Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:25 am BST

PDB ID	:	4O1N
Title	:	Crystal structure of Staphylococcal superantigen-like protein SAOUHSC_00383
Authors	:	Dutta, D.; Dutta, A.; Basak, A.; Das, A.K.
Deposited on	:	2013-12-16
Resolution	:	2.50 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 following versions of software and data (see references ①) were used in the production of this report:

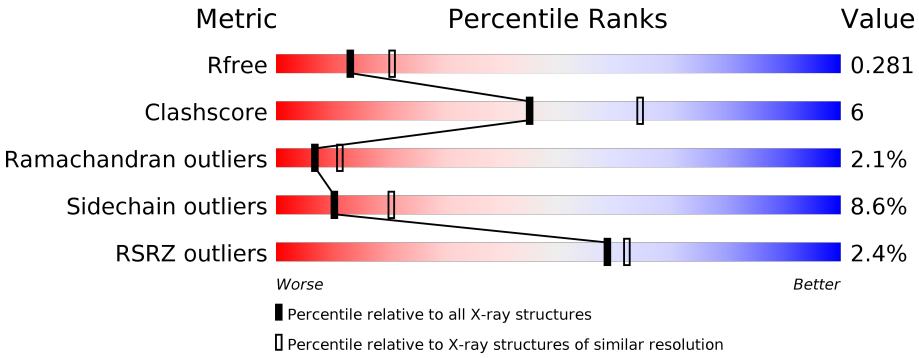
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	211	71% 16% • • 10%
1	B	211	2% 75% 10% • 10%
1	C	211	% 73% 12% • • 10%
1	D	211	% 75% 13% • 10%
1	E	211	5% 69% 15% • • 10%
1	F	211	3% 65% 22% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9217 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 Superantigen-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1513	947	260	303	3			
1	B	189	Total	C	N	O	S	0	0	0
			1520	949	260	308	3			
1	C	189	Total	C	N	O	S	0	0	0
			1523	955	260	305	3			
1	D	190	Total	C	N	O	S	0	0	0
			1502	936	261	302	3			
1	E	189	Total	C	N	O	S	0	0	0
			1489	934	255	297	3			
1	F	190	Total	C	N	O	S	0	0	0
			1499	940	255	301	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
A	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9
A	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
A	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9
A	1	SER	-	EXPRESSION TAG	UNP Q2G0X9
B	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
B	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
B	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9
B	1	SER	-	EXPRESSION TAG	UNP Q2G0X9
C	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
C	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9
C	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
C	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9
C	1	SER	-	EXPRESSION TAG	UNP Q2G0X9
D	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
D	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9
D	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
D	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9
D	1	SER	-	EXPRESSION TAG	UNP Q2G0X9
E	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
E	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9
E	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
E	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9
E	1	SER	-	EXPRESSION TAG	UNP Q2G0X9
F	-8	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-7	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-6	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-5	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-4	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-3	HIS	-	EXPRESSION TAG	UNP Q2G0X9
F	-2	GLY	-	EXPRESSION TAG	UNP Q2G0X9
F	-1	SER	-	EXPRESSION TAG	UNP Q2G0X9
F	0	GLY	-	EXPRESSION TAG	UNP Q2G0X9

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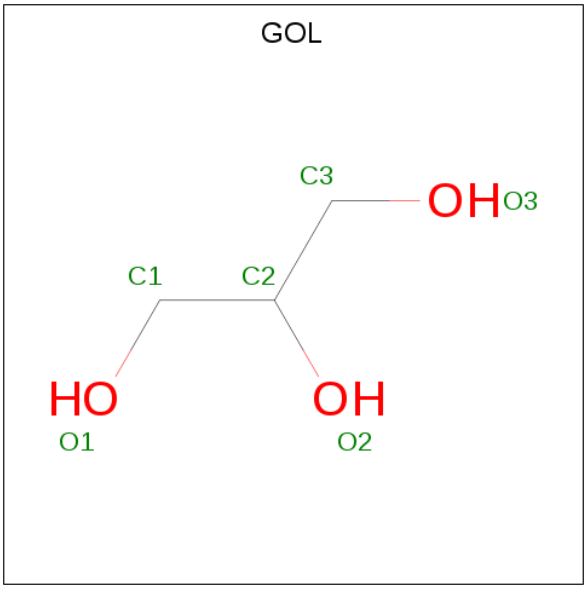
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	SER	-	EXPRESSION TAG	UNP Q2G0X9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

