Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 06:15 PM EDT

PDB ID	:	5UMN
Title	:	Crystal structure of C05 VPGSGW mutant bound to H3 influenza hemagglutinin, HA1 subunit
Authors	:	Wu, N.C.; Wilson, I.A.
Deposited on	:	2017-01-27
Resolution	:	1.97 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:

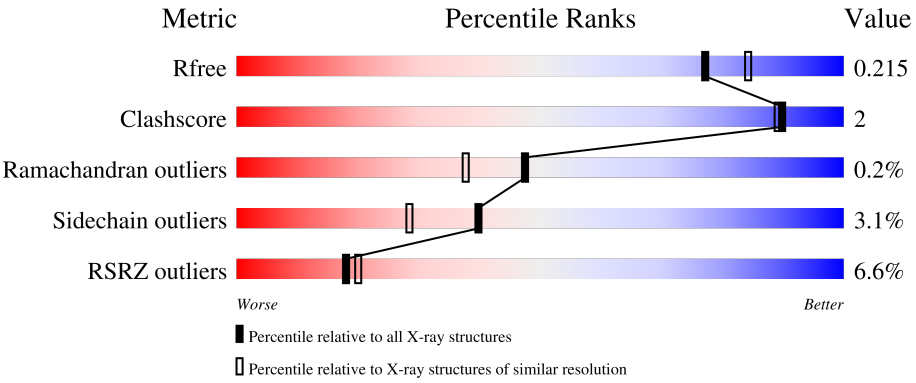
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	274	10% 93%
1	B	274	11% 80% 8% 11%
2	C	247	7% 91%
2	E	247	5% 89% 6%
3	D	214	2% 92% 7%

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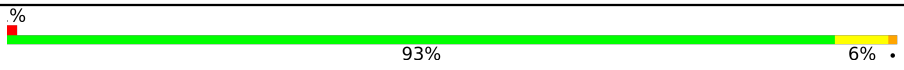
Mol	Chain	Length	Quality of chain
3	F	214	

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	NAG	A	402	-	-	-	X
7	FLC	C	301	-	-	-	X
7	FLC	C	302	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12093 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	2	0
			2087	1310	366	400	11			
1	B	243	Total	C	N	O	S	0	1	0
			1900	1194	333	361	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	expression tag	UNP Q91MA7
A	311	HIS	-	expression tag	UNP Q91MA7
A	312	HIS	-	expression tag	UNP Q91MA7
A	313	HIS	-	expression tag	UNP Q91MA7
A	314	HIS	-	expression tag	UNP Q91MA7
A	315	HIS	-	expression tag	UNP Q91MA7
A	316	HIS	-	expression tag	UNP Q91MA7
B	310	GLY	-	expression tag	UNP Q91MA7
B	311	HIS	-	expression tag	UNP Q91MA7
B	312	HIS	-	expression tag	UNP Q91MA7
B	313	HIS	-	expression tag	UNP Q91MA7
B	314	HIS	-	expression tag	UNP Q91MA7
B	315	HIS	-	expression tag	UNP Q91MA7
B	316	HIS	-	expression tag	UNP Q91MA7

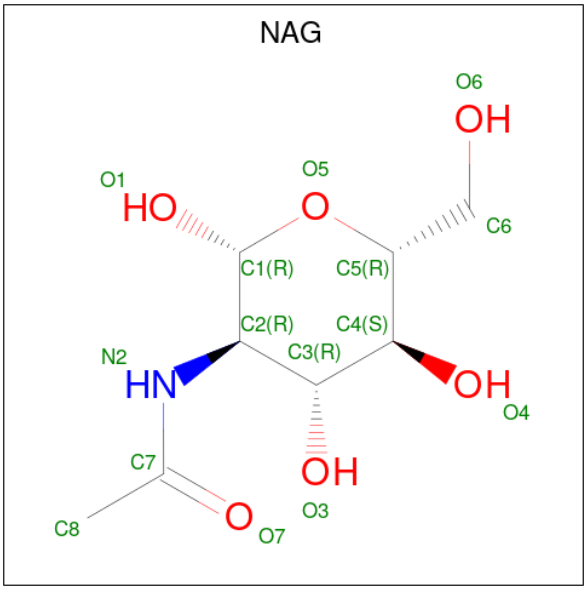
- Molecule 2 is a protein called Antibody C05 VPGSGW mutant, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	238	Total	C	N	O	S	0	3	0
			1791	1118	304	361	8			
2	E	238	Total	C	N	O	S	0	1	0
			1774	1110	298	357	9			

- Molecule 3 is a protein called Antibody C05, light chain.

