



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 19, 2023 – 12:55 PM EST

PDB ID : 3QEH  
Title : Crystal structure of human N12-i15, an ADCC and non-neutralizing anti-HIV-1 Env antibody  
Authors : Guan, Y.; DeVico, A.L.; Lewis, G.K.; Pazgier, M.  
Deposited on : 2011-01-20  
Resolution : 2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.36  
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) : 2.36

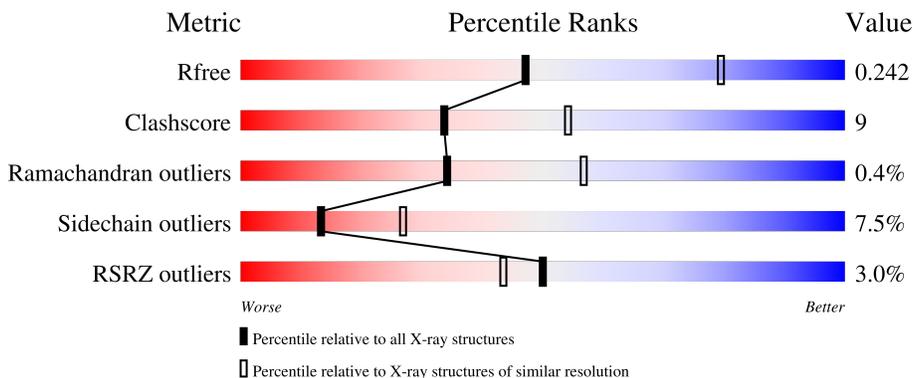
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	232	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">75%      14%      • 7%</p>
1	C	232	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">74%      14%      • 8%</p>
1	E	232	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">74%      13%      • • 8%</p>
1	G	232	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">66%      16%      • 17%</p>
2	B	218	<div style="display: flex; align-items: center;"> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 10px;">75%      21%      • •</p>

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Mol	Chain	Length	Quality of chain
2	D	218	 <p>% 81% 15% ..</p>
2	F	218	 <p>2% 80% 16% ..</p>
2	H	218	 <p>4% 62% 22% 5% 11%</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13446 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 Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1649	C 1043	N 281	O 318	S 7	0	0	0
1	C	213	Total 1630	C 1031	N 278	O 314	S 7	0	0	0
1	E	214	Total 1638	C 1037	N 279	O 315	S 7	0	0	0
1	G	192	Total 1475	C 939	N 250	O 279	S 7	0	0	0

- Molecule 2 is a protein called Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	215	Total 1655	C 1038	N 280	O 331	S 6	0	0	0
2	D	215	Total 1655	C 1038	N 280	O 331	S 6	0	0	0
2	F	212	Total 1631	C 1023	N 276	O 326	S 6	0	0	0
2	H	193	Total 1498	C 941	N 254	O 297	S 6	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

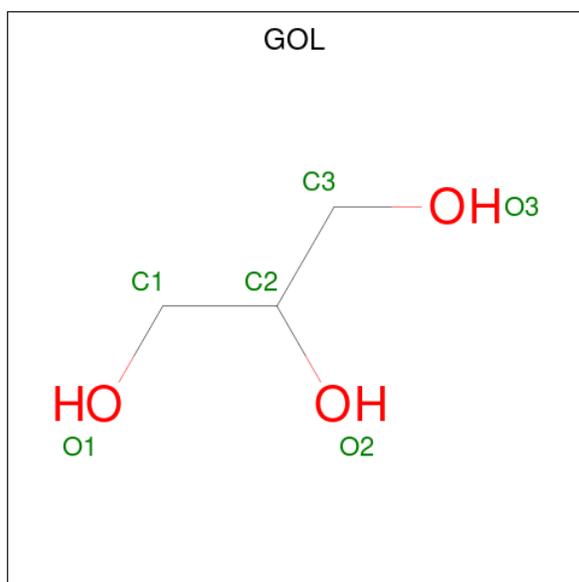


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	3	Total Cl 3 3	0	0
4	C	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	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	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

