wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MUG
Title	:	Crystal structure of human Fab PG16, a broadly reactive and potent HIV-1 neutralizing antibody
Authors	:	Pejchal, R.; Walker, L.M.; Burton, D.R.; Wilson, I.A.
Deposited on	:	2010-05-03
Resolution	:	2.49 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

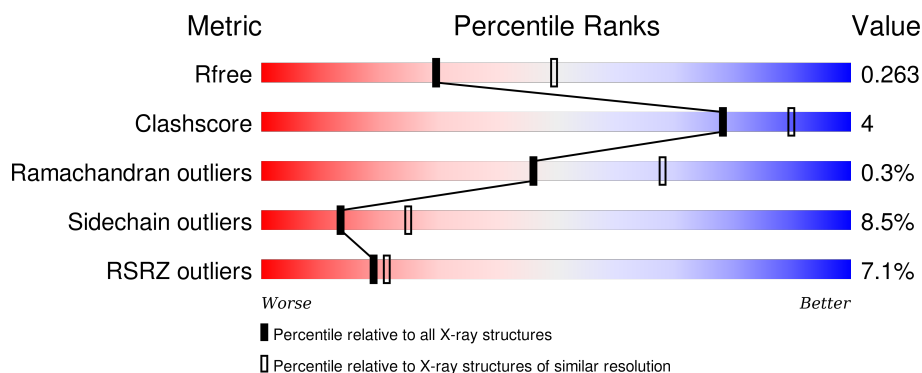|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.49 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		8.5%
RSRZ outliers		7.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	2% / 85% / 12% / ••
1	C	216	17% / 84% / 13% / ••
1	E	216	4% / 88% / 9% / •
1	G	216	2% / 87% / 11% / ••
1	I	216	4% / 83% / 14% / ••

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Mol	Chain	Length	Quality of chain
1	K	216	5% · · · · 85% · · · 12% · ·
2	B	241	6% · · · · 83% · · · 14% · ·
2	D	241	15% · · · · 86% · · · 12% ·
2	F	241	9% · · · · 86% · · · 11% · ·
2	H	241	5% · · · · 84% · · · 14% · ·
2	J	241	8% · · · · 79% · · · 20% · ·
2	L	241	5% · · · · 84% · · · 12% · ·

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
3	NAG	A	500	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20630 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 Antibody PG16 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total 1555	C 966	N 263	O 321	S 5	0	0	0
1	C	212	Total 1547	C 960	N 261	O 321	S 5	0	0	0
1	E	211	Total 1553	C 966	N 263	O 319	S 5	0	0	0
1	G	212	Total 1559	C 969	N 264	O 321	S 5	0	0	0
1	I	213	Total 1563	C 971	N 264	O 323	S 5	0	0	0
1	K	212	Total 1558	C 969	N 264	O 320	S 5	0	0	0

- Molecule 2 is a protein called Antibody PG16 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total 1795	C 1129	N 301	O 355	S 10	0	0	0
2	D	239	Total 1806	C 1139	N 302	O 355	S 10	0	0	0
2	F	238	Total 1796	C 1135	N 302	O 349	S 10	0	0	0
2	H	239	Total 1799	C 1132	N 302	O 355	S 10	0	0	0
2	J	239	Total 1806	C 1139	N 302	O 355	S 10	0	0	0
2	L	238	Total 1792	C 1134	N 301	O 347	S 10	0	0	0