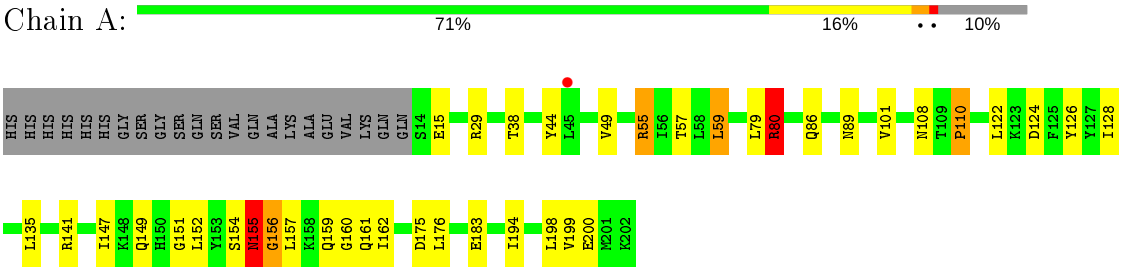
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	26	Total O 26 26	0	0
3	C	41	Total O 41 41	0	0
3	D	17	Total O 17 17	0	0
3	E	23	Total O 23 23	0	0
3	F	16	Total O 16 16	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

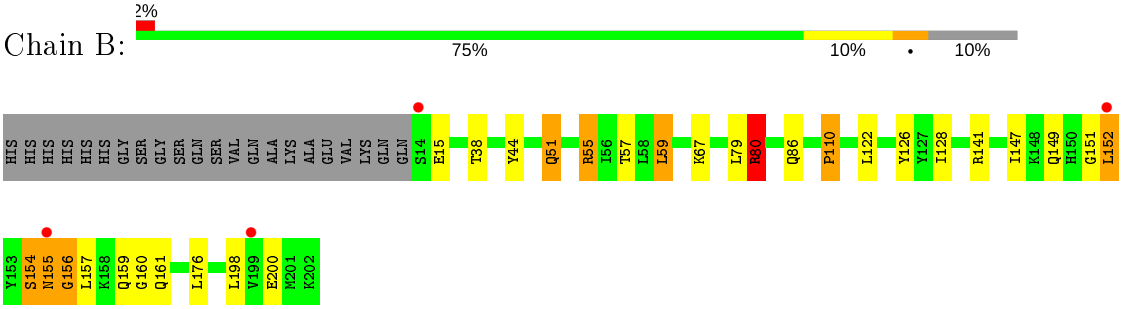
- Molecule 1: Superantigen-like protein

Chain A:



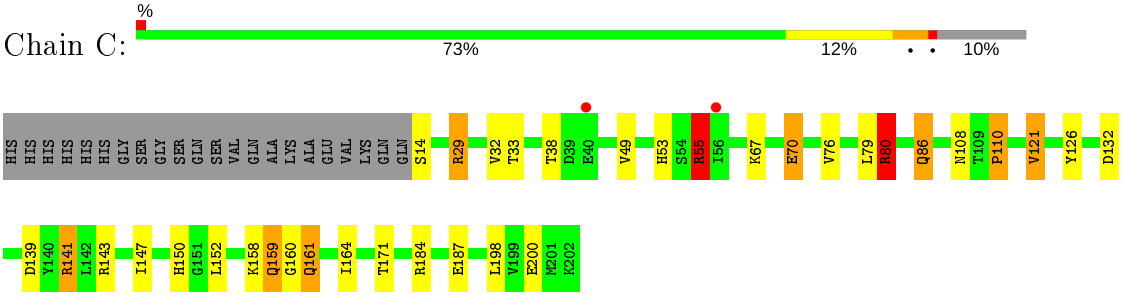
- Molecule 1: Superantigen-like protein

Chain B:



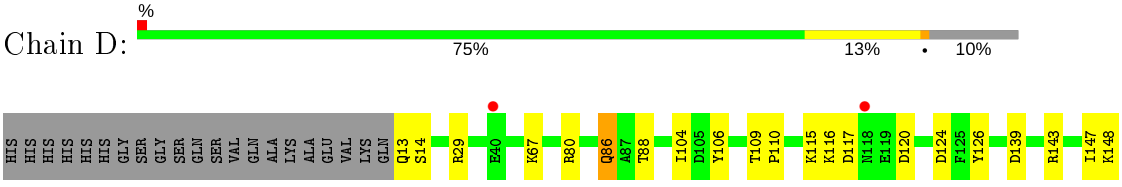
- Molecule 1: Superantigen-like protein

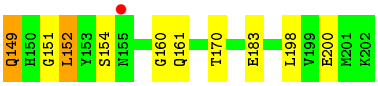
Chain C:



- Molecule 1: Superantigen-like protein

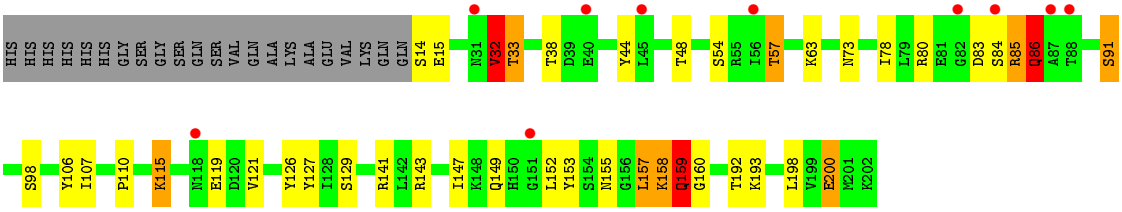
Chain D:





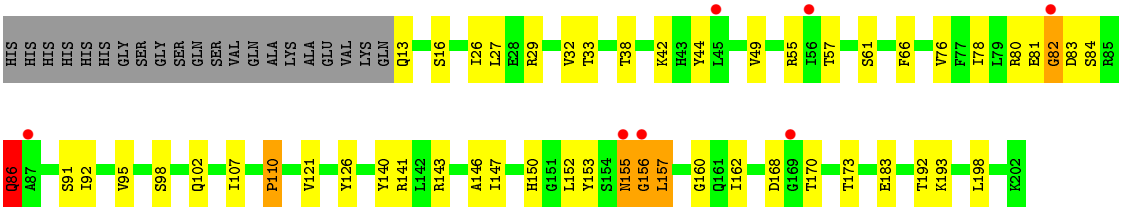
• Molecule 1: Superantigen-like protein

Chain E:



• Molecule 1: Superantigen-like protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.90Å 70.50Å 126.50Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	19.69 – 2.50 19.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.69-2.50) 99.6 (19.68-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.283 0.209 , 0.281	Depositor DCC
R_{free} test set	2300 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9217	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 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/1534	0.92	4/2060 (0.2%)
1	B	0.60	0/1541	0.84	2/2070 (0.1%)
1	C	0.67	0/1544	0.93	6/2071 (0.3%)
1	D	0.63	0/1519	0.83	2/2039 (0.1%)
1	E	0.60	0/1510	0.81	0/2029
1	F	0.58	0/1520	0.79	0/2043
All	All	0.62	0/9168	0.86	14/12312 (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	5
1	B	0	6
1	C	0	1
1	E	0	1
All	All	0	13

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	80	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	B	80	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	B	80	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	D	80	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	C	80	ARG	NE-CZ-NH1	6.56	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	80	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	55	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	80	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	55	ARG	CG-CD-NE	5.63	123.63	111.80
1	C	55	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	141	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	132	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	175	ASP	CB-CG-OD2	-5.10	113.71	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLY	Peptide
1	A	155	ASN	Peptide
1	A	156	GLY	Peptide
1	A	159	GLN	Peptide
1	A	161	GLN	Peptide
1	B	151	GLY	Peptide
1	B	152	LEU	Peptide
1	B	155	ASN	Peptide
1	B	156	GLY	Peptide
1	B	159	GLN	Peptide
1	B	161	GLN	Peptide
1	C	159	GLN	Peptide
1	E	157	LEU	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	1513	0	1495	19	0
1	B	1520	0	1492	14	0
1	C	1523	0	1516	18	0
1	D	1502	0	1458	13	0
1	E	1489	0	1453	26	0
1	F	1499	0	1458	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	8	1	0
2	B	6	0	8	0	0
2	E	6	0	8	0	0
3	A	30	0	0	2	0
3	B	26	0	0	3	0
3	C	41	0	0	2	0
3	D	17	0	0	0	0
3	E	23	0	0	0	0
3	F	16	0	0	1	0
All	All	9217	0	8896	116	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 6.