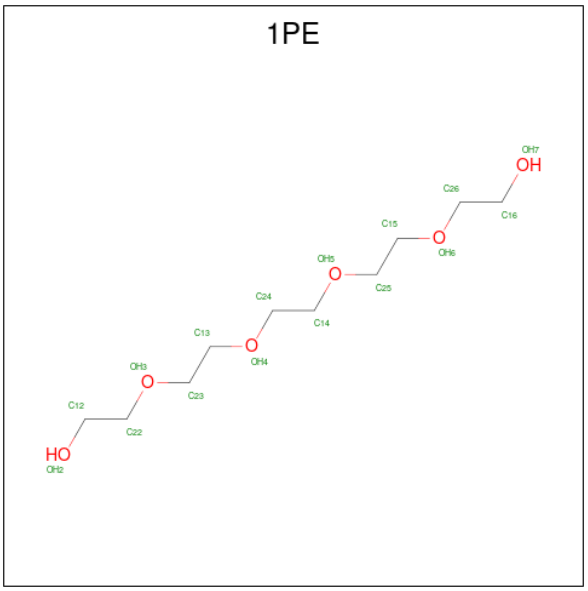
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	213	Total	C	N	O	S	0	0	0
			1637	1027	277	329	4			
3	F	213	Total	C	N	O	S	0	1	0
			1644	1031	278	331	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

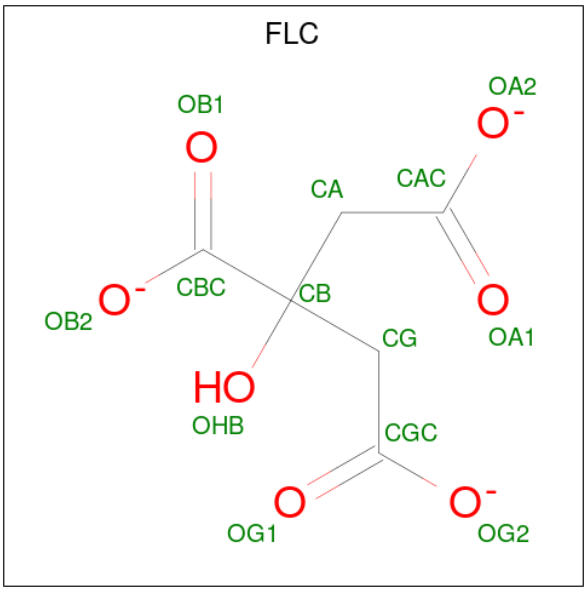


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 10 6	0	0
5	B	1	Total C O 16 10 6	0	0
5	B	1	Total C O 16 10 6	0	0
5	B	1	Total C O 16 10 6	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0

- Molecule 7 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 6 7	0	0
7	C	1	Total C O 13 6 7	0	0

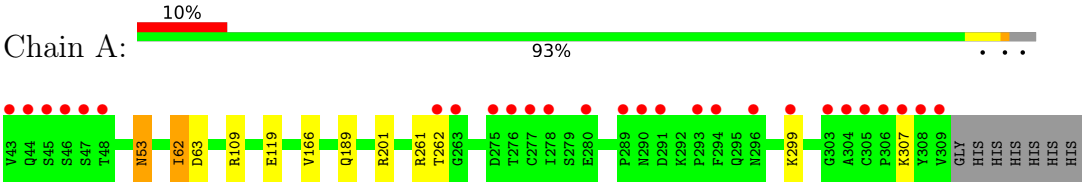
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	191	Total O 191 191	0	0
8	B	154	Total O 154 154	0	0
8	C	183	Total O 183 183	0	0
8	D	152	Total O 152 152	0	0
8	E	201	Total O 201 201	0	0
8	F	232	Total O 232 232	0	0

