Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 06:21 PM EDT

PDB ID	:	3EYF
Title	:	Crystal structure of anti-human cytomegalovirus antibody 8f9 plus gB peptide
Authors	:	Thomson, C.A.; Bryson, S.; McLean, G.R.; Creagh, A.L.; Pai, E.F.; Schrader, J.W.
Deposited on	:	2008-10-20
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

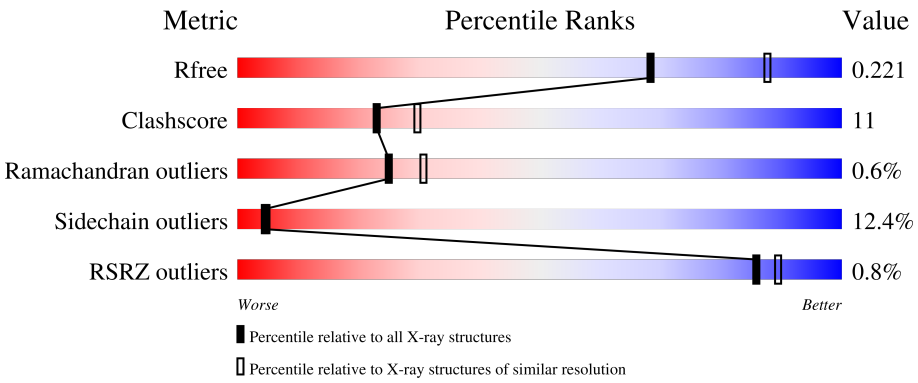
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	216	.% 70% 23% 5% •
1	C	216	.% 70% 24% 6%
2	B	242	63% 21% 5% • 10%
2	D	242	.% 64% 20% • 13%
3	E	11	55% 9% 18% 9% 9%

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Mol	Chain	Length	Quality of chain
3	F	11	73% 18% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7113 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 8f9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1660	1044	283	327	6	0	0	0
1	C	215	1660	1044	283	327	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	PDB 3EYF
C	0	MET	-	expression tag	PDB 3EYF

- Molecule 2 is a protein called AD-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1633	1021	283	319	10	0	0	0
2	D	211	1588	993	276	309	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	235	LEU	-	expression tag	PDB 3EYF
B	236	GLU	-	expression tag	PDB 3EYF
B	237	HIS	-	expression tag	PDB 3EYF
B	238	HIS	-	expression tag	PDB 3EYF
B	239	HIS	-	expression tag	PDB 3EYF
B	240	HIS	-	expression tag	PDB 3EYF
B	241	HIS	-	expression tag	PDB 3EYF
B	242	HIS	-	expression tag	PDB 3EYF
D	235	LEU	-	expression tag	PDB 3EYF
D	236	GLU	-	expression tag	PDB 3EYF

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Chain	Residue	Modelled	Actual	Comment	Reference
D	237	HIS	-	expression tag	PDB 3EYF
D	238	HIS	-	expression tag	PDB 3EYF
D	239	HIS	-	expression tag	PDB 3EYF
D	240	HIS	-	expression tag	PDB 3EYF
D	241	HIS	-	expression tag	PDB 3EYF
D	242	HIS	-	expression tag	PDB 3EYF

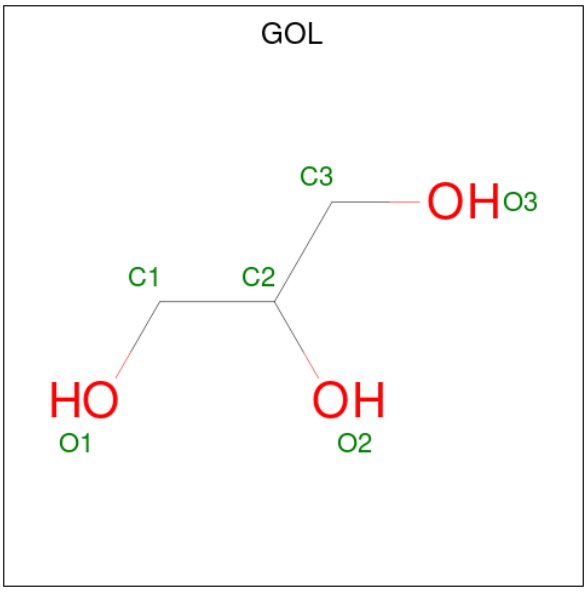
- Molecule 3 is a protein called Synthetic peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	10	79	52	12	15	0	0	1
3	F	10	79	52	12	15	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	11	NH2	-	amidation	UNP P13201
F	11	NH2	-	amidation	UNP P13201