All (116) 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:D:106:TYR:CE2	1:D:106:TYR:OH	2.03	1.10
1:C:110:PRO:HD2	1:C:126:TYR:O	1.49	1.10
1:A:110:PRO:HD2	1:A:126:TYR:O	1.56	1.04
1:E:153:TYR:HA	1:E:157:LEU:CB	1.98	0.93
1:B:110:PRO:HD2	1:B:126:TYR:O	1.68	0.92
1:E:107:ILE:HG23	1:E:192:THR:HG22	1.56	0.88
1:E:110:PRO:HD2	1:E:126:TYR:O	1.73	0.87
1:F:110:PRO:HD2	1:F:126:TYR:O	1.75	0.87
1:C:55:ARG:HH11	1:C:55:ARG:HG2	1.45	0.81
1:F:110:PRO:CD	1:F:126:TYR:O	2.30	0.78
1:E:110:PRO:CD	1:E:126:TYR:O	2.33	0.76
1:D:110:PRO:HD2	1:D:126:TYR:O	1.87	0.75
1:B:160:GLY:HA2	1:B:176:LEU:HB2	1.67	0.74
1:A:160:GLY:HA2	1:A:176:LEU:HB2	1.70	0.73
1:C:147:ILE:HA	1:C:152:LEU:O	1.89	0.72
1:C:110:PRO:CD	1:C:126:TYR:O	2.32	0.71
1:E:147:ILE:HA	1:E:152:LEU:O	1.91	0.71
1:A:15:GLU:OE2	1:A:156:GLY:HA2	1.93	0.68
1:C:70:GLU:HG3	3:C:317:HOH:O	1.94	0.67
1:D:151:GLY:O	1:D:152:LEU:HB3	1.96	0.65
1:A:29:ARG:HG3	1:A:49:VAL:HG11	1.78	0.65
1:F:76:VAL:HG11	1:F:78:ILE:HD11	1.79	0.65
1:B:160:GLY:O	1:B:200:GLU:O	2.15	0.63
1:E:158:LYS:O	1:E:159:GLN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:CD	1:A:126:TYR:O	2.41	0.61
1:E:157:LEU:O	1:E:158:LYS:CB	2.49	0.60
1:B:80:ARG:HG3	3:B:404:HOH:O	2.02	0.59
1:F:147:ILE:HA	1:F:152:LEU:O	2.03	0.59
1:E:153:TYR:CA	1:E:157:LEU:CB	2.79	0.58
1:B:141:ARG:HD2	3:B:412:HOH:O	2.02	0.58
1:F:107:ILE:HG23	1:F:192:THR:HG22	1.86	0.57
1:F:156:GLY:HA3	1:F:157:LEU:CB	2.36	0.56
1:E:80:ARG:NH2	1:E:86:GLN:O	2.39	0.56
1:D:147:ILE:HA	1:D:152:LEU:O	2.06	0.55
1:B:147:ILE:HA	1:B:152:LEU:O	2.07	0.54
1:F:81:GLU:O	1:F:82:GLY:O	2.26	0.54
1:F:13:GLN:N	3:F:309:HOH:O	2.41	0.54
1:A:147:ILE:HA	1:A:152:LEU:O	2.09	0.53
1:C:55:ARG:NH1	1:C:55:ARG:HG2	2.21	0.53
1:B:110:PRO:CD	1:B:126:TYR:O	2.49	0.52
1:B:57:THR:HG22	1:B:59:LEU:HD13	1.92	0.52
1:C:141:ARG:HD2	3:C:304:HOH:O	2.10	0.51
1:A:135:LEU:HD11	2:A:301:GOL:H2	1.92	0.51
1:A:57:THR:HG22	1:A:59:LEU:HD13	1.92	0.51
1:F:78:ILE:HG23	1:F:91:SER:HB2	1.94	0.50
1:F:110:PRO:HD3	1:F:126:TYR:O	2.10	0.50
1:F:80:ARG:NH2	1:F:86:GLN:O	2.45	0.49
1:E:78:ILE:HG23	1:E:91:SER:HB2	1.94	0.49
1:A:183:GLU:HB3	3:A:430:HOH:O	2.11	0.49
1:D:149:GLN:HE21	1:D:149:GLN:HA	1.78	0.49
1:F:76:VAL:CG1	1:F:78:ILE:HG13	2.43	0.49
1:B:154:SER:O	1:B:155:ASN:C	2.51	0.48
1:C:160:GLY:O	1:C:200:GLU:O	2.30	0.48
1:F:76:VAL:HG11	1:F:78:ILE:CD1	2.43	0.48
1:D:116:LYS:O	1:D:117:ASP:C	2.52	0.47
1:E:44:TYR:CE1	1:E:57:THR:HG22	2.49	0.47
1:E:84:SER:C	1:E:85:ARG:O	2.53	0.47
1:B:51:GLN:HG3	3:B:422:HOH:O	2.14	0.47
1:F:29:ARG:HG3	1:F:49:VAL:HG11	1.96	0.47
1:F:155:ASN:O	1:F:156:GLY:C	2.53	0.46
1:C:158:LYS:C	1:C:159:GLN:HG3	2.35	0.46
1:F:26:ILE:HD11	1:F:140:TYR:CE1	2.50	0.46
1:F:156:GLY:CA	1:F:157:LEU:CB	2.94	0.45