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	28	Total	O	0	0
			28	28		
5	C	7	Total	O	0	0
			7	7		
5	D	14	Total	O	0	0
			14	14		
5	E	53	Total	O	0	0
			53	53		
5	F	30	Total	O	0	0
			30	30		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	32	Total 32	O 32	0	0
5	H	39	Total 39	O 39	0	0
5	I	51	Total 51	O 51	0	0
5	J	33	Total 33	O 33	0	0
5	K	64	Total 64	O 64	0	0
5	L	57	Total 57	O 57	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
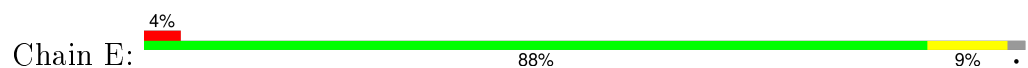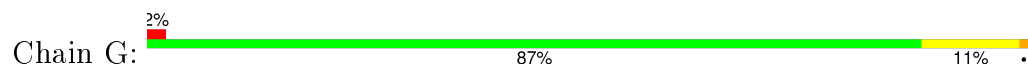
- Molecule 1: Antibody PG16 Light Chain
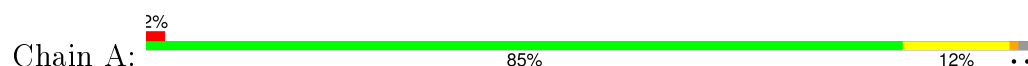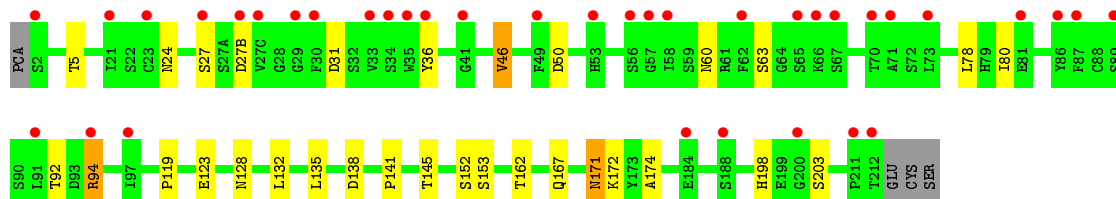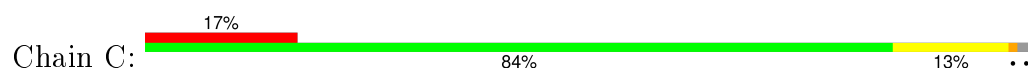
- Molecule 1: Antibody PG16 Light Chain

- Molecule 1: Antibody PG16 Light Chain

- Molecule 1: Antibody PG16 Light Chain

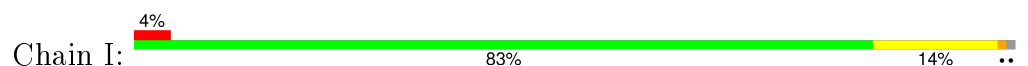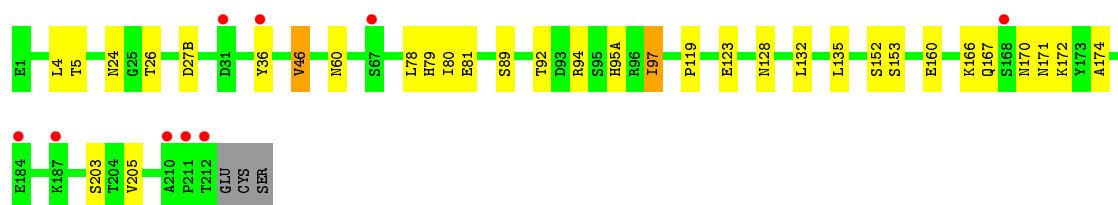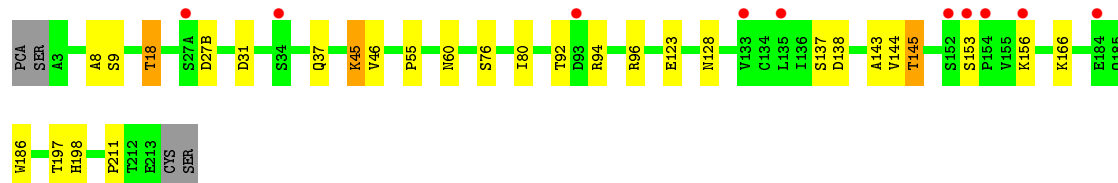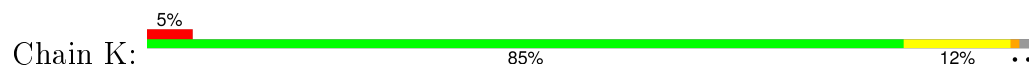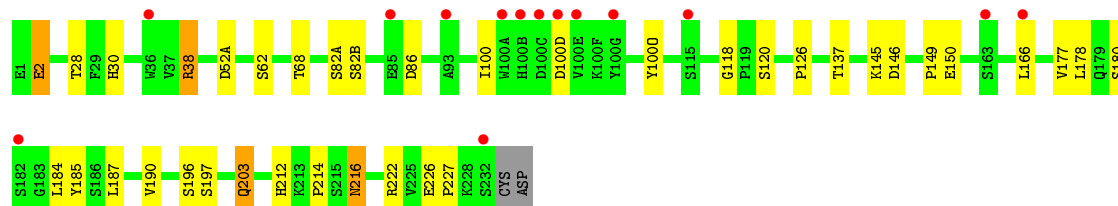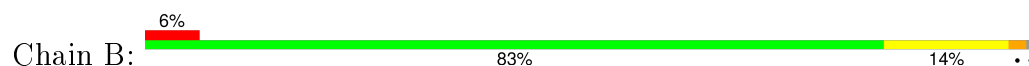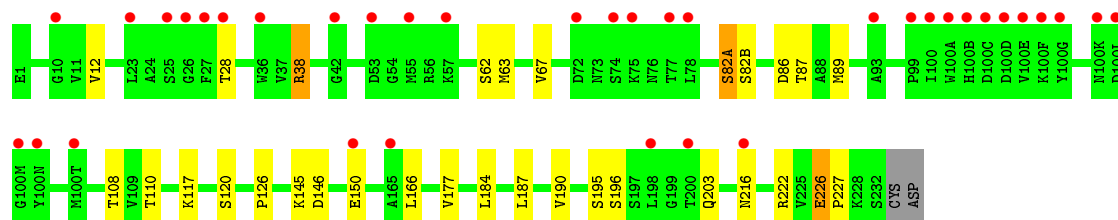- Molecule 1: Antibody PG16 Light Chain

