Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2024 – 06:58 pm GMT

PDB ID	:	8C7M
Title	:	Interleukin 12 receptor subunit beta-1 Fn domains in complex with antagonistic FAb fragment.
Authors	:	Bloch, Y.; Savvides, S.N.
Deposited on	:	2023-01-16
Resolution	:	2.56 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:

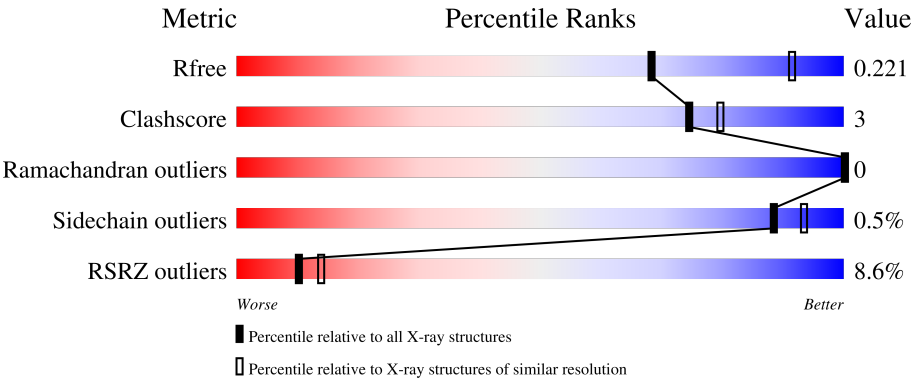
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	313	2% 83% 5% 12%
1	B	313	15% 81% 8% 11%
2	C	231	16% 84% 10% 6%
2	H	231	89% 7% .
3	D	212	15% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	L	212	97%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10911 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 Interleukin-12 receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2133	1339	378	403	13			
1	B	280	Total	C	N	O	S	0	0	0
			2155	1353	383	406	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	541	ASP	-	expression tag	UNP P42701
A	542	GLU	-	expression tag	UNP P42701
A	543	VAL	-	expression tag	UNP P42701
A	544	ASP	-	expression tag	UNP P42701
B	541	ASP	-	expression tag	UNP P42701
B	542	GLU	-	expression tag	UNP P42701
B	543	VAL	-	expression tag	UNP P42701
B	544	ASP	-	expression tag	UNP P42701

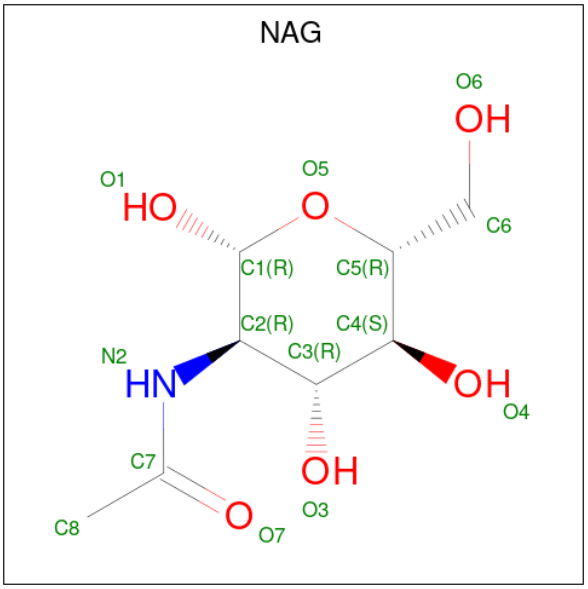
- Molecule 2 is a protein called FAb4 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1627	1026	273	322	6			
2	H	222	Total	C	N	O	S	0	0	0
			1660	1045	279	330	6			

- Molecule 3 is a protein called FAb4 Crystal Kappa Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1612	1014	266	327	5			
3	L	211	Total	C	N	O	S	0	0	0
			1628	1023	269	331	5			

- 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 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