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



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

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

- Molecule 5 is water.

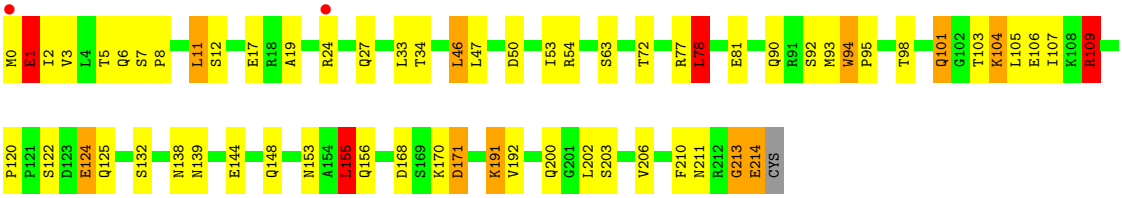
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	121	121	121	0	0
			Total	O		
5	B	93	93	93	0	0
			Total	O		
5	C	96	96	96	0	0
			Total	O		
5	D	82	82	82	0	0
			Total	O		
5	E	5	5	5	0	0
			Total	O		
5	F	5	5	5	0	0

3 Residue-property plots (i)

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

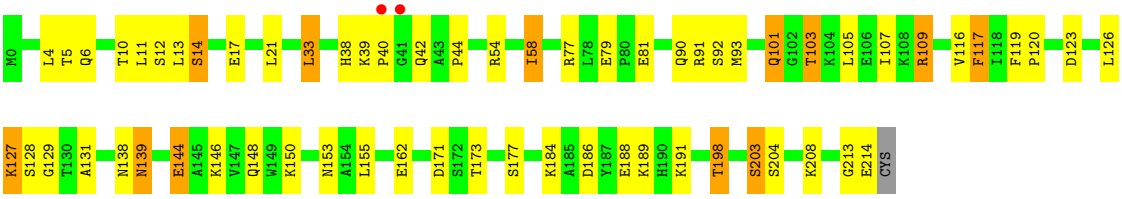
- Molecule 1: 8f9 Fab

Chain A:



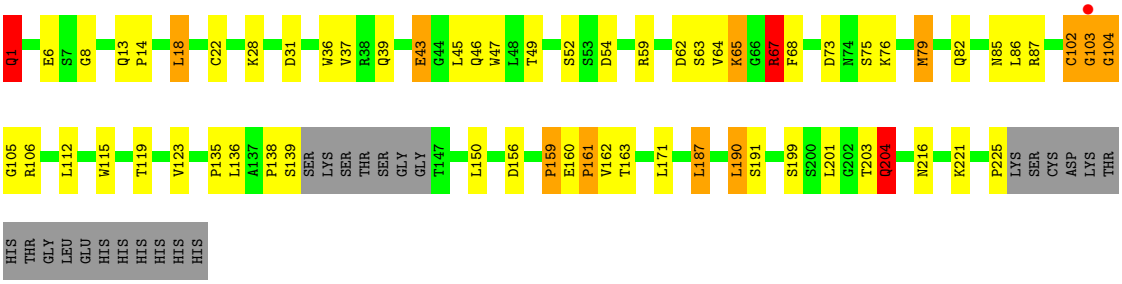
- Molecule 1: 8f9 Fab

Chain C:



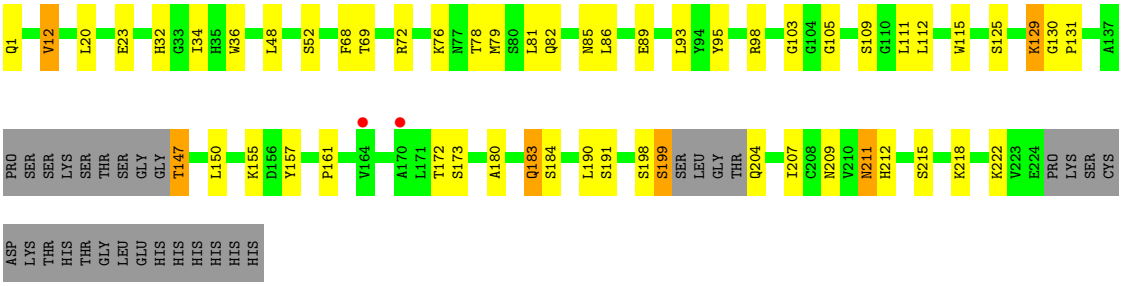
- Molecule 2: AD-2

Chain B:



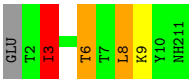
- Molecule 2: AD-2

Chain D:



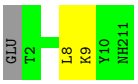
- Molecule 3: Synthetic peptide

Chain E:



- Molecule 3: Synthetic peptide

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.30Å 103.50Å 152.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.01 – 2.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 92.9 (49.01-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.230 0.219 , 0.221	Depositor DCC
R_{free} test set	2151 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NH2

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	1/1698 (0.1%)	1.14	8/2307 (0.3%)
1	C	0.97	0/1698	1.11	5/2307 (0.2%)
2	B	0.95	1/1670 (0.1%)	1.19	11/2265 (0.5%)
2	D	0.94	0/1622	1.09	4/2196 (0.2%)
3	E	1.05	0/79	1.31	1/107 (0.9%)
3	F	0.74	0/79	0.77	0/107
All	All	0.95	2/6846 (0.0%)	1.13	29/9289 (0.3%)

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	C	1	1
2	B	0	3
All	All	1	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	GLY	CA-C	-5.41	1.43	1.51
1	A	94	TRP	CB-CG	-5.40	1.40	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	GLY	N-CA-C	8.75	134.97	113.10
2	B	104	GLY	CA-C-N	-8.18	99.84	116.20
1	C	214	GLU	N-CA-C	-7.39	91.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	GLU	N-CA-C	7.22	130.49	111.00
1	C	203	SER	N-CA-CB	-6.94	100.08	110.50
1	A	1	GLU	N-CA-C	-6.71	92.88	111.00
2	D	111	LEU	CB-CG-CD1	-6.48	99.99	111.00
1	A	155	LEU	CA-CB-CG	-6.45	100.47	115.30
1	A	109	ARG	N-CA-CB	-5.94	99.91	110.60
2	B	102	CYS	N-CA-C	-5.87	95.15	111.00
2	B	203	THR	N-CA-CB	5.67	121.07	110.30
2	B	190	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	33	LEU	CA-CB-CG	-5.52	102.60	115.30
2	D	155	LYS	N-CA-C	5.47	125.77	111.00
2	B	136	LEU	N-CA-C	-5.44	96.32	111.00
1	A	47	LEU	CB-CG-CD1	-5.43	101.76	111.00
1	A	78	LEU	CA-CB-CG	5.42	127.77	115.30
3	E	3	ILE	N-CA-CB	-5.34	98.51	110.80
2	B	67	ARG	NE-CZ-NH1	-5.33	117.63	120.30
2	B	105	GLY	N-CA-C	-5.28	99.89	113.10
1	C	109	ARG	N-CA-CB	-5.19	101.25	110.60
2	D	147	THR	N-CA-C	5.14	124.88	111.00
2	D	103	GLY	N-CA-C	5.13	125.93	113.10
1	C	144	GLU	N-CA-CB	5.12	119.82	110.60
2	B	203	THR	CA-C-N	-5.08	106.01	117.20
1	A	46	LEU	CB-CG-CD2	5.07	119.62	111.00
1	A	213	GLY	N-CA-C	-5.06	100.44	113.10
2	B	203	THR	C-N-CA	5.06	134.34	121.70
2	B	1	GLN	CB-CA-C	5.03	120.47	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	38	HIS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	104	GLY	Mainchain
2	B	204	GLN	Mainchain
2	B	67	ARG	Sidechain
1	C	213	GLY	Mainchain