- Molecule 1: Antibody PG16 Light Chain

Chain K:

- Molecule 2: Antibody PG16 Heavy Chain

Chain B:

- Molecule 2: Antibody PG16 Heavy Chain

Chain D:

- Molecule 2: Antibody PG16 Heavy Chain
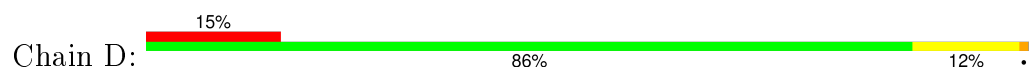
Chain F:

- Molecule 2: Antibody PG16 Heavy Chain
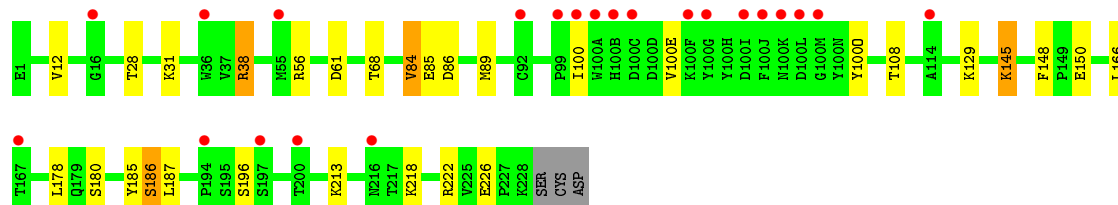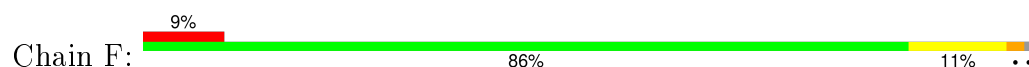
Chain H:
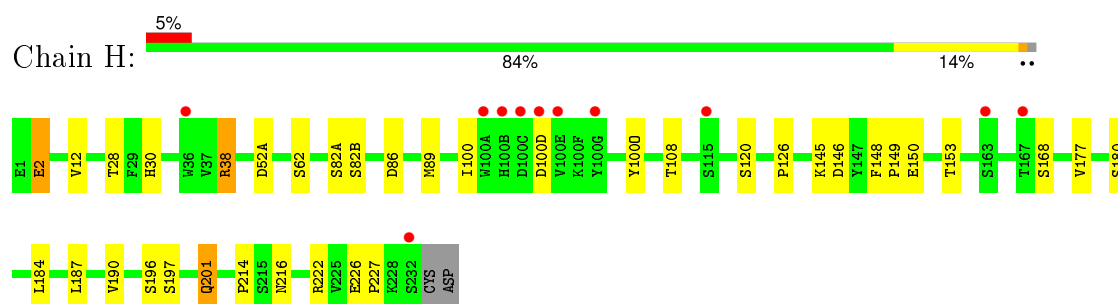
• Molecule 2: Antibody PG16 Heavy Chain
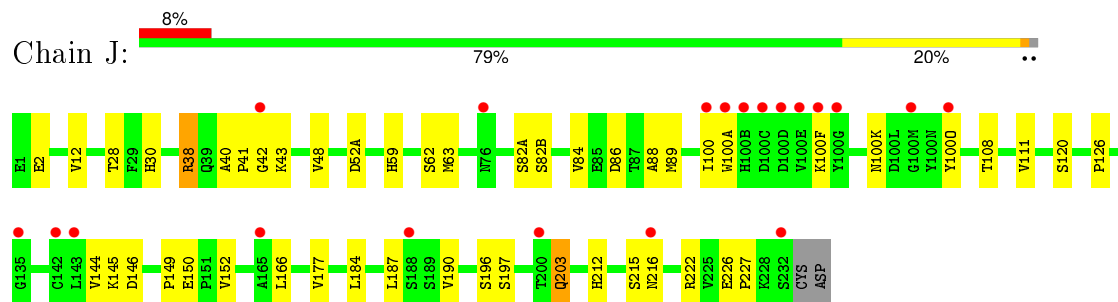
Chain J:

• Molecule 2: Antibody PG16 Heavy Chain

Chain L:
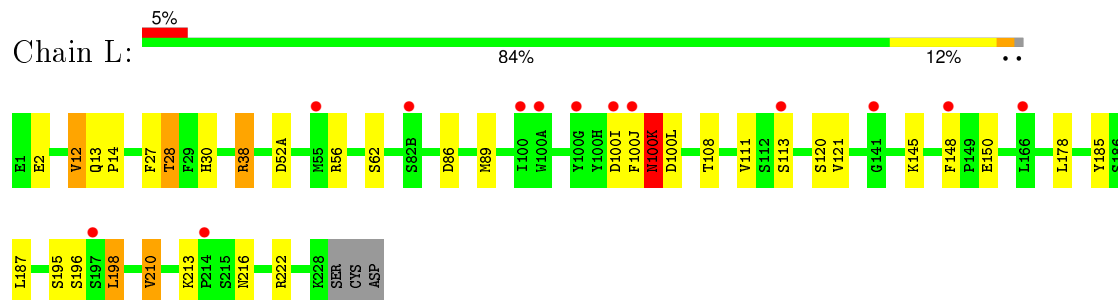
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	128.77Å 66.25Å 198.70Å 90.00° 98.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.49 24.97 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.97-2.49) 94.6 (24.97-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.207 , 0.248 0.221 , 0.263	Depositor DCC
R_{free} test set	5547 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 110628 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 75.82 % 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 1.1728e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PCA, NAG, TYS

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	0.46	0/1592	0.69	0/2171
1	C	0.46	0/1584	0.68	0/2163
1	E	0.54	0/1590	0.75	1/2167 (0.0%)
1	G	0.49	0/1596	0.70	0/2175
1	I	0.50	0/1593	0.72	0/2174
1	K	0.55	0/1595	0.75	0/2174
2	B	0.50	0/1819	0.75	0/2480
2	D	0.47	0/1832	0.75	1/2499 (0.0%)
2	F	0.52	0/1820	0.79	0/2480
2	H	0.50	0/1823	0.74	0/2484
2	J	0.50	0/1832	0.75	0/2499
2	L	0.57	0/1816	0.84	0/2474
All	All	0.51	0/20492	0.75	2/27940 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	82(A)	SER	N-CA-C	-5.50	96.15	111.00
1	E	145	THR	N-CA-CB	5.30	120.38	110.30

There are no chirality outliers.