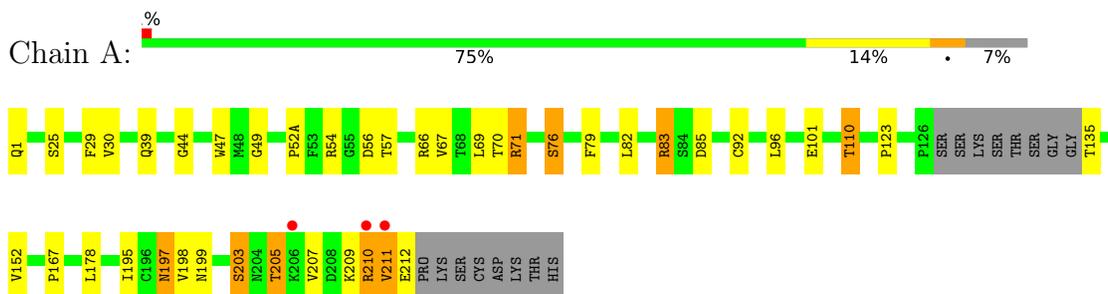
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	104	Total O 104 104	0	0
6	B	78	Total O 78 78	0	0
6	C	75	Total O 75 75	0	0
6	D	82	Total O 82 82	0	0
6	E	64	Total O 64 64	0	0
6	F	63	Total O 63 63	0	0
6	G	63	Total O 63 63	0	0
6	H	37	Total O 37 37	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.

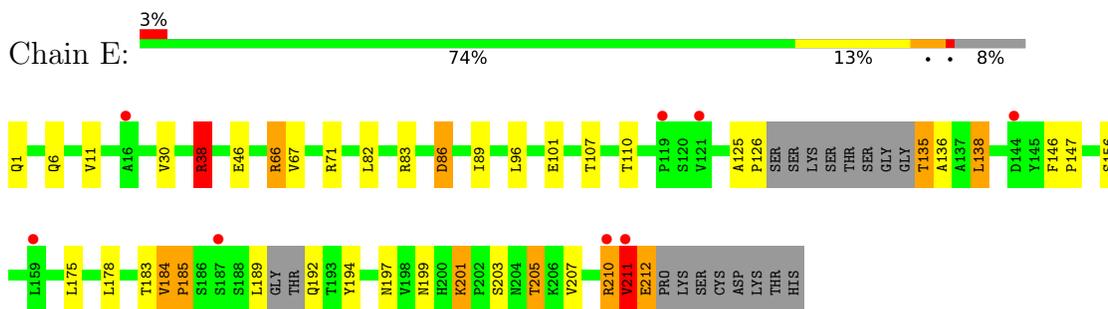
- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain



- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain

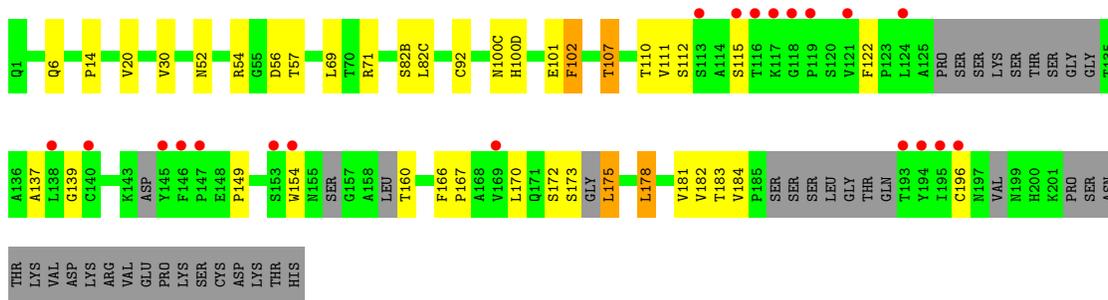


- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain

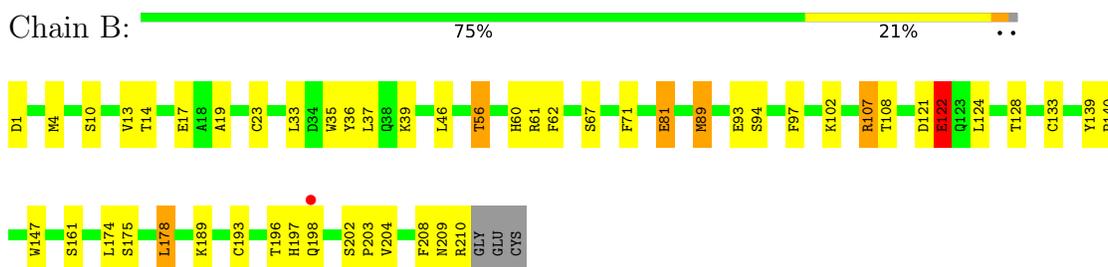


- Molecule 1: Fab fragment of human anti-HIV-1 Env antibody N12-i15, heavy chain

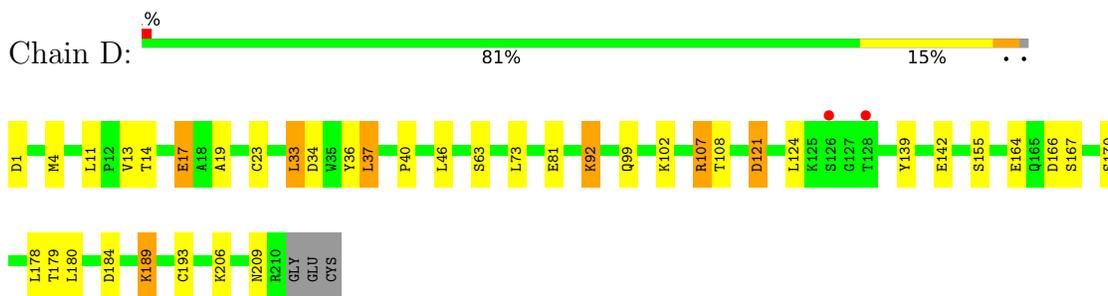




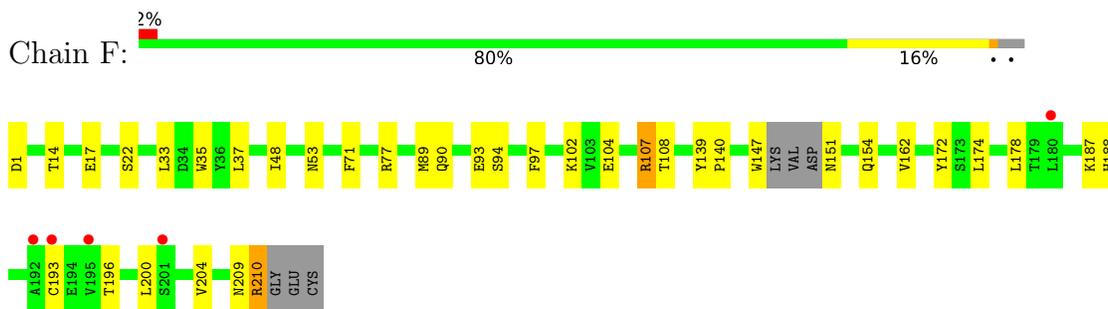
• Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain



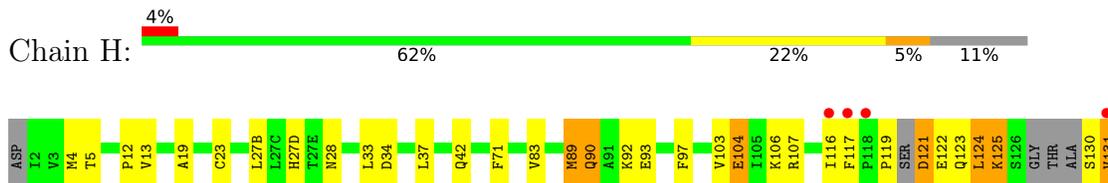
• Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain

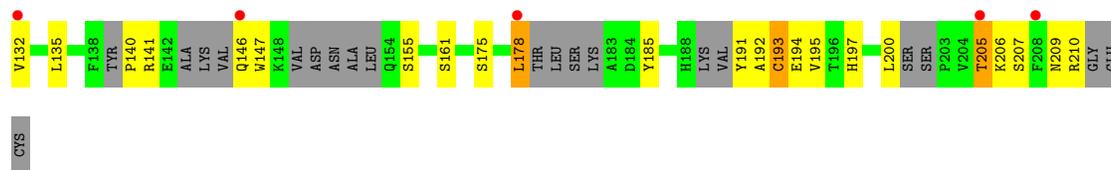


• Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain



• Molecule 2: Fab fragment of human anti-HIV-1 Env antibody N12-i15,light chain





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.12Å 125.12Å 149.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.59 40.18 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.59) 99.7 (40.18-2.59)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.216 , 0.254 0.199 , 0.242	Depositor DCC
$R_{free}$ test set	3614 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
Reported twinning fraction	0.941 for H, K, L 0.059 for K, H, -L	Depositor
Outliers	1 of 71531 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6355e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CL, GOL, SO4