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	1660	0	1628	47	0
1	C	1660	0	1628	34	0
2	B	1633	0	1586	45	0
2	D	1588	0	1540	23	0
3	E	79	0	79	6	0
3	F	79	0	79	1	0
4	C	12	0	16	1	0
5	A	121	0	0	12	0
5	B	93	0	0	3	0
5	C	96	0	0	7	0
5	D	82	0	0	7	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
All	All	7113	0	6556	151	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 11.

All (151) 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:A:90:GLN:NE2	1:A:93:MET:H	1.56	1.03
1:A:6:GLN:H	1:A:101:GLN:NE2	1.59	0.99
1:C:21:LEU:HD22	1:C:103:THR:HG21	1.52	0.90
2:B:73:ASP:OD1	2:B:76:LYS:HB2	1.73	0.89
2:B:103:GLY:CA	3:E:3:ILE:HD11	2.01	0.89
1:A:90:GLN:HE21	1:A:92:SER:N	1.73	0.87
2:B:106:ARG:HD3	5:C:366:HOH:O	1.76	0.85
1:A:90:GLN:HE22	1:A:93:MET:H	1.20	0.84
1:A:5:THR:HA	1:A:101:GLN:HE22	1.45	0.82
1:A:90:GLN:HE21	1:A:92:SER:H	1.26	0.80
2:D:129:LYS:HG3	2:D:130:GLY:N	1.97	0.79
2:B:67:ARG:NH1	2:B:87:ARG:HD2	1.99	0.77
1:A:104:LYS:HE3	5:A:299:HOH:O	1.85	0.76
2:B:43:GLU:OE1	2:B:43:GLU:HA	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:HIS:HE1	5:D:381:HOH:O	1.72	0.73
1:A:6:GLN:N	1:A:101:GLN:NE2	2.37	0.72
2:B:67:ARG:HH11	2:B:87:ARG:CD	2.04	0.71
2:B:1:GLN:NE2	5:B:289:HOH:O	2.23	0.71
1:A:170:LYS:HE2	5:A:291:HOH:O	1.91	0.71
1:A:101:GLN:OE1	5:A:322:HOH:O	2.08	0.71
1:C:198:THR:OG1	5:C:358:HOH:O	2.09	0.70
1:C:90:GLN:NE2	1:C:93:MET:H	1.91	0.69
2:D:69:THR:HG23	5:D:382:HOH:O	1.92	0.69
2:B:64:VAL:HG12	2:B:67:ARG:NH2	2.07	0.69
2:B:6:GLU:HB3	2:B:119:THR:HG22	1.75	0.68
2:B:103:GLY:HA3	3:E:3:ILE:HD11	1.74	0.68
2:B:67:ARG:HH11	2:B:87:ARG:HD2	1.57	0.68
1:C:12:SER:O	1:C:13:LEU:HD12	1.94	0.67
1:A:144:GLU:OE1	5:A:313:HOH:O	2.13	0.67
1:A:1:GLU:HA	5:A:292:HOH:O	1.96	0.66
1:A:106:GLU:HG2	1:A:107:ILE:N	2.12	0.65
2:D:207:ILE:HD13	2:D:222:LYS:HA	1.79	0.64
2:B:36:TRP:HE1	2:B:79:MET:CE	2.11	0.64
2:B:28:LYS:HD3	2:B:31:ASP:OD2	1.98	0.63
1:A:90:GLN:NE2	1:A:92:SER:N	2.45	0.63
2:B:28:LYS:HD3	2:B:31:ASP:CG	2.19	0.62
2:B:49:THR:OG1	2:B:59:ARG:O	2.12	0.62
2:B:156:ASP:HB3	2:B:187:LEU:HD12	1.81	0.62
1:C:184:LYS:O	1:C:188:GLU:HG3	2.00	0.61
2:B:36:TRP:HE1	2:B:79:MET:HE3	1.66	0.61
1:C:6:GLN:N	1:C:101:GLN:OE1	2.27	0.60
1:A:155:LEU:HG	1:A:156:GLN:N	2.16	0.60
2:D:211:ASN:ND2	5:D:307:HOH:O	2.33	0.60
2:B:139:SER:HB2	5:B:301:HOH:O	2.03	0.58
1:A:54:ARG:NH2	5:A:289:HOH:O	2.30	0.58
1:C:90:GLN:HE22	1:C:93:MET:H	1.51	0.58
2:D:105:GLY:O	5:D:310:HOH:O	2.17	0.58
2:B:139:SER:CB	5:B:301:HOH:O	2.52	0.58