There are no planarity outliers.

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	1555	0	1490	17	0
1	C	1547	0	1468	14	0
1	E	1553	0	1497	11	0
1	G	1559	0	1502	10	0
1	I	1563	0	1497	16	0
1	K	1558	0	1499	10	0
2	B	1795	0	1665	17	0
2	D	1806	0	1679	10	0
2	F	1796	0	1682	12	0
2	H	1799	0	1676	13	0
2	J	1806	0	1680	22	0
2	L	1792	0	1681	11	0
3	A	14	0	13	0	0
4	C	28	0	25	0	0
4	I	28	0	25	0	0
5	A	23	0	0	0	0
5	B	28	0	0	0	0
5	C	7	0	0	0	0
5	D	14	0	0	0	0
5	E	53	0	0	1	0
5	F	30	0	0	0	0
5	G	32	0	0	0	0
5	H	39	0	0	0	0
5	I	51	0	0	0	0
5	J	33	0	0	1	0
5	K	64	0	0	0	0
5	L	57	0	0	0	0
All	All	20630	0	19079	140	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 4.

The worst 5 of 140 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:97:ILE:CD1	1:A:97:ILE:CG1	1.74	1.61
1:A:135:LEU:HD13	2:B:190:VAL:HG11	1.49	0.95
1:I:135:LEU:HD13	2:J:190:VAL:HG11	1.50	0.90
1:E:8:ALA:HB2	1:E:145:THR:HG22	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD13	2:D:190:VAL:HG11	1.60	0.84

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	210/216 (97%)	200 (95%)	10 (5%)	0	100	100
1	C	210/216 (97%)	194 (92%)	15 (7%)	1 (0%)	34	55
1	E	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
1	G	210/216 (97%)	201 (96%)	9 (4%)	0	100	100
1	I	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	34	55
1	K	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
2	B	236/241 (98%)	226 (96%)	9 (4%)	1 (0%)	39	61
2	D	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	39	61
2	F	235/241 (98%)	222 (94%)	12 (5%)	1 (0%)	39	61
2	H	236/241 (98%)	228 (97%)	7 (3%)	1 (0%)	39	61
2	J	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	39	61
2	L	235/241 (98%)	221 (94%)	12 (5%)	2 (1%)	21	37
All	All	2674/2742 (98%)	2556 (96%)	109 (4%)	9 (0%)	46	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	171	ASN
2	L	100(K)	ASN
2	D	82(B)	SER
2	B	82(B)	SER

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Mol	Chain	Res	Type
2	H	82(B)	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	177/182 (97%)	166 (94%)	11 (6%)	23	41
1	C	175/182 (96%)	159 (91%)	16 (9%)	12	22
1	E	177/182 (97%)	167 (94%)	10 (6%)	26	47
1	G	178/182 (98%)	165 (93%)	13 (7%)	17	32
1	I	177/182 (97%)	164 (93%)	13 (7%)	17	32
1	K	177/182 (97%)	163 (92%)	14 (8%)	15	28
2	B	191/203 (94%)	173 (91%)	18 (9%)	11	20
2	D	193/203 (95%)	175 (91%)	18 (9%)	11	21
2	F	190/203 (94%)	173 (91%)	17 (9%)	12	23
2	H	192/203 (95%)	171 (89%)	21 (11%)	8	15
2	J	193/203 (95%)	176 (91%)	17 (9%)	12	23
2	L	189/203 (93%)	169 (89%)	20 (11%)	8	16
All	All	2209/2310 (96%)	2021 (92%)	188 (8%)	13	25

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	186	SER
2	H	28	THR
2	L	89	MET
2	F	196	SER
1	G	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	37	GLN
2	F	100(B)	HIS
2	J	212	HIS
2	D	179	GLN
1	I	189	HIS

