	0
6	J	71	0	0	0	0
6	K	39	0	0	0	0
6	L	30	0	0	0	0
All	All	17903	0	15921	59	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 2.

All (59) 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)
3:K:40:THR:HG22	3:K:88[A]:ILE:HD11	1.54	0.88
3:K:88[A]:ILE:HG22	3:K:88[A]:ILE:O	1.84	0.77
1:A:143:LYS:HG2	1:A:176[A]:THR:HG22	1.77	0.66
1:G:98:TRP:O	5:H:302:GOL:H2	1.96	0.65
1:C:99:ASP:HA	5:C:302:GOL:H31	1.78	0.65
3:K:79:PRO:O	3:K:82:VAL:HG12	2.00	0.61
3:K:88[A]:ILE:HG22	3:K:92:VAL:HG23	1.82	0.61
2:F:189:HIS:O	2:F:211:ARG:NH2	2.36	0.59
1:A:176[A]:THR:HG23	6:A:323:HOH:O	2.03	0.58
1:A:189:PRO:HB3	1:A:212:PRO:HG3	1.86	0.57
1:A:176[A]:THR:HG21	6:A:370:HOH:O	2.03	0.57
1:E:136:VAL:HG13	1:E:185:SER:HB3	1.86	0.56
2:F:94:TRP:CD2	2:F:95:PRO:HA	2.41	0.55
2:F:146:VAL:HG21	2:F:175:MET:HE2	1.88	0.55
3:K:88[A]:ILE:O	3:K:88[A]:ILE:CG2	2.52	0.54
2:D:94:TRP:CD2	2:D:95:PRO:HA	2.43	0.54
1:G:33:TYR:HB2	1:G:98:TRP:HB2	1.90	0.54
2:H:94:TRP:CD2	2:H:95:PRO:HA	2.43	0.54
1:C:34:TRP:HB3	1:C:78:TYR:CZ	2.43	0.53
2:B:94:TRP:CD2	2:B:95:PRO:HA	2.44	0.53
1:C:33:TYR:HB2	1:C:98:TRP:HB2	1.90	0.52
5:C:302:GOL:H12	6:D:410:HOH:O	2.09	0.51
3:J:46:ASN:OD1	3:J:59:ASN:ND2	2.43	0.51
2:H:104:LEU:C	2:H:104:LEU:HD23	2.31	0.51
1:C:71[A]:ARG:NH1	6:C:403:HOH:O	2.44	0.50
3:L:106:ASN:OD1	3:L:112:ARG:HD3	2.12	0.50
1:G:34:TRP:HB3	1:G:78:TYR:CZ	2.47	0.49
2:H:136:LEU:N	2:H:136:LEU:HD12	2.26	0.49
1:C:99:ASP:HA	5:C:302:GOL:C3	2.40	0.49
1:G:78:TYR:OH	1:G:95:CYS:HB2	2.13	0.48
1:A:34:TRP:HB3	1:A:78:TYR:CZ	2.48	0.48
3:L:17:LEU:HD22	3:L:28:TRP:CE2	2.49	0.48
2:B:13:VAL:HG22	2:B:19:VAL:HG11	1.95	0.48
1:C:184:PRO:O	1:C:187:THR:HB	2.13	0.48
3:K:40:THR:O	3:K:84:LEU:HA	2.14	0.47
1:A:189:PRO:HB3	1:A:212:PRO:CG	2.45	0.47
3:K:127:CYS:O	3:K:128:ARG:HB2	2.14	0.47
1:E:79:TYR:CZ	3:L:112:ARG:HD2	2.51	0.46
3:L:111:TRP:CD1	3:L:115:CYS:HB2	2.50	0.46
2:D:184:ASP:O	2:D:188:ARG:HG3	2.15	0.45
2:F:136:LEU:HD21	2:F:146:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:303:GOL:H31	2:D:164:THR:HG21	2.00	0.44
2:B:183:LYS:O	2:B:187:GLU:HG3	2.18	0.44
1:E:34:TRP:HB3	1:E:78:TYR:CZ	2.53	0.44
1:C:18:LEU:HD13	1:C:109:VAL:HG11	2.01	0.43
2:F:83:PHE:HB3	2:F:106:ILE:HG12	2.01	0.43
1:E:121:VAL:HG21	1:E:206:VAL:CG2	2.49	0.42
3:K:111:TRP:CD1	3:K:115:CYS:HB2	2.54	0.42
1:C:78:TYR:OH	1:C:95:CYS:HB2	2.19	0.42
1:E:33:TYR:HB2	1:E:98:TRP:HB2	2.02	0.42
2:D:49:LYS:HD2	2:D:55:ILE:CD1	2.51	0.41
2:H:179:LEU:HD11	2:H:181:LEU:HD21	2.00	0.41