1:A:90:GLN:NE2	1:A:93:MET:N	2.41	0.57
1:A:211:ASN:OD1	5:A:227:HOH:O	2.17	0.57
2:B:103:GLY:HA2	3:E:3:ILE:HD11	1.87	0.57
3:E:8:LEU:HG	3:E:9:LYS:H	1.70	0.57
2:B:22:CYS:HB3	2:B:79:MET:SD	2.45	0.57
1:C:54:ARG:HD3	5:C:316:HOH:O	2.03	0.56
1:A:77:ARG:HD2	5:A:286:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG13	2:B:46:GLN:O	2.06	0.56
1:A:138:ASN:HB3	1:A:139:ASN:HD22	1.69	0.56
1:A:8:PRO:O	1:A:103:THR:OG1	2.15	0.56
1:C:79:GLU:OE1	5:C:350:HOH:O	2.18	0.55
1:A:122:SER:HB2	1:A:124:GLU:HG2	1.89	0.55
1:C:90:GLN:HE21	1:C:92:SER:H	1.55	0.55
1:C:162:GLU:HA	1:C:177:SER:O	2.07	0.55
1:A:6:GLN:H	1:A:101:GLN:HE21	1.49	0.55
1:C:5:THR:HA	1:C:101:GLN:OE1	2.07	0.54
2:B:62:ASP:OD2	2:B:65:LYS:NZ	2.40	0.54
1:A:202:LEU:HD13	1:A:206:VAL:HG23	1.90	0.54
1:C:138:ASN:OD1	1:C:139:ASN:ND2	2.41	0.53
2:B:135:PRO:HD3	2:B:221:LYS:HE2	1.90	0.53
2:D:89:GLU:HG2	5:D:342:HOH:O	2.08	0.53
1:A:90:GLN:NE2	1:A:92:SER:H	2.02	0.53
1:A:12:SER:HB3	1:A:106:GLU:OE1	2.10	0.52
1:A:125:GLN:HE22	1:A:132:SER:HB2	1.75	0.52
2:D:212:HIS:ND1	2:D:215:SER:OG	2.40	0.52
2:B:102:CYS:HB2	3:E:6:THR:HG22	1.91	0.52
1:C:14:SER:O	1:C:17:GLU:HG3	2.10	0.52
2:B:87:ARG:O	2:B:123:VAL:HG21	2.10	0.52
2:B:8:GLY:O	2:B:18:LEU:HD21	2.10	0.52
1:A:90:GLN:OE1	1:A:98:THR:HG22	2.10	0.51
2:B:138:PRO:HG2	2:B:225:PRO:HG3	1.91	0.51
1:C:11:LEU:HG	1:C:13:LEU:HD13	1.93	0.51
2:B:37:VAL:HG22	2:B:47:TRP:HA	1.93	0.51
1:C:127:LYS:O	1:C:129:GLY:N	2.44	0.50
1:A:72:THR:HG22	5:A:219:HOH:O	2.11	0.50
1:C:171:ASP:HB3	1:C:173:THR:HG23	1.93	0.50
3:F:9:LYS:HE3	5:F:265:HOH:O	2.11	0.49
2:B:187:LEU:HD23	2:B:187:LEU:N	2.26	0.49
2:B:201:LEU:HD23	2:B:201:LEU:N	2.27	0.49
1:A:213:GLY:O	1:A:214:GLU:HB3	2.13	0.49
2:B:115:TRP:CD1	2:B:115:TRP:N	2.81	0.49
2:D:32:HIS:CE1	5:D:381:HOH:O	2.55	0.49
1:C:38:HIS:HD2	1:C:42:GLN:O	1.96	0.49
2:D:131:PRO:HB3	2:D:157:TYR:HB3	1.94	0.49
1:A:148:GLN:HG2	1:A:155:LEU:CD1	2.42	0.49
2:B:68:PHE:HA	2:B:82:GLN:O	2.12	0.48
2:D:211:ASN:OD1	2:D:218:LYS:HE2	2.14	0.48
1:C:54:ARG:HG2	1:C:58:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ASP:HA	1:C:189:LYS:HD2	1.96	0.47
1:A:17:GLU:O	1:A:78:LEU:HD22	2.15	0.47
1:C:146:LYS:HB2	5:C:368:HOH:O	2.14	0.47
1:A:109:ARG:NH2	5:A:248:HOH:O	2.41	0.47
1:A:191:LYS:CE	1:A:211:ASN:HD22	2.27	0.47
1:C:148:GLN:HE22	1:C:155:LEU:HD21	1.80	0.47
1:A:122:SER:HB2	1:A:124:GLU:CG	2.44	0.47
2:D:180:ALA:HB2	2:D:190:LEU:HD23	1.96	0.47
2:B:13:GLN:HG2	2:B:14:PRO:HD2	1.97	0.46
1:C:126:LEU:CD2	1:C:131:ALA:HB2	2.46	0.46