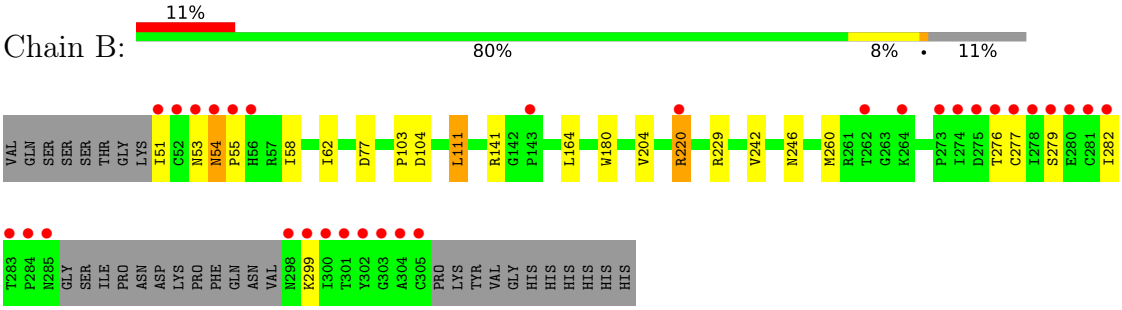
3 Residue-property plots (i)

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.

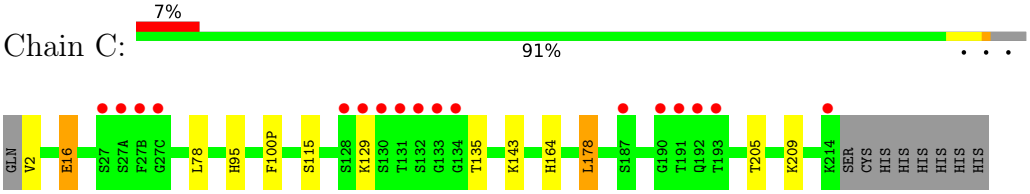
• Molecule 1: Hemagglutinin



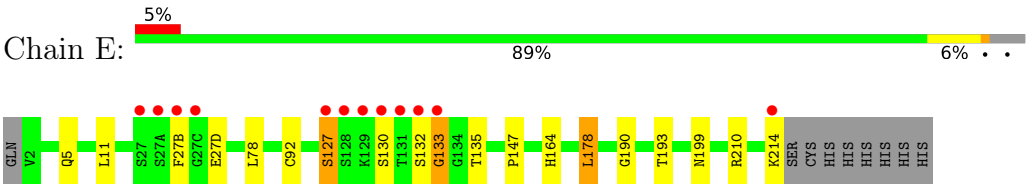
• Molecule 1: Hemagglutinin



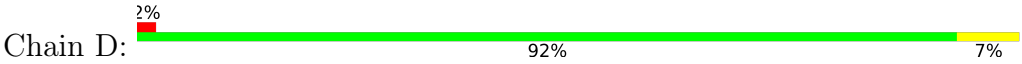
• Molecule 2: Antibody C05 VPGSGW mutant, heavy chain



• Molecule 2: Antibody C05 VPGSGW mutant, heavy chain

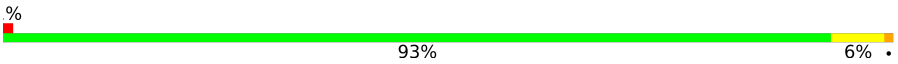


• Molecule 3: Antibody C05, light chain



• Molecule 3: Antibody C05, light chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	88.34Å 88.34Å 255.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.34 – 1.97 39.51 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (88.34-1.97) 99.5 (39.51-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.208 0.189 , 0.215	Depositor DCC
R_{free} test set	6721 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12093	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: 1PE, NAG, NA, FLC