1:E:110:PRO:HD3	1:E:126:TYR:O	2.15	0.45
1:E:85:ARG:O	1:E:86:GLN:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:OD1	1:A:155:ASN:O	2.35	0.45
1:A:80:ARG:HE	1:A:89:ASN:ND2	2.14	0.45
1:E:107:ILE:CG2	1:E:192:THR:HG22	2.35	0.45
1:E:107:ILE:HD12	1:E:129:SER:C	2.37	0.45
1:A:110:PRO:HG3	1:A:128:ILE:HD11	1.99	0.44
1:B:44:TYR:CD1	1:B:55:ARG:HD3	2.52	0.44
1:E:32:VAL:HG13	1:E:33:THR:N	2.31	0.44
1:A:160:GLY:O	1:A:200:GLU:O	2.36	0.44
1:C:79:LEU:C	1:C:79:LEU:HD23	2.38	0.44
1:F:27:LEU:HB3	1:F:78:ILE:HB	2.00	0.44
1:A:80:ARG:HD3	3:A:426:HOH:O	2.18	0.44
1:A:110:PRO:HB3	1:A:194:ILE:O	2.18	0.44
1:B:79:LEU:C	1:B:79:LEU:HD23	2.38	0.44
1:E:143:ARG:NH1	1:E:153:TYR:OH	2.51	0.43
1:F:183:GLU:CD	1:F:183:GLU:H	2.20	0.43
1:D:115:LYS:HE2	1:D:120:ASP:OD1	2.18	0.43
1:D:86:GLN:H	1:D:86:GLN:NE2	2.16	0.43
1:F:146:ALA:O	1:F:150:HIS:HB2	2.18	0.43
1:E:158:LYS:O	1:E:159:GLN:CB	2.66	0.43
1:B:15:GLU:OE2	1:B:156:GLY:CA	2.67	0.43
1:F:66:PHE:CZ	1:F:95:VAL:HG12	2.54	0.42
1:B:110:PRO:HG3	1:B:128:ILE:HD11	2.01	0.42
1:C:53:HIS:NE2	1:D:88:THR:OG1	2.51	0.42
1:E:73:ASN:HD22	1:E:73:ASN:HA	1.68	0.42
1:D:13:GLN:O	1:D:14:SER:HB3	2.20	0.42
1:F:143:ARG:NH1	1:F:153:TYR:OH	2.53	0.42
1:C:184:ARG:HA	1:C:187:GLU:HG2	2.02	0.41
1:C:80:ARG:NH2	1:C:86:GLN:O	2.31	0.41
1:E:15:GLU:CG	1:E:153:TYR:O	2.68	0.41
1:D:139:ASP:OD1	1:D:143:ARG:NE	2.49	0.41
1:D:151:GLY:O	1:D:152:LEU:CB	2.64	0.41
1:E:160:GLY:HA3	1:E:200:GLU:O	2.20	0.41
1:C:29:ARG:HD2	1:C:49:VAL:HG11	2.03	0.41
1:C:55:ARG:HH11	1:C:55:ARG:CG	2.23	0.41
1:F:81:GLU:HG3	1:F:92:ILE:HD12	2.03	0.41
1:F:168:ASP:OD1	1:F:170:THR:OG1	2.36	0.41
1:E:115:LYS:HE3	1:E:121:VAL:HG22	2.02	0.41
1:A:79:LEU:HD23	1:A:79:LEU:C	2.41	0.41
1:A:162:ILE:HG12	1:A:199:VAL:HG22	2.03	0.41
1:A:44:TYR:CD1	1:A:55:ARG:HD3	2.56	0.40
1:C:164:ILE:O	1:C:171:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LEU:HA	1:E:153:TYR:HA	1.92	0.40
1:F:44:TYR:CE1	1:F:55:ARG:NH2	2.90	0.40
1:A:80:ARG:HE	1:A:89:ASN:HD22	1.70	0.40
1:C:139:ASP:O	1:C:143:ARG:HG3	2.22	0.40
1:F:76:VAL:CG1	1:F:78:ILE:CD1	2.98	0.40
1:C:121:VAL:HG11	1:C:150:HIS:CD2	2.57	0.40
1:D:160:GLY:HA3	1:D:200:GLU:O	2.21	0.40
1:E:106:TYR:CE1	1:E:127:TYR:HB3	2.56	0.40
1:E:44:TYR:CE1	1:E:57:THR:CG2	3.05	0.40
1:F:162:ILE:O	1:F:173:THR:HA	2.22	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	187/211 (89%)	175 (94%)	8 (4%)	4 (2%)	7 11
1	B	187/211 (89%)	174 (93%)	11 (6%)	2 (1%)	14 26
1	C	187/211 (89%)	180 (96%)	5 (3%)	2 (1%)	14 26
1	D	188/211 (89%)	177 (94%)	9 (5%)	2 (1%)	14 26
1	E	187/211 (89%)	167 (89%)	14 (8%)	6 (3%)	4 5
1	F	188/211 (89%)	166 (88%)	14 (7%)	8 (4%)	2 3
All	All	1124/1266 (89%)	1039 (92%)	61 (5%)	24 (2%)	7 11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	PRO
1	C	110	PRO