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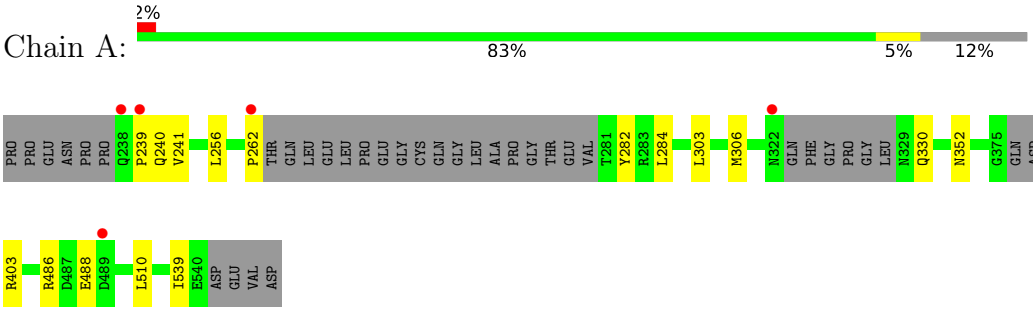
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	H	10	Total O 10 10	0	0
6	L	11	Total O 11 11	0	0

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.

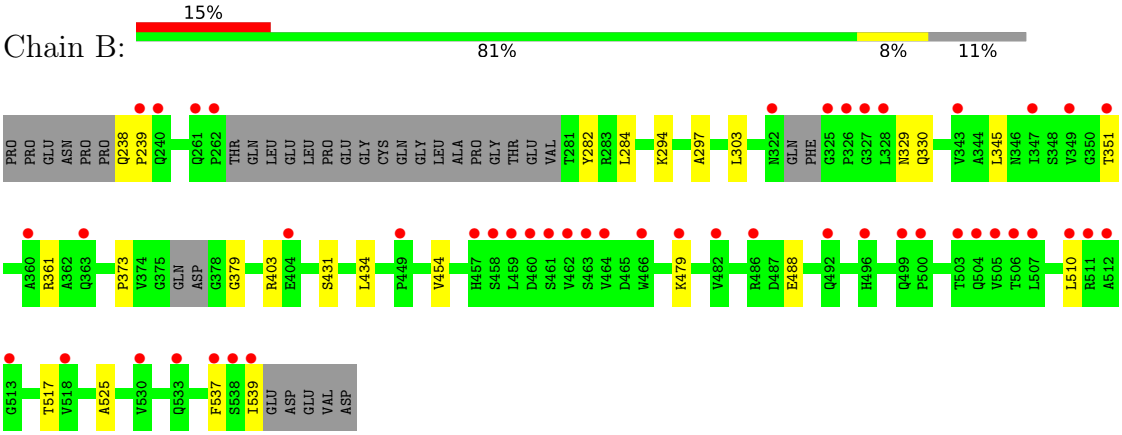
• Molecule 1: Interleukin-12 receptor subunit beta-1

Chain A:



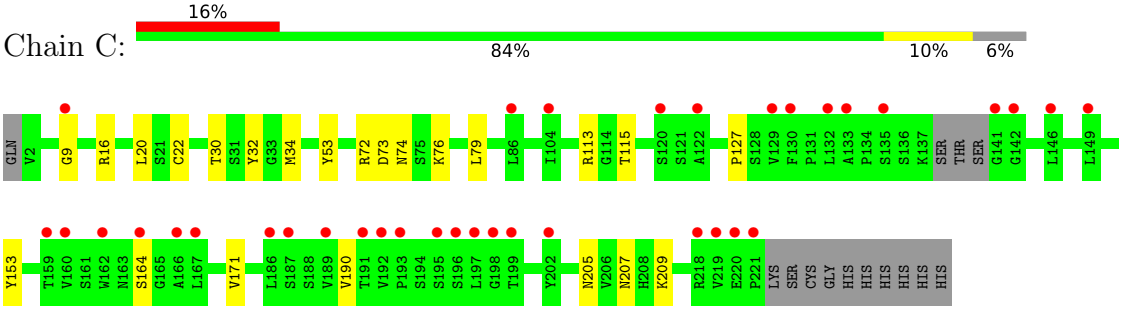
• Molecule 1: Interleukin-12 receptor subunit beta-1

Chain B:



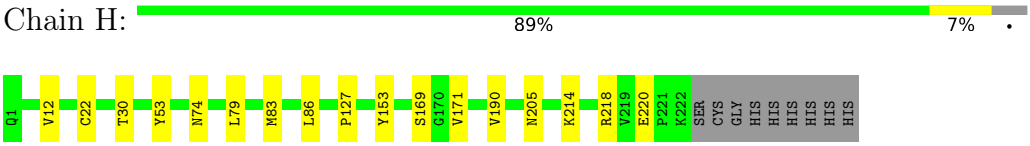
• Molecule 2: FAb4 Heavy chain

Chain C:



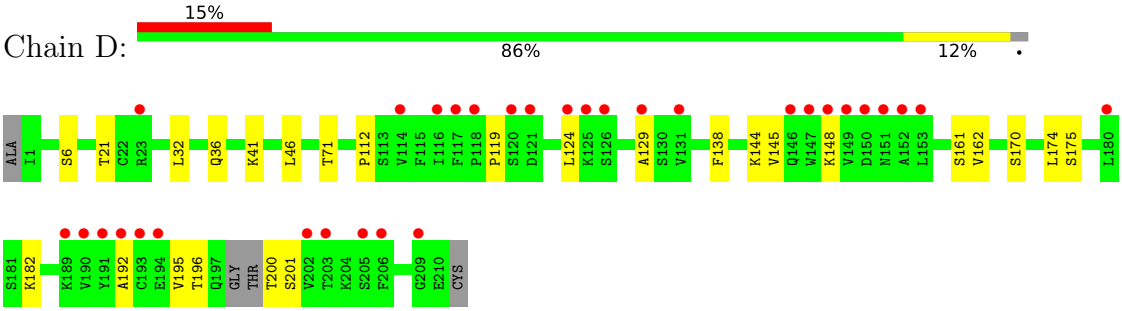
• Molecule 2: FAb4 Heavy chain

Chain H:



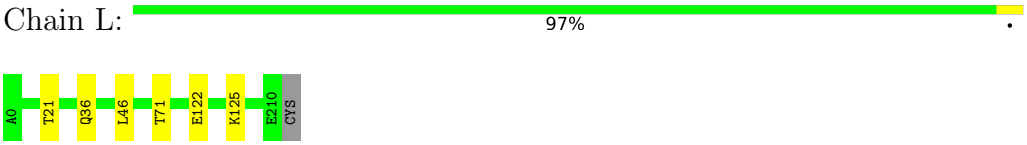
• Molecule 3: FAb4 Crystal Kappa Light chain

Chain D:



• Molecule 3: FAb4 Crystal Kappa Light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.66Å 140.18Å 219.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.09 – 2.56 70.09 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (70.09-2.56) 99.7 (70.09-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.203 , 0.228 0.202 , 0.221	Depositor DCC
R_{free} test set	1999 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.0	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	0.95	EDS
Total number of atoms	10911	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: CL, NAG

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	0.24	0/2188	0.51	0/2985
1	B	0.25	0/2211	0.51	0/3016
2	C	0.25	0/1666	0.51	0/2271
2	H	0.26	0/1700	0.52	0/2318
3	D	0.27	0/1648	0.49	0/2237
3	L	0.27	0/1665	0.50	0/2262
All	All	0.26	0/11078	0.51	0/15089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2133	0	2064	12	0
1	B	2155	0	2091	17	0
2	C	1627	0	1571	14	0
2	H	1660	0	1607	8	0
3	D	1612	0	1557	17	0
3	L	1628	0	1573	4	0
4	A	56	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
5	A	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	H	10	0	0	0	0
6	L	11	0	0	0	0
All	All	10911	0	10528	69	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 3.