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	0.61	0/2139	0.76	2/2914 (0.1%)
1	B	0.62	0/1946	0.76	3/2649 (0.1%)
2	C	0.68	1/1830 (0.1%)	0.80	2/2489 (0.1%)
2	E	0.68	1/1813 (0.1%)	0.84	2/2466 (0.1%)
3	D	0.60	0/1671	0.77	1/2266 (0.0%)
3	F	0.68	0/1678	0.85	2/2276 (0.1%)
All	All	0.65	2/11077 (0.0%)	0.80	12/15060 (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	E	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	16	GLU	CD-OE1	8.34	1.34	1.25
2	E	92	CYS	CB-SG	-5.29	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	178	LEU	CA-CB-CG	7.89	133.44	115.30
2	C	178	LEU	CB-CG-CD2	7.11	123.08	111.00
3	F	28	ASP	CB-CG-OD1	6.94	124.54	118.30
2	C	178	LEU	CA-CB-CG	6.53	130.32	115.30
1	B	220	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	229	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	109	ARG	NE-CZ-NH1	5.75	123.17	120.30
3	D	28	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	220	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	201	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	E	210	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	F	28	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	132	SER	Peptide
2	E	190	GLY	Peptide
2	E	27(B)	PHE	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	2087	0	2022	5	0
1	B	1900	0	1838	10	0
2	C	1791	0	1733	6	0
2	E	1774	0	1721	5	1
3	D	1637	0	1602	9	1
3	F	1644	0	1608	8	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	16	0	22	0	0
5	B	48	0	66	0	0
6	B	1	0	0	0	0
7	C	26	0	10	0	0
8	A	191	0	0	0	0
8	B	154	0	0	0	0
8	C	183	0	0	3	0
8	D	152	0	0	1	0
8	E	201	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	232	0	0	1	0
All	All	12093	0	10674	38	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (38) 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)
2:C:2:VAL:N	8:C:401:HOH:O	2.20	0.74
3:F:155:GLN:HE21	3:F:158:ASN:HD21	1.40	0.68
2:C:16:GLU:HG2	8:C:578:HOH:O	2.00	0.61
3:F:55:GLN:HE21	3:F:55:GLN:HA	1.66	0.61
2:E:127:SER:N	2:E:130:SER:OG	2.35	0.60
1:B:77:ASP:OD2	1:B:141:ARG:NH1	2.36	0.59
1:B:54:ASN:HD22	1:B:55:PRO:HA	1.68	0.58
1:A:189:GLN:HE21	2:E:27(D):GLU:H	1.53	0.56
3:F:40:PRO:CG	3:F:165:GLU:HG3	2.39	0.52
2:C:209:LYS:NZ	8:C:403:HOH:O	2.42	0.52
2:C:164:HIS:CD2	3:D:137:ASN:HD21	2.28	0.51
3:D:83:VAL:HG12	3:D:106:ILE:HG12	1.94	0.50
3:F:40:PRO:CB	3:F:165:GLU:HG3	2.43	0.49
2:E:164:HIS:CD2	3:F:137:ASN:HD21	2.31	0.48
3:D:155:GLN:CG	3:D:158:ASN:HD21	2.27	0.48
3:F:12:SER:HA	3:F:105:VAL:O	2.14	0.48
2:C:164:HIS:HD2	3:D:137:ASN:HD21	1.64	0.46
3:D:55:GLN:HA	3:D:55:GLN:HE21	1.80	0.45
3:F:11:LEU:HD12	3:F:11:LEU:C	2.38	0.44
3:D:124:GLN:NE2	8:D:307:HOH:O	2.50	0.44
2:C:95:HIS:CE1	2:C:100(P):PHE:CE1	3.05	0.44
1:B:58:ILE:HD11	1:B:282:ILE:HD13	1.98	0.44
3:D:78:LEU:HD21	3:D:106:ILE:HD13	2.00	0.43
3:D:83:VAL:CG1	3:D:106:ILE:HG12	2.48	0.43
1:A:119:GLU:OE2	1:A:261:ARG:NH2	2.49	0.43
1:B:111:LEU:C	1:B:111:LEU:HD12	2.39	0.43
3:F:45:LYS:NZ	8:F:310:HOH:O	2.51	0.43
1:A:189:GLN:HE21	2:E:27(D):GLU:N	2.15	0.43
1:B:103:PRO:O	1:B:104:ASP:CB	2.65	0.43
1:B:180:TRP:CE2	1:B:204:VAL:HG21	2.54	0.42
1:B:51:ILE:HG23	1:B:282:ILE:CG2	2.49	0.42
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:HG23	1:B:276:THR:O	2.20	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.36	0.41
1:A:53:ASN:C	1:A:53:ASN:HD22	2.23	0.41
1:B:164:LEU:O	1:B:246:ASN:HA	2.21	0.40
2:E:11:LEU:HB2	2:E:147:PRO:HG3	2.03	0.40
1:B:111:LEU:HD13	1:B:260[B]:MET:HE1	2.03	0.40

