



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:30 PM UTC

PDB ID : 3Q1S / pdb_00003q1s
Title : HIV-1 neutralizing antibody Z13e1 in complex with epitope display protein
Authors : Stanfield, R.L.; Julien, J.-P.; Pejchal, R.; Gach, J.S.; Zwick, M.B.; Wilson, I.A.
Deposited on : 2010-12-17
Resolution : 2.15 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

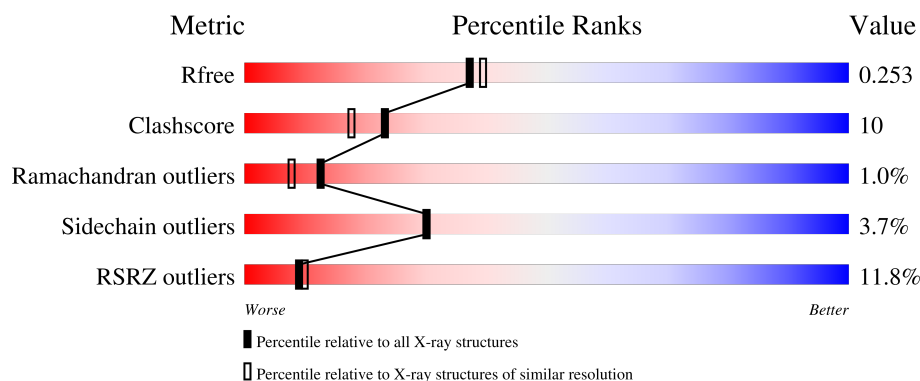
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	L	212	85% 12% ..
2	H	230	4% 77% 12% 8%
3	I	151	34% 48% 19% 7% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IPA	L	2	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4387 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 Z13e1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	209	Total	C	N	O	S	0	0	0
			1604	1002	277	321	4			

- Molecule 2 is a protein called Z13e1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1603	1025	263	309	6			

- Molecule 3 is a protein called Interleukin-22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	113	Total	C	N	O	S	0	0	0
			909	572	160	169	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	64	TRP	SER	engineered mutation	UNP Q9GZX6
I	65	ASN	LEU	engineered mutation	UNP Q9GZX6
I	66	TRP	ALA	engineered mutation	UNP Q9GZX6
I	68	ASP	ASN	engineered mutation	UNP Q9GZX6
I	69	ILE	ASN	engineered mutation	UNP Q9GZX6

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



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

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



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

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

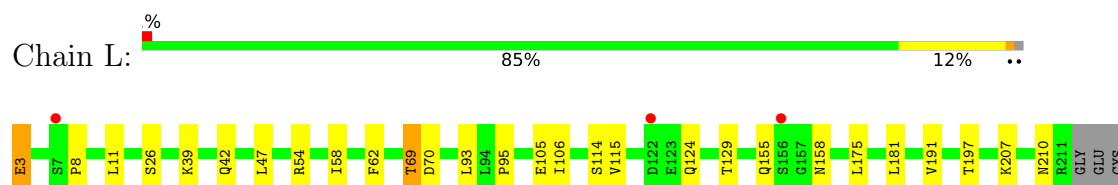
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	85	Total O 85 85	0	0
6	H	93	Total O 93 93	0	0
6	I	25	Total O 25 25	0	0

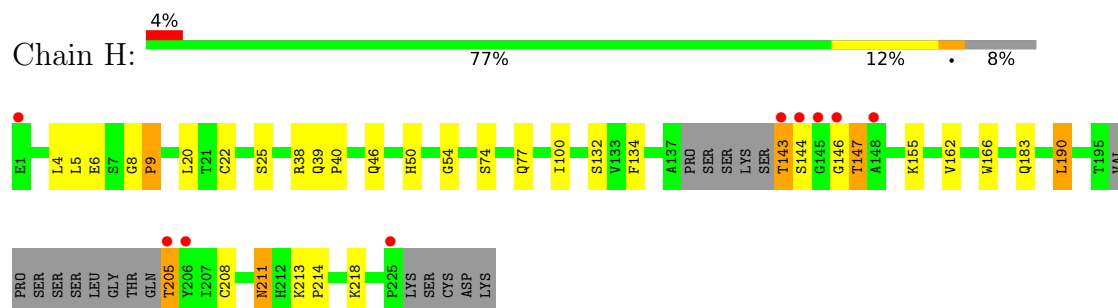
3 Residue-property plots [i](#)

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.