All (69) 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:32:TYR:O	2:C:72:ARG:NH2	2.20	0.73
3:D:162:VAL:HG22	3:D:174:LEU:HD23	1.71	0.72
1:B:345:LEU:HD11	1:B:434:LEU:HD11	1.75	0.68
1:B:373:PRO:CG	1:B:379:GLY:HA3	2.25	0.67
1:A:239:PRO:O	1:A:330:GLN:NE2	2.28	0.66
3:D:200:THR:HG22	3:D:201:SER:N	2.11	0.66
1:A:403:ARG:NH2	3:D:170:SER:OG	2.29	0.66
1:B:238:GLN:N	1:B:282:TYR:HH	1.95	0.64
1:B:373:PRO:HG3	1:B:379:GLY:HA3	1.79	0.64
3:D:148:LYS:HB2	3:D:192:ALA:HB3	1.77	0.64
1:B:284:LEU:HB2	1:B:303:LEU:HD23	1.78	0.64
2:C:20:LEU:HD22	2:C:115:THR:HG21	1.81	0.63
1:A:284:LEU:HB2	1:A:303:LEU:HD23	1.82	0.61
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.84	0.60
2:C:72:ARG:NH1	2:C:74:ASN:OD1	2.35	0.59
2:C:164:SER:H	2:C:205:ASN:HD21	1.51	0.59
3:D:21:THR:HG22	3:D:71:THR:HG22	1.85	0.58
2:C:73:ASP:OD2	2:C:76:LYS:HE2	2.03	0.58
3:L:36:GLN:HB2	3:L:46:LEU:HD11	1.85	0.58
1:B:479:LYS:HE3	1:B:525:ALA:HA	1.85	0.58
2:H:30:THR:HG22	2:H:74:ASN:HB3	1.85	0.57
3:D:200:THR:HG22	3:D:201:SER:H	1.69	0.56
3:L:122:GLU:HA	3:L:125:LYS:NZ	2.21	0.56
3:D:144:LYS:HB3	3:D:196:THR:OG1	2.06	0.55
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PRO:O	1:B:330:GLN:NE2	2.40	0.54
1:B:373:PRO:HG2	1:B:379:GLY:HA3	1.90	0.54
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.90	0.54
1:B:488:GLU:OE2	1:B:517:THR:OG1	2.20	0.54
1:A:240:GLN:HB3	1:A:262:PRO:HA	1.90	0.53
3:D:36:GLN:HB2	3:D:46:LEU:HD11	1.89	0.53
2:C:171:VAL:HG22	2:C:190:VAL:HG22	1.90	0.53
1:B:294:LYS:HE2	1:B:297:ALA:HA	1.90	0.53
3:D:200:THR:CG2	3:D:201:SER:N	2.74	0.50
1:B:454:VAL:HG11	1:B:537:PHE:CG	2.46	0.50
3:D:145:VAL:HG12	3:D:195:VAL:HG12	1.92	0.50
3:L:122:GLU:HA	3:L:125:LYS:HZ3	1.77	0.50
1:B:510:LEU:HB2	1:B:539:ILE:HD11	1.94	0.50
1:B:239:PRO:HD3	1:B:282:TYR:CZ	2.46	0.49
3:D:200:THR:CG2	3:D:201:SER:H	2.25	0.48
2:C:207:ASN:HD21	2:C:209:LYS:HE2	1.78	0.48
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.96	0.48
2:H:171:VAL:HG22	2:H:190:VAL:HG22	1.95	0.47
3:L:21:THR:HG22	3:L:71:THR:HG22	1.95	0.47
1:A:510:LEU:HB2	1:A:539:ILE:HD11	1.97	0.46
2:C:113:ARG:HH22	3:D:41:LYS:NZ	2.13	0.46
2:C:9:GLY:HA3	2:C:115:THR:OG1	2.16	0.46
1:B:351:THR:O	1:B:403:ARG:HD3	2.17	0.45
1:B:361:ARG:NH1	1:B:431:SER:OG	2.51	0.44
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.98	0.44
2:H:83:MET:HB3	2:H:86:LEU:HD21	2.00	0.43
1:A:486:ARG:NH1	1:A:488:GLU:OE1	2.52	0.43
1:A:239:PRO:HD3	1:A:282:TYR:CE1	2.53	0.43
3:D:124:LEU:O	3:D:182:LYS:HD2	2.19	0.43
1:A:241:VAL:HG22	1:A:330:GLN:NE2	2.34	0.42
2:C:16:ARG:HA	2:C:16:ARG:HD3	1.84	0.42