All (1) 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)
3:D:17:ASP:OD1	2:E:133:GLY:O[1_645]	1.85	0.35

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	267/274 (97%)	260 (97%)	6 (2%)	1 (0%)	34 22
1	B	240/274 (88%)	228 (95%)	11 (5%)	1 (0%)	34 22
2	C	239/247 (97%)	233 (98%)	6 (2%)	0	100 100
2	E	237/247 (96%)	228 (96%)	8 (3%)	1 (0%)	34 22
3	D	211/214 (99%)	205 (97%)	6 (3%)	0	100 100
3	F	212/214 (99%)	206 (97%)	6 (3%)	0	100 100
All	All	1406/1470 (96%)	1360 (97%)	43 (3%)	3 (0%)	47 38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	133	GLY
1	A	62	ILE

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Mol	Chain	Res	Type
1	B	62	ILE

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	238/242 (98%)	233 (98%)	5 (2%)	53	47
1	B	215/242 (89%)	207 (96%)	8 (4%)	34	22
2	C	201/207 (97%)	194 (96%)	7 (4%)	36	24
2	E	199/207 (96%)	191 (96%)	8 (4%)	31	19
3	D	186/187 (100%)	181 (97%)	5 (3%)	44	35
3	F	187/187 (100%)	182 (97%)	5 (3%)	44	35
All	All	1226/1272 (96%)	1188 (97%)	38 (3%)	40	28

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	166	VAL
1	A	262	THR
1	A	299	LYS
1	A	307	LYS
1	B	53	ASN
1	B	54	ASN
1	B	111	LEU
1	B	220	ARG
1	B	242	VAL
1	B	277	CYS
1	B	279	SER
1	B	299	LYS
2	C	78	LEU
2	C	115	SER
2	C	129	LYS
2	C	135	THR

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Mol	Chain	Res	Type
2	C	143	LYS
2	C	178	LEU
2	C	205	THR
3	D	55	GLN
3	D	126	LYS
3	D	129	THR
3	D	142	ARG
3	D	145	LYS
2	E	5	GLN
2	E	78	LEU
2	E	127	SER
2	E	135	THR
2	E	178	LEU
2	E	193	THR
2	E	199	ASN
2	E	214	LYS
3	F	55	GLN
3	F	129	THR
3	F	137	ASN
3	F	145	LYS
3	F	154	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	53	ASN
1	A	54	ASN
1	A	80	GLN
1	A	171	ASN
1	A	189	GLN
1	B	54	ASN
1	B	56	HIS
1	B	171	ASN
1	B	298	ASN
2	C	192	GLN
3	D	55	GLN
3	D	124	GLN
3	D	137	ASN
3	D	138	ASN
3	D	155	GLN
3	D	199	GLN
3	F	55	GLN