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	0.95	1/1688 (0.1%)	0.87	1/2299 (0.0%)
1	C	0.94	0/1668	0.89	3/2270 (0.1%)
1	E	0.87	0/1676	0.87	5/2281 (0.2%)
1	G	0.85	2/1506 (0.1%)	0.82	0/2042
2	B	0.92	4/1691 (0.2%)	0.88	2/2295 (0.1%)
2	D	0.93	1/1691 (0.1%)	0.88	4/2295 (0.2%)
2	F	0.88	3/1666 (0.2%)	0.80	0/2260
2	H	0.82	0/1525	0.83	0/2055
All	All	0.90	11/13111 (0.1%)	0.86	15/17797 (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
1	A	0	1
1	E	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	CYS	CB-SG	-6.42	1.71	1.82
2	B	122	GLU	CB-CG	6.11	1.63	1.52
1	G	92	CYS	CB-SG	-6.04	1.72	1.82
2	F	71	PHE	CE1-CZ	5.79	1.48	1.37
2	B	193	CYS	CB-SG	-5.66	1.72	1.81

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	C	71	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	D	33	LEU	CA-CB-CG	-5.92	101.68	115.30
2	D	37	LEU	CB-CG-CD2	5.89	121.01	111.00
1	E	38	ARG	NE-CZ-NH2	-5.86	117.37	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	SER	Peptide
1	E	211	VAL	Peptide

## 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	1649	0	1615	34	0
1	C	1630	0	1593	27	0
1	E	1638	0	1604	26	0
1	G	1475	0	1434	27	0
2	B	1655	0	1620	30	0
2	D	1655	0	1620	18	0
2	F	1631	0	1593	19	0
2	H	1498	0	1448	40	0
3	A	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	1	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	1
4	H	1	0	0	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	6	0	8	0	0
6	A	104	0	0	6	0
6	B	78	0	0	1	0
6	C	75	0	0	3	0
6	D	82	0	0	2	0
6	E	64	0	0	1	2
6	F	63	0	0	0	3
6	G	63	0	0	0	0
6	H	37	0	0	1	0
All	All	13446	0	12559	217	3

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 9.

The worst 5 of 217 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:E:210:ARG:O	1:E:210:ARG:HD3	1.41	1.20
2:H:141:ARG:O	2:H:141:ARG:HG2	1.50	1.08
1:E:199:ASN:OD1	1:E:205:THR:HG22	1.66	0.95
1:G:166:PHE:O	1:G:178:LEU:HD21	1.67	0.95
1:G:170:LEU:HD11	1:G:175:LEU:HD13	1.49	0.94

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:226:HOH:O	6:F:565:HOH:O[4_555]	1.41	0.79
6:E:558:HOH:O	6:F:384:HOH:O[4_555]	1.57	0.63
4:G:222:CL:CL	6:F:446:HOH:O[3_554]	1.75	0.45

## 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	212/232 (91%)	198 (93%)	13 (6%)	1 (0%)	29	52
1	C	207/232 (89%)	194 (94%)	11 (5%)	2 (1%)	15	32
1	E	208/232 (90%)	198 (95%)	9 (4%)	1 (0%)	29	52
1	G	176/232 (76%)	165 (94%)	10 (6%)	1 (1%)	25	47
2	B	213/218 (98%)	208 (98%)	4 (2%)	1 (0%)	29	52
2	D	213/218 (98%)	202 (95%)	11 (5%)	0	100	100
2	F	208/218 (95%)	201 (97%)	7 (3%)	0	100	100
2	H	175/218 (80%)	170 (97%)	5 (3%)	0	100	100
All	All	1612/1800 (90%)	1536 (95%)	70 (4%)	6 (0%)	34	57

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	185	PRO
2	B	61	ARG
1	C	156	SER
1	C	202	PRO
1	A	76	SER