3:D:112:PRO:HB3	3:D:138:PHE:HB3	2.01	0.42
1:A:352:ASN:ND2	4:A:602:NAG:O7	2.51	0.42
2:H:12:VAL:HG11	2:H:86:LEU:HD13	2.02	0.42
2:H:218:ARG:HD2	2:H:220:GLU:OE2	2.20	0.41
1:A:241:VAL:HG22	1:A:330:GLN:HE22	1.86	0.41
3:D:119:PRO:HG3	3:D:129:ALA:HB1	2.02	0.41
1:B:239:PRO:HD3	1:B:282:TYR:CE2	2.55	0.41
2:C:30:THR:HG22	2:C:74:ASN:HB3	2.01	0.41
1:A:256:LEU:O	1:A:306:MET:HB3	2.21	0.41
3:D:174:LEU:HD22	3:D:175:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:O	1:B:329:ASN:OD1	2.39	0.40
1:A:403:ARG:HH22	3:D:170:SER:HG	1.67	0.40
2:H:205:ASN:HB3	2:H:214:LYS:HE3	2.03	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	267/313 (85%)	260 (97%)	7 (3%)	0	100	100
1	B	272/313 (87%)	263 (97%)	9 (3%)	0	100	100
2	C	213/231 (92%)	208 (98%)	5 (2%)	0	100	100
2	H	220/231 (95%)	215 (98%)	5 (2%)	0	100	100
3	D	204/212 (96%)	196 (96%)	8 (4%)	0	100	100
3	L	209/212 (99%)	203 (97%)	6 (3%)	0	100	100
All	All	1385/1512 (92%)	1345 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	234/264 (89%)	234 (100%)	0	100 100
1	B	235/264 (89%)	235 (100%)	0	100 100
2	C	180/194 (93%)	179 (99%)	1 (1%)	86 92
2	H	184/194 (95%)	182 (99%)	2 (1%)	73 83
3	D	183/185 (99%)	180 (98%)	3 (2%)	62 76
3	L	184/185 (100%)	184 (100%)	0	100 100
All	All	1200/1286 (93%)	1194 (100%)	6 (0%)	88 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	53	TYR
3	D	6	SER
3	D	32	LEU
3	D	161	SER
2	H	53	TYR
2	H	169	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	172	HIS
2	C	205	ASN
2	C	207	ASN
3	D	146	GLN
3	D	197	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	NAG	A	603	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	601	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	A	604	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	A	602	1	14,14,15	0.40	0	17,19,21	0.53	0
4	NAG	A	601	1	14,14,15	0.33	0	17,19,21	0.46	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	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	NAG	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	275/313 (87%)	0.39	6 (2%) 62 70	60, 83, 137, 189	0
1	B	280/313 (89%)	0.92	48 (17%) 1 1	77, 126, 221, 247	0
2	C	217/231 (93%)	0.81	36 (16%) 1 1	92, 141, 203, 249	0
2	H	222/231 (96%)	0.52	0 100 100	42, 64, 88, 101	0
3	D	208/212 (98%)	0.75	32 (15%) 2 3	77, 116, 197, 215	0
3	L	211/212 (99%)	0.40	0 100 100	39, 66, 87, 108	0
All	All	1413/1512 (93%)	0.63	122 (8%) 10 14	39, 91, 189, 249	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	VAL	9.3
1	B	327	GLY	7.9
2	C	199	THR	7.5
1	A	380	LEU	6.8