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Mol	Chain	Res	Type
3	F	124	GLN
3	F	137	ASN
3	F	138	ASN
3	F	155	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	1PE	B	404	-	15,15,15	0.49	0	14,14,14	0.26	0
4	NAG	B	401	1	14,14,15	0.77	0	17,19,21	1.06	2 (11%)
4	NAG	A	402	1	14,14,15	0.57	0	17,19,21	1.07	1 (5%)
5	1PE	A	403	-	15,15,15	0.56	0	14,14,14	0.40	0
7	FLC	C	301	-	12,12,12	1.00	0	17,17,17	1.23	2 (11%)
4	NAG	B	402	1	14,14,15	0.60	0	17,19,21	1.22	3 (17%)
7	FLC	C	302	-	12,12,12	1.04	0	17,17,17	1.22	2 (11%)
4	NAG	A	401	1	14,14,15	0.76	0	17,19,21	1.95	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	1PE	B	403	-	15,15,15	0.53	0	14,14,14	0.37	0
5	1PE	B	405	-	15,15,15	0.53	0	14,14,14	0.34	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	1PE	B	404	-	-	3/13/13/13	-
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	1PE	A	403	-	-	5/13/13/13	-
7	FLC	C	301	-	-	0/16/16/16	-
4	NAG	B	402	1	-	2/6/23/26	0/1/1/1
7	FLC	C	302	-	-	6/16/16/16	-
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	1PE	B	403	-	-	5/13/13/13	-
5	1PE	B	405	-	-	2/13/13/13	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	NAG	C1-O5-C5	6.46	120.94	112.19
7	C	301	FLC	OB2-CBC-CB	3.30	118.78	113.05
4	A	401	NAG	O5-C1-C2	2.97	115.97	111.29
7	C	302	FLC	OB2-CBC-CB	2.68	117.71	113.05
4	B	402	NAG	C1-O5-C5	2.58	115.69	112.19
4	A	402	NAG	O5-C5-C6	2.37	110.92	107.20
4	B	402	NAG	O5-C5-C6	2.34	110.88	107.20
4	A	401	NAG	C2-N2-C7	2.25	126.10	122.90
4	B	401	NAG	C2-N2-C7	2.24	126.09	122.90
7	C	301	FLC	OB1-CBC-CB	-2.22	119.11	122.25
4	B	402	NAG	C4-C3-C2	-2.04	108.02	111.02
4	B	401	NAG	C1-O5-C5	2.03	114.94	112.19
7	C	302	FLC	OA1-CAC-CA	-2.02	117.04	122.94

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	NAG	O5-C5-C6-O6
4	B	402	NAG	C4-C5-C6-O6
5	B	405	1PE	OH4-C13-C23-OH3
5	A	403	1PE	OH4-C13-C23-OH3
5	B	404	1PE	OH7-C16-C26-OH6
5	B	403	1PE	OH2-C12-C22-OH3
5	A	403	1PE	OH5-C14-C24-OH4
5	B	403	1PE	OH7-C16-C26-OH6
7	C	302	FLC	OHB-CB-CBC-OB1
7	C	302	FLC	OHB-CB-CBC-OB2
5	A	403	1PE	OH6-C15-C25-OH5
7	C	302	FLC	CA-CB-CBC-OB1
7	C	302	FLC	CA-CB-CBC-OB2
5	B	403	1PE	C23-C13-OH4-C24
5	B	405	1PE	C16-C26-OH6-C15
7	C	302	FLC	CG-CB-CBC-OB2
5	A	403	1PE	C12-C22-OH3-C23
5	B	403	1PE	C16-C26-OH6-C15
5	A	403	1PE	C25-C15-OH6-C26
5	B	404	1PE	OH5-C14-C24-OH4
7	C	302	FLC	CG-CB-CBC-OB1
5	B	403	1PE	C15-C25-OH5-C14
5	B	404	1PE	OH6-C15-C25-OH5

There are no ring outliers.

No monomer is involved in short contacts.