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Mol	Chain	Res	Type
1	E	85	ARG
1	E	86	GLN
1	F	61	SER
1	F	82	GLY
1	F	157	LEU
1	A	157	LEU
1	E	159	GLN
1	F	86	GLN
1	F	156	GLY
1	A	155	ASN
1	F	84	SER
1	F	110	PRO
1	A	110	PRO
1	D	152	LEU
1	D	124	ASP
1	E	83	ASP
1	E	158	LYS
1	A	124	ASP
1	B	157	LEU
1	C	161	GLN
1	F	160	GLY
1	E	32	VAL

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	168/191 (88%)	157 (94%)	11 (6%)	17 33
1	B	169/191 (88%)	158 (94%)	11 (6%)	17 33
1	C	170/191 (89%)	154 (91%)	16 (9%)	8 17
1	D	162/191 (85%)	150 (93%)	12 (7%)	13 27
1	E	161/191 (84%)	141 (88%)	20 (12%)	4 9
1	F	162/191 (85%)	147 (91%)	15 (9%)	9 17
All	All	992/1146 (87%)	907 (91%)	85 (9%)	10 20

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	55	ARG
1	A	59	LEU
1	A	80	ARG
1	A	86	GLN
1	A	101	VAL
1	A	108	ASN
1	A	122	LEU
1	A	149	GLN
1	A	154	SER
1	A	198	LEU
1	B	38	THR
1	B	51	GLN
1	B	55	ARG
1	B	59	LEU
1	B	67	LYS
1	B	80	ARG
1	B	86	GLN
1	B	122	LEU
1	B	149	GLN
1	B	154	SER
1	B	198	LEU
1	C	14	SER
1	C	29	ARG
1	C	32	VAL
1	C	33	THR
1	C	38	THR
1	C	55	ARG
1	C	67	LYS
1	C	70	GLU
1	C	76	VAL
1	C	80	ARG
1	C	86	GLN
1	C	108	ASN
1	C	121	VAL
1	C	141	ARG
1	C	161	GLN
1	C	198	LEU
1	D	29	ARG
1	D	67	LYS
1	D	86	GLN
1	D	104	ILE