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

13 non-standard protein/DNA/RNA residues 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	PCA	B	1	2	7,8,9	0.77	0	9,10,12	1.59	3 (33%)
2	TYS	B	100(H)	2	15,16,17	1.62	2 (13%)	16,22,24	1.44	2 (12%)
2	PCA	D	1	2	7,8,9	0.77	0	9,10,12	1.84	2 (22%)
2	TYS	D	100(H)	2	15,16,17	2.00	1 (6%)	16,22,24	1.68	3 (18%)
2	PCA	F	1	2	7,8,9	0.95	1 (14%)	9,10,12	0.85	0
2	TYS	F	100(H)	2	15,16,17	2.21	1 (6%)	16,22,24	1.29	2 (12%)
2	PCA	H	1	2	7,8,9	0.77	0	9,10,12	1.51	2 (22%)
2	TYS	H	100(H)	2	15,16,17	1.58	2 (13%)	16,22,24	1.53	3 (18%)
1	PCA	I	1	1	7,8,9	1.14	1 (14%)	9,10,12	1.09	0
2	PCA	J	1	2	7,8,9	0.91	0	9,10,12	1.53	2 (22%)
2	TYS	J	100(H)	2	15,16,17	2.17	2 (13%)	16,22,24	1.53	4 (25%)
2	PCA	L	1	2	7,8,9	0.73	0	9,10,12	1.46	1 (11%)
2	TYS	L	100(H)	2	15,16,17	2.69	4 (26%)	16,22,24	1.89	5 (31%)

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	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	TYS	B	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	D	1	2	-	0/0/11/13	0/1/1/1
2	TYS	D	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1
2	TYS	F	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	TYS	H	100(H)	2	-	0/9/11/13	0/1/1/1
1	PCA	I	1	1	-	0/0/11/13	0/1/1/1
2	PCA	J	1	2	-	0/0/11/13	0/1/1/1
2	TYS	J	100(H)	2	-	0/9/11/13	0/1/1/1
2	PCA	L	1	2	-	0/0/11/13	0/1/1/1
2	TYS	L	100(H)	2	-	0/9/11/13	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	100(H)	TYS	OH-S	-8.73	1.47	1.63
2	F	100(H)	TYS	OH-S	-7.57	1.49	1.63
2	J	100(H)	TYS	OH-S	-7.55	1.49	1.63
2	D	100(H)	TYS	OH-S	-6.60	1.51	1.63
2	H	100(H)	TYS	OH-S	-4.72	1.55	1.63

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	100(H)	TYS	CG-CB-CA	-3.62	106.03	114.21
2	F	100(H)	TYS	CG-CB-CA	-3.06	107.31	114.21
2	H	1	PCA	CA-N-CD	-2.98	103.83	113.81
2	J	1	PCA	CA-N-CD	-2.97	103.86	113.81
2	B	100(H)	TYS	CG-CB-CA	-2.95	107.55	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

4 carbohydrates 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	NAG	C	500	1,4	14,14,15	2.07	5 (35%)	15,19,21	1.51	2 (13%)
4	NAG	C	501	4	14,14,15	2.82	6 (42%)	15,19,21	2.56	6 (40%)
4	NAG	I	500	1,4	14,14,15	1.95	3 (21%)	15,19,21	2.17	5 (33%)
4	NAG	I	501	4	14,14,15	2.83	8 (57%)	15,19,21	3.41	10 (66%)

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	NAG	C	500	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	501	4	-	0/6/23/26	0/1/1/1
4	NAG	I	500	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	501	4	-	0/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	500	NAG	O4-C4	2.07	1.47	1.43
4	C	501	NAG	C4-C3	2.07	1.57	1.52
4	I	501	NAG	C6-C5	2.25	1.60	1.51
4	I	500	NAG	C3-C2	2.69	1.58	1.52
4	I	500	NAG	C4-C3	2.71	1.59	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	501	NAG	C3-C4-C5	-3.45	104.18	110.20
4	I	500	NAG	C2-N2-C7	-3.17	118.97	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	NAG	C3-C4-C5	-2.13	106.49	110.20
4	I	500	NAG	C1-O5-C5	2.06	114.86	112.25
4	I	501	NAG	C6-C5-C4	2.08	118.16	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