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

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	267/274 (97%)	0.54	27 (10%) 7 7	16, 27, 64, 78	0
1	B	243/274 (88%)	1.13	31 (12%) 3 4	19, 32, 137, 166	0
2	C	238/247 (96%)	0.42	17 (7%) 16 17	20, 28, 63, 98	0
2	E	238/247 (96%)	0.29	12 (5%) 28 31	19, 27, 58, 100	0
3	D	213/214 (99%)	0.08	4 (1%) 66 68	22, 32, 54, 76	0
3	F	213/214 (99%)	-0.05	2 (0%) 84 85	17, 24, 35, 53	0
All	All	1412/1470 (96%)	0.42	93 (6%) 18 20	16, 28, 63, 166	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	CYS	16.7
1	B	52	CYS	15.7
1	B	282	ILE	15.2
1	B	300	ILE	14.2
1	B	278	ILE	14.0
1	B	283	THR	13.9
1	B	302	TYR	13.7
1	B	304	ALA	13.4
1	B	281	CYS	12.4
1	B	277	CYS	11.3
2	E	27(B)	PHE	10.7
1	B	301	THR	10.6
2	E	128	SER	10.4
1	B	303	GLY	10.4
2	E	132	SER	10.3
1	B	279	SER	9.6
2	E	130	SER	8.4
1	B	285	ASN	8.3
1	B	284	PRO	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	275	ASP	8.0
2	E	131	THR	7.9
2	C	133	GLY	7.9
2	C	27(B)	PHE	7.8
1	B	276	THR	7.8
1	B	51	ILE	7.3
2	C	128	SER	7.1
1	B	55	PRO	6.8
1	B	299	LYS	6.6
1	B	54	ASN	6.4
1	B	298	ASN	6.4
1	B	280	GLU	6.2
2	E	27(C)	GLY	6.1
2	E	133	GLY	5.9
2	E	27	SER	5.8
1	B	53	ASN	5.3
2	C	190	GLY	5.2
1	A	294	PHE	5.2
2	C	134	GLY	4.9
1	A	291	ASP	4.9
1	A	307	LYS	4.8
2	E	27(A)	SER	4.6
2	C	131	THR	4.4
1	A	277	CYS	4.3
2	C	132	SER	4.3
1	A	48	THR	4.2
1	A	276	THR	4.2
1	A	305	CYS	4.2
2	C	27(C)	GLY	4.0
1	A	46	SER	4.0
2	E	127	SER	4.0
2	C	130	SER	3.9
2	C	191	THR	3.9
1	B	274	ILE	3.9
1	B	264	LYS	3.8
1	B	56	HIS	3.7
1	A	309	VAL	3.7
2	C	27(A)	SER	3.7
2	E	129	LYS	3.6
1	A	43	VAL	3.6
3	D	212	GLY	3.6
2	C	193	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	47	SER	3.3
1	A	293	PRO	3.3
1	A	304	ALA	3.1
1	A	308	TYR	3.0
2	C	192	GLN	3.0
2	C	27	SER	3.0
1	A	299	LYS	2.9
1	A	45	SER	2.8
2	E	214	LYS	2.7
3	D	213	GLU	2.7
1	A	262	THR	2.7
1	A	306	PRO	2.7
2	C	214	LYS	2.5
1	A	275	ASP	2.5
1	B	262	THR	2.4
1	A	290	ASN	2.4
1	A	303	GLY	2.4
2	C	129	LYS	2.4
1	A	289	PRO	2.3
3	D	156	SER	2.3
3	F	56	ARG	2.2
1	B	143	PRO	2.2
1	B	220	ARG	2.2
1	A	278	ILE	2.2
1	B	273	PRO	2.1
1	A	296	ASN	2.1
1	A	44	GLN	2.1
1	A	263	GLY	2.1
3	D	188	LYS	2.1
3	F	212	GLY	2.1
1	A	280	GLU	2.0
2	C	187	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
5	1PE	A	403	16/16	0.53	0.30	69,73,79,79	0
7	FLC	C	302	13/13	0.62	0.41	47,73,77,80	0
4	NAG	A	401	14/15	0.66	0.33	64,74,79,80	0
5	1PE	B	405	16/16	0.69	0.27	71,81,86,88	0
5	1PE	B	403	16/16	0.70	0.29	70,76,82,82	0
7	FLC	C	301	13/13	0.72	0.42	70,80,85,88	0
4	NAG	B	401	14/15	0.73	0.25	60,68,70,73	0
4	NAG	A	402	14/15	0.79	0.50	65,70,74,75	0
5	1PE	B	404	16/16	0.81	0.25	74,78,80,80	0
4	NAG	B	402	14/15	0.81	0.41	74,83,87,87	0
6	NA	B	406	1/1	0.90	0.27	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.