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.02	0.41
2:B:132:VAL:HG13	2:B:209:PHE:HE1	1.85	0.41
3:L:63:TRP:CE2	3:L:98:ILE:HG12	2.56	0.41
1:A:121:VAL:HG21	1:A:206:VAL:CG2	2.51	0.41
3:I:63:TRP:CE2	3:I:98:ILE:HG12	2.56	0.40
3:J:63:TRP:CE2	3:J:98:ILE:HG12	2.57	0.40
1:C:195[A]:CYS:SG	1:C:208:LYS:HB3	2.62	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	207/213 (97%)	205 (99%)	2 (1%)	0	100	100
1	C	206/213 (97%)	204 (99%)	2 (1%)	0	100	100
1	E	203/213 (95%)	201 (99%)	2 (1%)	0	100	100
1	G	202/213 (95%)	198 (98%)	4 (2%)	0	100	100
2	B	214/213 (100%)	210 (98%)	4 (2%)	0	100	100
2	D	212/213 (100%)	209 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	212/213 (100%)	208 (98%)	4 (2%)	0	100	100
2	H	214/213 (100%)	206 (96%)	8 (4%)	0	100	100
3	I	128/129 (99%)	127 (99%)	1 (1%)	0	100	100
3	J	128/129 (99%)	127 (99%)	1 (1%)	0	100	100
3	K	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
3	L	122/129 (95%)	122 (100%)	0	0	100	100
All	All	2172/2220 (98%)	2137 (98%)	35 (2%)	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	184/190 (97%)	182 (99%)	2 (1%)	73	73
1	C	184/190 (97%)	184 (100%)	0	100	100
1	E	182/190 (96%)	182 (100%)	0	100	100
1	G	180/190 (95%)	178 (99%)	2 (1%)	73	73
2	B	190/191 (100%)	188 (99%)	2 (1%)	73	73
2	D	185/191 (97%)	183 (99%)	2 (1%)	73	73
2	F	184/191 (96%)	181 (98%)	3 (2%)	62	60
2	H	186/191 (97%)	181 (97%)	5 (3%)	44	38
3	I	103/106 (97%)	102 (99%)	1 (1%)	76	76
3	J	103/106 (97%)	103 (100%)	0	100	100
3	K	98/106 (92%)	93 (95%)	5 (5%)	24	14
3	L	99/106 (93%)	99 (100%)	0	100	100
All	All	1878/1948 (96%)	1856 (99%)	22 (1%)	73	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	213	ARG
2	B	24	ARG
2	B	142	LYS
3	I	103	ASN
2	D	107	LYS
2	D	213	GLU
2	F	76	ASN
2	F	105	GLU
2	F	191	SER
3	K	19	ASN
3	K	79	PRO
3	K	103	ASN
3	K	112	ARG
3	K	114	ARG
1	G	177	LEU
1	G	208	LYS
2	H	45[A]	ARG
2	H	45[B]	ARG
2	H	77	SER
2	H	105[A]	GLU
2	H	105[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	171	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	GOL	J	201	-	5,5,5	0.30	0	5,5,5	0.70	0
5	GOL	C	303	-	5,5,5	0.28	0	5,5,5	0.62	0
5	GOL	H	302	-	5,5,5	0.45	0	5,5,5	0.73	0
5	GOL	E	301	-	5,5,5	0.20	0	5,5,5	0.42	0
5	GOL	C	302	-	5,5,5	0.74	0	5,5,5	1.06	0
5	GOL	C	301	-	5,5,5	0.25	0	5,5,5	0.57	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	GOL	J	201	-	-	2/4/4/4	-
5	GOL	C	303	-	-	1/4/4/4	-
5	GOL	H	302	-	-	4/4/4/4	-
5	GOL	E	301	-	-	2/4/4/4	-
5	GOL	C	302	-	-	4/4/4/4	-