1 ligand is 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	$\#|Z| > 2$
3	NAG	A	500	1	14,14,15	1.55	3 (21%)	15,19,21	1.46	4 (26%)

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
3	NAG	A	500	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAG	C4-C5	2.00	1.57	1.53
3	A	500	NAG	C3-C2	2.58	1.58	1.52
3	A	500	NAG	C4-C3	2.77	1.59	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	500	NAG	C1-O5-C5	2.13	114.95	112.25
3	A	500	NAG	O4-C4-C3	2.35	115.62	110.34
3	A	500	NAG	C4-C3-C2	2.48	115.08	111.23
3	A	500	NAG	C3-C2-N2	2.62	116.85	110.56

There are no chirality outliers.

There are no torsion outliers.

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, 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	212/216 (98%)	0.10	5 (2%)	62	66	31, 56, 80, 99	0
1	C	212/216 (98%)	0.84	37 (17%)	2	2	36, 74, 112, 129	0
1	E	211/216 (97%)	0.13	8 (3%)	44	49	38, 53, 81, 89	0
1	G	212/216 (98%)	0.04	5 (2%)	62	66	31, 50, 71, 81	0
1	I	212/216 (98%)	0.12	9 (4%)	40	45	29, 47, 78, 105	0
1	K	212/216 (98%)	0.02	10 (4%)	35	40	35, 47, 77, 89	0
2	B	237/241 (98%)	0.23	14 (5%)	26	29	25, 58, 87, 122	0
2	D	237/241 (98%)	0.76	36 (15%)	3	3	42, 67, 122, 186	0
2	F	236/241 (97%)	0.52	22 (9%)	11	11	45, 67, 100, 128	0
2	H	237/241 (98%)	0.20	11 (4%)	36	41	25, 51, 83, 120	0
2	J	237/241 (98%)	0.44	20 (8%)	14	14	37, 59, 89, 154	0
2	L	236/241 (97%)	0.16	13 (5%)	29	32	39, 56, 78, 99	0
All	All	2691/2742 (98%)	0.30	190 (7%)	19	21	25, 57, 93, 186	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	100(A)	TRP	9.7
2	F	100(A)	TRP	9.1
2	D	100(M)	GLY	8.3
2	J	100(G)	TYR	7.5
2	F	100	ILE	7.4

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

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	TYS	L	100(H)	16/17	0.91	0.17	-	68,76,93,94	0
2	PCA	J	1	8/9	0.65	0.45	-	88,92,95,98	0
2	PCA	H	1	8/9	0.95	0.19	-	63,69,74,75	0
2	PCA	L	1	8/9	0.91	0.23	-	59,62,65,69	0
2	PCA	B	1	8/9	0.95	0.17	-	60,65,69,70	0
2	PCA	F	1	8/9	0.84	0.22	-	76,79,80,80	0
2	PCA	D	1	8/9	0.63	0.52	-	111,118,125,129	0
2	TYS	B	100(H)	16/17	0.93	0.12	-	53,65,84,84	0
1	PCA	I	1	8/9	0.81	0.38	-	83,86,87,88	0
2	TYS	F	100(H)	16/17	0.84	0.23	-	114,120,128,130	0
2	TYS	D	100(H)	16/17	0.84	0.24	-	134,143,157,162	0
2	TYS	J	100(H)	16/17	0.81	0.30	-	94,108,128,131	0
2	TYS	H	100(H)	16/17	0.96	0.11	-	46,58,78,79	0

6.3 Carbohydrates (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
4	NAG	I	500	14/15	0.91	0.14	0.09	52,55,60,63	0
4	NAG	C	500	14/15	0.78	0.18	-0.79	88,94,103,106	0
4	NAG	I	501	14/15	0.86	0.29	-	63,69,72,73	0
4	NAG	C	501	14/15	0.61	0.41	-	107,115,119,121	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	500	14/15	0.73	0.51	12.12	109,113,120,122	0

6.5 Other polymers (i)

There are no such residues in this entry.