1:C:38:HIS:CE1	5:C:356:HOH:O	2.68	0.46
2:D:199:SER:HB3	5:D:360:HOH:O	2.14	0.45
1:C:40:PRO:HD3	5:C:351:HOH:O	2.17	0.45
1:C:116:VAL:HG12	1:C:208:LYS:HG3	1.98	0.45
2:D:36:TRP:NE1	2:D:79:MET:HE1	2.31	0.45
2:B:79:MET:HB2	2:B:79:MET:HE2	1.77	0.45
1:C:150:LYS:NZ	4:C:300:GOL:O2	2.49	0.45
2:B:13:GLN:HG2	2:B:14:PRO:CD	2.47	0.45
2:D:115:TRP:CD1	2:D:115:TRP:N	2.84	0.45
1:A:94:TRP:HB2	1:A:95:PRO:HA	2.00	0.44
2:B:86:LEU:HD23	2:B:86:LEU:HA	1.74	0.44
1:C:148:GLN:OE1	1:C:155:LEU:HD11	2.17	0.44
2:B:52:SER:OG	2:B:54:ASP:OD2	2.32	0.44
1:A:120:PRO:HB3	1:A:210:PHE:CZ	2.53	0.44
1:A:19:ALA:HB2	1:A:78:LEU:HD21	2.00	0.43
1:A:90:GLN:HE22	1:A:93:MET:N	2.00	0.43
2:D:183:GLN:HE21	2:D:183:GLN:HB2	1.47	0.43
1:A:168:ASP:OD2	1:A:171:ASP:HB2	2.19	0.43
1:A:191:LYS:HE3	1:A:211:ASN:HD22	1.84	0.43
2:B:112:LEU:HD12	2:B:112:LEU:N	2.33	0.43
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.81	0.43
1:C:90:GLN:NE2	1:C:92:SER:H	2.16	0.43
2:B:64:VAL:HG12	2:B:67:ARG:HH22	1.81	0.43
2:B:36:TRP:HE1	2:B:79:MET:HE1	1.83	0.42
2:D:93:LEU:HD23	2:D:95:TYR:CZ	2.54	0.42
1:A:124:GLU:HG2	1:A:124:GLU:H	1.42	0.42
2:B:36:TRP:NE1	2:B:79:MET:HE3	2.33	0.42
2:B:39:GLN:HB2	2:B:45:LEU:HD23	2.01	0.42
2:D:98:ARG:O	2:D:112:LEU:HA	2.20	0.42
1:C:117:PHE:CD2	1:C:117:PHE:N	2.88	0.42
1:A:50:ASP:HB2	1:A:53:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:SER:O	2:D:72:ARG:NH1	2.53	0.42
2:D:68:PHE:HA	2:D:82:GLN:O	2.19	0.42
2:D:12:VAL:HG11	2:D:86:LEU:CD1	2.51	0.41
1:C:119:PHE:HA	1:C:120:PRO:HD3	1.80	0.41
2:D:81:LEU:HD12	2:D:81:LEU:HA	1.84	0.41
2:B:36:TRP:NE1	2:B:79:MET:CE	2.82	0.41
1:C:91:ARG:NH1	2:D:109:SER:O	2.49	0.41
1:A:200:GLN:NE2	5:A:316:HOH:O	2.32	0.41
1:A:2:ILE:HD11	1:A:93:MET:CB	2.51	0.41
1:A:2:ILE:O	1:A:98:THR:HG21	2.20	0.41
1:A:11:LEU:HB3	1:A:105:LEU:HD13	2.02	0.40
5:A:296:HOH:O	3:E:8:LEU:HD11	2.20	0.40
1:C:39:LYS:HA	1:C:40:PRO:HD2	1.48	0.40
2:B:160:GLU:HA	2:B:161:PRO:HA	1.84	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	213/216 (99%)	202 (95%)	10 (5%)	1 (0%)	29	35
1	C	213/216 (99%)	204 (96%)	7 (3%)	2 (1%)	17	20
2	B	214/242 (88%)	202 (94%)	10 (5%)	2 (1%)	17	20
2	D	205/242 (85%)	198 (97%)	7 (3%)	0	100	100
3	E	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
3	F	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
All	All	861/938 (92%)	819 (95%)	37 (4%)	5 (1%)	25	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
2	B	204	GLN
1	C	128	SER
1	C	139	ASN
2	B	159	PRO