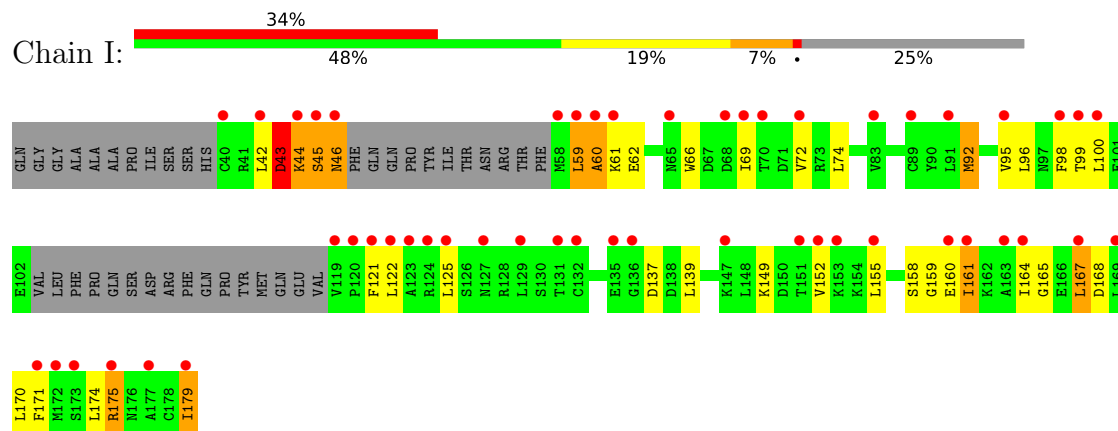
- Molecule 1: Z13e1 Fab light chain



- Molecule 2: Z13e1 Fab heavy chain



- Molecule 3: Interleukin-22



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.62Å 99.22Å 105.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 2.15 49.63 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.63-2.15) 99.8 (49.63-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.207 , 0.260 0.241 , 0.253	Depositor DCC
R_{free} test set	1672 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4387	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: IPA, 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	L	0.98	0/1637	0.94	0/2223
2	H	1.09	1/1644 (0.1%)	1.04	5/2245 (0.2%)
3	I	0.76	0/919	1.00	2/1228 (0.2%)
All	All	0.99	1/4200 (0.0%)	0.99	7/5696 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	40	PRO	CA-C	5.27	1.54	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	43	ASP	N-CA-C	7.21	121.15	109.40
2	H	147	THR	N-CA-C	6.12	123.84	110.80
2	H	6	GLU	CB-CA-C	-5.55	100.16	109.65
2	H	39	GLN	CA-C-N	5.42	123.61	119.66
2	H	39	GLN	C-N-CA	5.42	123.61	119.66
2	H	46	GLN	CA-CB-CG	-5.33	103.44	114.10
3	I	59	LEU	N-CA-C	-5.21	105.69	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	146	GLY	Peptide

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	L	1604	0	1572	28	0
2	H	1603	0	1578	27	0
3	I	909	0	920	34	0
4	L	8	0	16	6	0
5	H	24	0	32	6	0
5	I	12	0	16	2	0
5	L	24	0	32	5	0
6	H	93	0	0	1	0
6	I	25	0	0	1	0
6	L	85	0	0	0	0
All	All	4387	0	4166	85	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 10.