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Mol	Chain	Res	Type
1	D	109	THR
1	D	148	LYS
1	D	149	GLN
1	D	154	SER
1	D	161	GLN
1	D	170	THR
1	D	183	GLU
1	D	198	LEU
1	E	14	SER
1	E	32	VAL
1	E	33	THR
1	E	38	THR
1	E	48	THR
1	E	54	SER
1	E	57	THR
1	E	63	LYS
1	E	86	GLN
1	E	91	SER
1	E	98	SER
1	E	115	LYS
1	E	119	GLU
1	E	141	ARG
1	E	149	GLN
1	E	155	ASN
1	E	159	GLN
1	E	193	LYS
1	E	198	LEU
1	E	200	GLU
1	F	16	SER
1	F	32	VAL
1	F	33	THR
1	F	38	THR
1	F	42	LYS
1	F	57	THR
1	F	83	ASP
1	F	86	GLN
1	F	98	SER
1	F	102	GLN
1	F	121	VAL
1	F	141	ARG
1	F	155	ASN
1	F	193	LYS

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Mol	Chain	Res	Type
1	F	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	86	GLN
1	A	89	ASN
1	A	155	ASN
1	B	73	ASN
1	B	86	GLN
1	B	89	ASN
1	C	86	GLN
1	C	89	ASN
1	D	23	ASN
1	D	43	HIS
1	D	86	GLN
1	D	149	GLN
1	E	23	ASN
1	E	73	ASN
1	F	23	ASN
1	F	73	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
2	GOL	A	301	-	5,5,5	0.60	0	5,5,5	1.06	0
2	GOL	B	301	-	5,5,5	0.67	0	5,5,5	1.13	0
2	GOL	E	301	-	5,5,5	0.59	0	5,5,5	1.14	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
2	GOL	A	301	-	-	2/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	E	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	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, 95^{th} 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	A	189/211 (89%)	-0.12	1 (0%)	91	91	22, 36, 56, 65	0
1	B	189/211 (89%)	0.08	4 (2%)	63	66	27, 44, 70, 86	0
1	C	189/211 (89%)	-0.16	2 (1%)	80	82	23, 36, 57, 75	0
1	D	190/211 (90%)	0.07	3 (1%)	72	74	27, 47, 72, 85	0
1	E	189/211 (89%)	0.28	10 (5%)	26	28	30, 51, 73, 92	0
1	F	190/211 (90%)	0.32	7 (3%)	41	45	34, 53, 76, 84	0
All	All	1136/1266 (89%)	0.08	27 (2%)	59	62	22, 44, 71, 92	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	156	GLY	3.8
1	E	118	ASN	3.8
1	E	87	ALA	3.5
1	D	155	ASN	3.4
1	E	56	ILE	3.4
1	E	82	GLY	3.3
1	F	56	ILE	3.3
1	F	87	ALA	3.0
1	E	45	LEU	2.7
1	E	40	GLU	2.7
1	E	88	THR	2.5
1	B	14	SER	2.5
1	B	152	LEU	2.5
1	F	155	ASN	2.5
1	E	151	GLY	2.4
1	E	84	SER	2.4
1	D	118	ASN	2.4
1	C	56	ILE	2.3
1	F	45	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	82	GLY	2.3
1	B	199	VAL	2.3
1	F	169	GLY	2.3
1	B	155	ASN	2.2
1	C	40	GLU	2.2
1	A	45	LEU	2.1
1	E	31	ASN	2.0
1	D	40	GLU	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 carbohydrates 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^{th} 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^2)	Q<0.9
2	GOL	A	301	6/6	0.79	0.28	46,55,56,60	0
2	GOL	E	301	6/6	0.89	0.21	38,47,53,59	0
2	GOL	B	301	6/6	0.94	0.17	37,42,45,49	0

6.5 Other polymers (i)

There are no such residues in this entry.