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	186/187 (100%)	163 (88%)	23 (12%)	4 5
1	C	186/187 (100%)	164 (88%)	22 (12%)	5 5
2	B	183/204 (90%)	163 (89%)	20 (11%)	6 7
2	D	177/204 (87%)	153 (86%)	24 (14%)	3 3
3	E	9/10 (90%)	6 (67%)	3 (33%)	0 0
3	F	9/10 (90%)	8 (89%)	1 (11%)	6 7
All	All	750/802 (94%)	657 (88%)	93 (12%)	4 5

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	1	GLU
1	A	3	VAL
1	A	7	SER
1	A	11	LEU
1	A	24	ARG
1	A	27	GLN
1	A	33	LEU
1	A	34	THR
1	A	46	LEU
1	A	63	SER
1	A	78	LEU
1	A	81	GLU
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	104	LYS
1	A	109	ARG
1	A	124	GLU
1	A	153	ASN
1	A	155	LEU
1	A	171	ASP
1	A	191	LYS
1	A	192	VAL
1	A	203	SER
2	B	1	GLN
2	B	18	LEU
2	B	43	GLU
2	B	63	SER
2	B	65	LYS
2	B	75	SER
2	B	79	MET
2	B	85	ASN
2	B	150	LEU
2	B	159	PRO
2	B	161	PRO
2	B	162	VAL
2	B	163	THR
2	B	171	LEU
2	B	187	LEU
2	B	190	LEU
2	B	191	SER
2	B	199	SER
2	B	204	GLN
2	B	216	ASN
1	C	4	LEU
1	C	10	THR
1	C	14	SER
1	C	33	LEU
1	C	44	PRO
1	C	58	ILE
1	C	77	ARG
1	C	81	GLU
1	C	101	GLN
1	C	103	THR
1	C	105	LEU
1	C	107	ILE
1	C	109	ARG