All (85) 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:L:93:LEU:HD11	4:L:2:IPA:C1	1.70	1.21
1:L:93:LEU:CD1	4:L:2:IPA:H11	1.81	1.09
1:L:93:LEU:HD11	4:L:2:IPA:H11	1.13	1.09
3:I:42:LEU:HD13	3:I:125:LEU:HD22	1.50	0.92
1:L:42:GLN:NE2	5:L:217:GOL:O3	2.12	0.82
1:L:3:GLU:HA	1:L:93:LEU:HD21	1.61	0.81
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.71	0.71
1:L:197:THR:HG23	5:L:215:GOL:C1	2.23	0.68
1:L:115:VAL:H	2:H:143:THR:N	1.94	0.65
2:H:5:LEU:HD23	2:H:5:LEU:C	2.22	0.65
2:H:74:SER:O	5:H:231:GOL:H11	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:THR:HG23	5:L:215:GOL:H11	1.80	0.64
3:I:99:THR:HG21	3:I:170:LEU:CD2	2.27	0.63
1:L:95:PRO:HD2	4:L:2:IPA:H2	1.81	0.63
3:I:96:LEU:CD1	3:I:122:LEU:HD22	2.30	0.62
3:I:96:LEU:HD11	3:I:122:LEU:HD22	1.81	0.62
3:I:61:LYS:O	5:I:9:GOL:C1	2.49	0.60
3:I:152:VAL:O	3:I:152:VAL:HG12	2.00	0.60
3:I:46:ASN:H	3:I:46:ASN:HD22	1.50	0.58
3:I:161:ILE:N	3:I:161:ILE:HD13	2.17	0.58
1:L:3:GLU:N	1:L:26:SER:HG	2.00	0.58
1:L:39:LYS:HD2	5:L:217:GOL:H12	1.86	0.57
1:L:155:GLN:HE21	1:L:158:ASN:HD21	1.53	0.57
1:L:69:THR:HG23	1:L:70:ASP:OD1	2.05	0.57
3:I:99:THR:HG21	3:I:170:LEU:HD21	1.88	0.56
2:H:5:LEU:HD23	2:H:5:LEU:O	2.06	0.56
2:H:9:PRO:CD	2:H:9:PRO:O	2.54	0.55
2:H:205:THR:O	2:H:205:THR:HG22	2.05	0.55
1:L:191:VAL:HG22	1:L:210:ASN:ND2	2.22	0.55
1:L:197:THR:HG23	5:L:215:GOL:H12	1.87	0.54
3:I:152:VAL:O	3:I:152:VAL:CG1	2.56	0.54
3:I:72:VAL:HG23	6:I:189:HOH:O	2.07	0.54
2:H:8:GLY:HA3	2:H:20:LEU:CD2	2.37	0.53
1:L:93:LEU:CG	4:L:2:IPA:H11	2.39	0.53
1:L:54:ARG:NH1	1:L:62:PHE:O	2.37	0.52
1:L:69:THR:CG2	1:L:70:ASP:OD1	2.58	0.52
3:I:164:ILE:O	3:I:167:LEU:HD12	2.10	0.52
2:H:213:LYS:HB2	2:H:214:PRO:CD	2.41	0.51
3:I:121:PHE:CD2	3:I:171:PHE:HE2	2.30	0.50
3:I:98:PHE:CD1	3:I:149:LYS:HG2	2.47	0.49
2:H:38:ARG:HH21	5:H:232:GOL:H11	1.78	0.49
2:H:9:PRO:O	2:H:9:PRO:HD2	2.14	0.48
1:L:114:SER:OG	2:H:144:SER:HB2	2.13	0.48
1:L:3:GLU:HB3	4:L:2:IPA:H32	1.96	0.48
1:L:175:LEU:C	1:L:175:LEU:HD23	2.39	0.48
1:L:207:LYS:HE2	2:H:143:THR:HG23	1.96	0.47
2:H:211:ASN:HD21	2:H:218:LYS:NZ	2.12	0.47
3:I:96:LEU:O	3:I:99:THR:HG22	2.14	0.47
1:L:8:PRO:CG	1:L:11:LEU:HD13	2.45	0.47
2:H:155:LYS:NZ	2:H:183:GLN:OE1	2.48	0.47
2:H:213:LYS:HB2	2:H:214:PRO:HD3	1.96	0.47
3:I:43:ASP:O	3:I:46:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:175:ARG:O	3:I:179:ILE:HD13	2.14	0.47
3:I:99:THR:HG23	3:I:100:LEU:H	1.80	0.46
3:I:59:LEU:O	3:I:60:ALA:HB3	2.16	0.46
3:I:59:LEU:O	3:I:62:GLU:HG2	2.16	0.46
1:L:8:PRO:HG3	1:L:11:LEU:HD13	1.99	0.45
5:H:233:GOL:HO1	3:I:66:TRP:HE3	1.65	0.45
3:I:74:LEU:HD13	3:I:152:VAL:HG22	1.98	0.44
1:L:124:GLN:HG2	1:L:129:THR:O	2.17	0.44
2:H:54:GLY:O	5:H:233:GOL:H32	2.18	0.44
2:H:50:HIS:CD2	2:H:50:HIS:C	2.96	0.44
3:I:137:ASP:OD2	3:I:139:LEU:HB2	2.18	0.43
1:L:3:GLU:HA	1:L:93:LEU:CD2	2.42	0.43
2:H:5:LEU:C	2:H:5:LEU:CD2	2.91	0.43
3:I:92:MET:HE3	3:I:170:LEU:HD12	1.99	0.43
1:L:47:LEU:HD12	1:L:58:ILE:HD12	2.01	0.43
2:H:132:SER:HB3	2:H:134:PHE:CZ	2.54	0.43
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.59	0.42
3:I:168:ASP:N	3:I:168:ASP:OD1	2.43	0.42
2:H:162:VAL:CG2	2:H:190:LEU:HD13	2.49	0.42
2:H:77:GLN:NE2	6:H:311:HOH:O	2.53	0.42
3:I:161:ILE:O	3:I:165:GLY:N	2.52	0.42
2:H:74:SER:O	5:H:231:GOL:C1	2.67	0.42
2:H:166:TRP:CH2	2:H:208:CYS:HB3	2.55	0.41
3:I:61:LYS:O	5:I:9:GOL:H12	2.18	0.41
2:H:100:ILE:HD13	3:I:69:ILE:HG21	2.02	0.41
2:H:54:GLY:C	5:H:233:GOL:H32	2.44	0.41
3:I:155:LEU:HB2	3:I:159:GLY:CA	2.51	0.41
3:I:96:LEU:HD22	3:I:174:LEU:HD11	2.01	0.41
3:I:96:LEU:C	3:I:99:THR:HG22	2.46	0.41
1:L:105:GLU:HG2	1:L:106:ILE:N	2.36	0.41
3:I:44:LYS:O	3:I:45:SER:C	2.64	0.41
3:I:95:VAL:O	3:I:99:THR:HG22	2.20	0.40
3:I:99:THR:HG23	3:I:100:LEU:N	2.37	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	L	207/212 (98%)	199 (96%)	8 (4%)	0	100	100
2	H	205/230 (89%)	194 (95%)	10 (5%)	1 (0%)	24	20
3	I	107/151 (71%)	97 (91%)	6 (6%)	4 (4%)	2	0
All	All	519/593 (88%)	490 (94%)	24 (5%)	5 (1%)	12	8