### 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	186/200 (93%)	174 (94%)	12 (6%)	17	34
1	C	184/200 (92%)	169 (92%)	15 (8%)	11	22
1	E	185/200 (92%)	167 (90%)	18 (10%)	8	15
1	G	164/200 (82%)	153 (93%)	11 (7%)	16	33
2	B	189/191 (99%)	177 (94%)	12 (6%)	18	36
2	D	189/191 (99%)	176 (93%)	13 (7%)	15	31
2	F	186/191 (97%)	175 (94%)	11 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	171/191 (90%)	154 (90%)	17 (10%)	8 15
All	All	1454/1564 (93%)	1345 (92%)	109 (8%)	13 27

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	110	THR
2	F	22	SER
2	H	107	ARG
1	E	138	LEU
1	E	203	SER

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

Mol	Chain	Res	Type
1	E	164	HIS
2	F	123	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 [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 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	F	214	-	5,5,5	0.48	0	5,5,5	1.05	0
5	GOL	H	214	-	5,5,5	0.64	0	5,5,5	0.24	0
3	SO4	G	221	-	4,4,4	0.14	0	6,6,6	0.21	0
5	GOL	E	222	-	5,5,5	0.62	0	5,5,5	0.54	0
3	SO4	A	221	-	4,4,4	0.22	0	6,6,6	0.72	0
5	GOL	D	214	-	5,5,5	0.32	0	5,5,5	0.62	0
3	SO4	E	221	-	4,4,4	0.22	0	6,6,6	0.55	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	E	222	-	-	2/4/4/4	-
5	GOL	F	214	-	-	0/4/4/4	-
5	GOL	D	214	-	-	2/4/4/4	-
5	GOL	H	214	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	214	GOL	C1-C2-C3-O3
5	E	222	GOL	O1-C1-C2-C3
5	H	214	GOL	O1-C1-C2-O2
5	H	214	GOL	O1-C1-C2-C3
5	D	214	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	221	SO4	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 [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	216/232 (93%)	-0.04	3 (1%) 75 71	12, 29, 62, 72	0
1	C	213/232 (91%)	0.10	2 (0%) 84 82	12, 30, 68, 78	0
1	E	214/232 (92%)	0.26	8 (3%) 41 34	13, 37, 73, 89	0
1	G	192/232 (82%)	0.46	20 (10%) 6 4	14, 45, 81, 91	0
2	B	215/218 (98%)	-0.08	1 (0%) 91 89	11, 32, 49, 59	0
2	D	215/218 (98%)	-0.14	2 (0%) 84 82	12, 33, 57, 70	0
2	F	212/218 (97%)	0.22	5 (2%) 59 53	15, 40, 84, 94	0
2	H	193/218 (88%)	0.30	9 (4%) 31 25	21, 48, 91, 103	0
All	All	1670/1800 (92%)	0.13	50 (2%) 50 43	11, 35, 77, 103	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	196	CYS	5.5
1	G	121	VAL	4.4
1	G	124	LEU	4.4
1	G	154	TRP	4.1
1	E	210	ARG	3.9

### 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
4	CL	B	216	1/1	0.84	0.14	50,50,50,50	0
5	GOL	F	214	6/6	0.89	0.23	38,41,48,51	0
4	CL	C	222	1/1	0.90	0.39	58,58,58,58	0
5	GOL	H	214	6/6	0.91	0.18	53,54,54,55	0
4	CL	B	214	1/1	0.93	0.09	51,51,51,51	0
4	CL	B	215	1/1	0.94	0.21	65,65,65,65	0
5	GOL	D	214	6/6	0.95	0.20	50,51,51,53	0
5	GOL	E	222	6/6	0.95	0.22	43,47,48,49	0
4	CL	D	215	1/1	0.96	0.08	50,50,50,50	0
4	CL	F	215	1/1	0.96	0.17	63,63,63,63	0
4	CL	A	222	1/1	0.97	0.36	46,46,46,46	0
3	SO4	A	221	5/5	0.97	0.14	55,55,56,59	0
4	CL	C	221	1/1	0.97	0.23	43,43,43,43	0
4	CL	H	215	1/1	0.97	0.13	59,59,59,59	0
4	CL	G	222	1/1	0.98	0.28	54,54,54,54	0
3	SO4	E	221	5/5	0.98	0.15	53,54,55,58	0
3	SO4	G	221	5/5	0.98	0.11	63,63,64,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.