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	123	ASP
1	C	127	LYS
1	C	144	GLU
1	C	153	ASN
1	C	191	LYS
1	C	198	THR
1	C	203	SER
1	C	204	SER
2	D	1	GLN
2	D	12	VAL
2	D	20	LEU
2	D	23	GLU
2	D	34	ILE
2	D	48	LEU
2	D	76	LYS
2	D	78	THR
2	D	85	ASN
2	D	125	SER
2	D	129	LYS
2	D	147	THR
2	D	150	LEU
2	D	161	PRO
2	D	172	THR
2	D	173	SER
2	D	183	GLN
2	D	184	SER
2	D	191	SER
2	D	198	SER
2	D	199	SER
2	D	204	GLN
2	D	209	ASN
2	D	211	ASN
3	E	3	ILE
3	E	6	THR
3	E	8	LEU
3	F	8	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	90	GLN
1	A	101	GLN
1	A	125	GLN
1	A	138	ASN
1	A	139	ASN
1	A	190	HIS
1	A	200	GLN
1	A	211	ASN
2	B	77	ASN
2	B	176	HIS
2	B	183	GLN
1	C	38	HIS
1	C	42	GLN
1	C	90	GLN
1	C	125	GLN
1	C	161	GLN
1	C	200	GLN
2	D	32	HIS
2	D	216	ASN
3	F	5	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
4	GOL	C	300	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	C	301	-	5,5,5	0.79	0	5,5,5	0.95	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
4	GOL	C	300	-	-	4/4/4/4	-
4	GOL	C	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	300	GOL	O1-C1-C2-O2
4	C	300	GOL	O1-C1-C2-C3
4	C	300	GOL	C1-C2-C3-O3
4	C	300	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-O2
4	C	301	GOL	O1-C1-C2-C3
4	C	301	GOL	C1-C2-C3-O3
4	C	301	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
4	C	300	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 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	A	215/216 (99%)	-0.13	2 (0%)	84	88	32, 43, 56, 89	0
1	C	215/216 (99%)	-0.09	2 (0%)	84	88	31, 44, 62, 84	0
2	B	218/242 (90%)	-0.08	1 (0%)	91	94	32, 46, 69, 79	0
2	D	211/242 (87%)	-0.09	2 (0%)	84	88	30, 43, 66, 81	0
3	E	9/11 (81%)	0.47	0	100	100	59, 64, 70, 74	0
3	F	9/11 (81%)	0.37	0	100	100	40, 42, 54, 58	0
All	All	877/938 (93%)	-0.09	7 (0%)	86	89	30, 44, 65, 89	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	MET	4.6
2	D	170	ALA	4.2
2	B	103	GLY	2.9
2	D	164	VAL	2.2
1	C	40	PRO	2.1
1	A	24	ARG	2.1
1	C	41	GLY	2.1

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, 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(Å^2)	Q<0.9
4	GOL	C	300	6/6	0.66	0.28	71,72,73,73	0
4	GOL	C	301	6/6	0.84	0.21	72,75,76,78	0

6.5 Other polymers (i)

There are no such residues in this entry.