1	B	262	PRO	6.3
3	D	120	SER	6.2
3	D	190	VAL	6.0
2	C	202	TYR	6.0
1	B	537	PHE	5.6
1	A	262	PRO	5.5
2	C	167	LEU	5.4
2	C	198	GLY	5.3
1	A	239	PRO	5.2
1	B	462	VAL	5.1
2	C	191	THR	4.8
1	B	530	VAL	4.7
2	C	219	VAL	4.7
3	D	209	GLY	4.6
1	B	326	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	459	LEU	4.5
2	C	195	SER	4.5
3	D	149	VAL	4.4
3	D	191	TYR	4.3
3	D	189	LYS	4.3
1	B	463	SER	4.3
2	C	220	GLU	4.2
2	C	146	LEU	4.2
3	D	125	LYS	4.1
3	D	116	ILE	4.1
1	B	325	GLY	4.0
1	B	505	VAL	4.0
1	B	496	HIS	3.9
2	C	221	PRO	3.9
3	D	206	PHE	3.9
3	D	148	LYS	3.8
3	D	203	THR	3.8
1	B	261	GLN	3.7
3	D	180	LEU	3.7
1	B	510	LEU	3.7
3	D	151	ASN	3.6
1	A	322	ASN	3.6
3	D	146	GLN	3.6
3	D	118	PRO	3.5
3	D	117	PHE	3.5
1	B	239	PRO	3.5
2	C	149	LEU	3.4
2	C	197	LEU	3.4
3	D	150	ASP	3.4
1	B	351	THR	3.4
1	B	461	SER	3.3
1	B	482	VAL	3.3
2	C	135	SER	3.3
1	B	322	ASN	3.2
2	C	133	ALA	3.2
3	D	124	LEU	3.2
2	C	132	LEU	3.2
2	C	218	ARG	3.2
2	C	189	VAL	3.1
1	B	486	ARG	3.1
2	C	160	VAL	3.1
3	D	193	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	121	ASP	3.0
1	B	363	GLN	3.0
1	B	347	ILE	3.0
3	D	126	SER	3.0
3	D	129	ALA	3.0
2	C	159	THR	2.9
1	B	539	ILE	2.9
1	B	506	THR	2.9
2	C	129	VAL	2.9
1	B	464	VAL	2.9
1	A	489	ASP	2.9
1	A	238	GLN	2.8
1	B	512	ALA	2.8
3	D	147	TRP	2.8
3	D	153	LEU	2.8
1	B	240	GLN	2.7
1	B	457	HIS	2.7
1	B	499	GLN	2.7
1	B	504	GLN	2.7
1	B	533	GLN	2.7
1	B	349	VAL	2.7
3	D	152	ALA	2.7
3	D	192	ALA	2.6
3	D	114	VAL	2.6
3	D	131	VAL	2.5
1	B	511	ARG	2.4
2	C	162	TRP	2.4
1	B	328	LEU	2.4
1	B	507	LEU	2.4
2	C	164	SER	2.4
2	C	104	ILE	2.3
1	B	492	GLN	2.3
2	C	196	SER	2.3
3	D	205	SER	2.3
1	B	449	PRO	2.2
1	B	343	VAL	2.2
3	D	194	GLU	2.2
2	C	193	PRO	2.2
2	C	142	GLY	2.2
1	B	503	THR	2.2
1	B	460	ASP	2.2
1	B	360	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	166	ALA	2.2
2	C	192	VAL	2.2
1	B	479	LYS	2.1
1	B	466	TRP	2.1
3	D	23	ARG	2.1
1	B	500	PRO	2.1
1	B	404	GLU	2.1
2	C	86	LEU	2.1
2	C	187	SER	2.0
2	C	130	PHE	2.0
2	C	141	GLY	2.0
3	D	202	VAL	2.0
1	B	458	SER	2.0
1	B	538	SER	2.0
2	C	120	SER	2.0
1	B	513	GLY	2.0
2	C	122	ALA	2.0
2	C	9	GLY	2.0
2	C	186	LEU	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
4	NAG	A	601	14/15	0.92	0.13	88,94,107,108	0
4	NAG	A	603	14/15	0.92	0.12	101,106,114,118	0
4	NAG	B	601	14/15	0.92	0.17	115,135,138,142	0
5	CL	A	605	1/1	0.92	0.26	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	H	301	1/1	0.94	0.16	92,92,92,92	0
4	NAG	A	604	14/15	0.95	0.18	86,97,104,107	0
4	NAG	A	602	14/15	0.95	0.18	70,85,101,103	0

6.5 Other polymers (i)

There are no such residues in this entry.