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	THR
3	I	167	LEU
3	I	45	SER
3	I	44	LYS
3	I	60	ALA

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	L	180/182 (99%)	177 (98%)	3 (2%)	53	60
2	H	180/198 (91%)	174 (97%)	6 (3%)	33	34
3	I	102/135 (76%)	94 (92%)	8 (8%)	11	7
All	All	462/515 (90%)	445 (96%)	17 (4%)	30	30

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	GLU
1	L	69	THR
1	L	181	LEU
2	H	9	PRO
2	H	25	SER
2	H	143	THR
2	H	190	LEU
2	H	205	THR
2	H	211	ASN
3	I	43	ASP
3	I	46	ASN
3	I	92	MET
3	I	158	SER
3	I	160	GLU
3	I	161	ILE
3	I	175	ARG
3	I	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	38	GLN
1	L	42	GLN
1	L	89	GLN
1	L	124	GLN
1	L	155	GLN
2	H	39	GLN
2	H	77	GLN
2	H	211	ASN
3	I	46	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	GOL	H	232	-	5,5,5	0.59	0	5,5,5	0.74	0
5	GOL	L	215	-	5,5,5	0.52	0	5,5,5	0.61	0
5	GOL	L	218	-	5,5,5	0.90	0	5,5,5	0.70	0
5	GOL	L	217	-	5,5,5	0.48	0	5,5,5	1.09	0
4	IPA	L	2	-	3,3,3	0.69	0	3,3,3	0.49	0
4	IPA	L	1	-	3,3,3	0.70	0	3,3,3	0.29	0
5	GOL	L	216	-	5,5,5	0.56	0	5,5,5	1.11	0
5	GOL	H	233	-	5,5,5	0.48	0	5,5,5	1.00	0
5	GOL	I	9	-	5,5,5	0.48	0	5,5,5	0.70	0
5	GOL	H	234	-	5,5,5	0.48	0	5,5,5	0.52	0
5	GOL	I	2	-	5,5,5	0.59	0	5,5,5	0.46	0
5	GOL	H	231	-	5,5,5	0.90	0	5,5,5	1.26	1 (20%)