5	GOL	C	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	302	GOL	C1-C2-C3-O3
5	C	302	GOL	O2-C2-C3-O3
5	E	301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	H	302	GOL	C1-C2-C3-O3
5	C	302	GOL	O1-C1-C2-C3
5	H	302	GOL	O1-C1-C2-C3
5	E	301	GOL	O2-C2-C3-O3
5	H	302	GOL	O1-C1-C2-O2
5	C	302	GOL	O1-C1-C2-O2
5	H	302	GOL	O2-C2-C3-O3
5	J	201	GOL	O2-C2-C3-O3
5	J	201	GOL	C1-C2-C3-O3
5	C	303	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	303	GOL	1	0
5	H	302	GOL	1	0
5	C	302	GOL	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	208/213 (97%)	0.01	2 (0%) 82 84	15, 26, 42, 50	0
1	C	207/213 (97%)	-0.02	1 (0%) 91 92	14, 26, 40, 48	0
1	E	207/213 (97%)	-0.01	0 100 100	19, 29, 42, 50	0
1	G	206/213 (96%)	0.04	0 100 100	17, 32, 50, 61	0
2	B	212/213 (99%)	-0.09	0 100 100	15, 22, 33, 44	0
2	D	213/213 (100%)	-0.02	0 100 100	15, 24, 39, 46	0
2	F	212/213 (99%)	0.13	2 (0%) 84 85	17, 28, 50, 56	0
2	H	212/213 (99%)	0.28	6 (2%) 53 56	19, 32, 49, 70	0
3	I	129/129 (100%)	-0.14	1 (0%) 86 87	17, 31, 44, 53	0
3	J	129/129 (100%)	-0.15	3 (2%) 60 63	16, 25, 39, 59	0
3	K	125/129 (96%)	0.84	14 (11%) 5 6	24, 35, 51, 62	0
3	L	126/129 (97%)	0.06	3 (2%) 59 62	22, 37, 54, 65	0
All	All	2186/2220 (98%)	0.07	32 (1%) 73 76	14, 28, 47, 70	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	129	LEU	5.6
3	L	129	LEU	4.1
3	K	29	VAL	3.7
3	J	71	GLY	3.4
3	K	108	TRP	3.3
1	A	127	GLY	3.3
2	H	194	CYS	3.3
3	K	69	THR	3.3
2	F	209	PHE	3.1
3	J	129	LEU	3.1
3	K	47	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	163	TRP	2.9
3	J	72	SER	2.8
3	K	6	CYS	2.8
2	H	160	LEU	2.8
1	A	213	ARG	2.7
3	K	115	CYS	2.6
3	K	123	TRP	2.6
2	F	188	ARG	2.6
3	K	3	TYR	2.5
3	K	111	TRP	2.4
2	H	143	ASP	2.3
3	L	47	THR	2.2
3	L	126	GLY	2.2
2	H	122	SER	2.2
3	K	28	TRP	2.1
3	K	107	ALA	2.1
1	C	211	VAL	2.1
3	K	51	THR	2.1
3	K	10	ALA	2.0
3	K	62	TRP	2.0
2	H	126	THR	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(Å <sup>2</sup> )	Q<0.9
5	GOL	C	302	6/6	0.83	0.24	29,30,32,33	0
5	GOL	E	301	6/6	0.85	0.26	44,51,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	H	302	6/6	0.86	0.19	35,37,38,38	0
5	GOL	C	303	6/6	0.87	0.22	41,44,45,49	0
5	GOL	J	201	6/6	0.87	0.26	44,49,51,53	0
5	GOL	C	301	6/6	0.89	0.20	38,44,45,48	0
4	CL	H	301	1/1	0.98	0.10	29,29,29,29	0
4	CL	F	301	1/1	0.99	0.07	24,24,24,24	0
4	CL	D	301	1/1	0.99	0.08	22,22,22,22	0
4	CL	B	301	1/1	1.00	0.07	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.