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	H	232	-	-	0/4/4/4	-
5	GOL	L	215	-	-	0/4/4/4	-
5	GOL	L	218	-	-	1/4/4/4	-
5	GOL	L	217	-	-	0/4/4/4	-
5	GOL	L	216	-	-	2/4/4/4	-
5	GOL	H	233	-	-	0/4/4/4	-
5	GOL	I	9	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	H	234	-	-	4/4/4/4	-
5	GOL	I	2	-	-	0/4/4/4	-
5	GOL	H	231	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	231	GOL	O1-C1-C2	2.39	121.15	110.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	234	GOL	O1-C1-C2-C3
5	H	234	GOL	C1-C2-C3-O3
5	L	216	GOL	C1-C2-C3-O3
5	H	234	GOL	O1-C1-C2-O2
5	H	234	GOL	O2-C2-C3-O3
5	L	216	GOL	O2-C2-C3-O3
5	L	218	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	232	GOL	1	0
5	L	215	GOL	3	0
5	L	217	GOL	2	0
4	L	2	IPA	6	0
5	H	233	GOL	3	0
5	I	9	GOL	2	0
5	H	231	GOL	2	0

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	L	209/212 (98%)	0.27	3 (1%) 73 77	23, 37, 60, 71	0
2	H	211/230 (91%)	0.48	9 (4%) 40 45	20, 35, 69, 79	0
3	I	113/151 (74%)	2.06	51 (45%) 0 1	43, 75, 122, 135	0
All	All	533/593 (89%)	0.74	63 (11%) 9 10	20, 40, 94, 135	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	144	SER	9.3
2	H	143	THR	7.2
3	I	163	ALA	5.8
3	I	59	LEU	5.6
2	H	145	GLY	5.4
3	I	60	ALA	4.8
3	I	171	PHE	4.7
3	I	164	ILE	4.5
3	I	58	MET	4.0
3	I	121	PHE	3.9
3	I	119	VAL	3.9
3	I	125	LEU	3.7
3	I	99	THR	3.6
3	I	161	ILE	3.5
3	I	169	LEU	3.4
3	I	132	CYS	3.2
3	I	70	THR	3.2
3	I	120	PRO	3.1
3	I	152	VAL	3.1
3	I	177	ALA	3.1
3	I	122	LEU	3.1
3	I	179	ILE	3.1
3	I	175	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	100	LEU	2.9
3	I	44	LYS	2.9
3	I	123	ALA	2.8
3	I	135	GLU	2.8
3	I	83	VAL	2.8
2	H	146	GLY	2.7
2	H	1	GLU	2.7
3	I	42	LEU	2.6
3	I	46	ASN	2.6
2	H	225	PRO	2.6
3	I	129	LEU	2.6
3	I	98	PHE	2.6
3	I	172	MET	2.6
3	I	65	ASN	2.5
3	I	61	LYS	2.5
3	I	69	ILE	2.5
3	I	151	THR	2.5
2	H	205	THR	2.4
3	I	173	SER	2.4
3	I	127	ASN	2.4
3	I	167	LEU	2.3
3	I	95	VAL	2.3
1	L	7	SER	2.3
3	I	124	ARG	2.3
3	I	91	LEU	2.2
3	I	131	THR	2.2
2	H	148	ALA	2.2
3	I	136	GLY	2.1
3	I	45	SER	2.1
1	L	122	ASP	2.1
3	I	147	LYS	2.1
3	I	68	ASP	2.1
2	H	206	TYR	2.1
3	I	153	LYS	2.1
1	L	156	SER	2.1
3	I	160	GLU	2.1
3	I	155	LEU	2.0
3	I	40	CYS	2.0
3	I	89	CYS	2.0
3	I	72	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 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	IPA	L	1	4/4	0.65	0.19	41,41,42,43	0
5	GOL	I	2	6/6	0.72	0.19	39,44,46,46	0
5	GOL	H	234	6/6	0.76	0.17	40,46,47,49	0
5	GOL	L	216	6/6	0.78	0.21	45,46,48,48	0
5	GOL	H	231	6/6	0.79	0.16	36,36,40,41	0
5	GOL	I	9	6/6	0.79	0.21	42,46,49,49	0
5	GOL	H	233	6/6	0.80	0.18	44,45,47,47	0
5	GOL	L	218	6/6	0.81	0.13	43,47,47,48	0
5	GOL	L	217	6/6	0.81	0.24	33,39,42,43	0
5	GOL	H	232	6/6	0.82	0.20	39,42,47,47	0
5	GOL	L	215	6/6	0.83	0.14	42,46,46,49	0
4	IPA	L	2	4/4	0.84	0.16	41,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.