Full wwPDB X-ray Structure Validation Report (i)

Apr 9, 2024 – 12:35 PM EDT

PDB ID	:	9B7B
Title	:	Crystal structure of humanized 44H10 Fab Version 22 in complex with HLA-DR (HLA-DRA*01:01/HLA-DRB1*04:01)
Deposited on	:	2024-03-27
Resolution	:	3.08 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

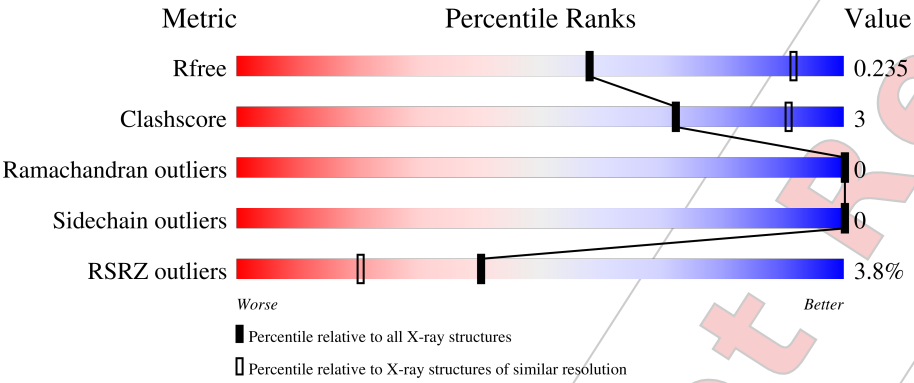
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	190	88% 8% .
1	E	190	% 89% 7% .
2	B	226	5% 80% 8% 12%
2	F	226	8% 77% 10% 13%

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Mol	Chain	Length	Quality of chain
3	C	223	3% 91% 9%
3	G	223	4% 92% 7%
4	D	214	89% 10%
4	H	214	8% 86% 13%

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
5	NAG	B	301	-	-	-	X
6	SO4	H	301	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12878 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1506	973	245	283	5			
1	E	184	Total	C	N	O	S	0	0	0
			1506	973	245	283	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP P01903
A	183	SER	-	expression tag	UNP P01903
A	184	GLY	-	expression tag	UNP P01903
A	185	GLU	-	expression tag	UNP P01903
A	186	ASN	-	expression tag	UNP P01903
A	187	LEU	-	expression tag	UNP P01903
A	188	TYR	-	expression tag	UNP P01903
A	189	PHE	-	expression tag	UNP P01903
A	190	GLN	-	expression tag	UNP P01903
E	182	THR	-	expression tag	UNP P01903
E	183	SER	-	expression tag	UNP P01903
E	184	GLY	-	expression tag	UNP P01903
E	185	GLU	-	expression tag	UNP P01903
E	186	ASN	-	expression tag	UNP P01903
E	187	LEU	-	expression tag	UNP P01903
E	188	TYR	-	expression tag	UNP P01903
E	189	PHE	-	expression tag	UNP P01903
E	190	GLN	-	expression tag	UNP P01903

- Molecule 2 is a protein called Hemagglutinin HA1 chain, HLA class II histocompatibility antigen DR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	198	Total	C	N	O	S	0	0	0
			1629	1032	286	306	5			
2	F	196	Total	C	N	O	S	0	0	0
			1612	1022	282	303	5			

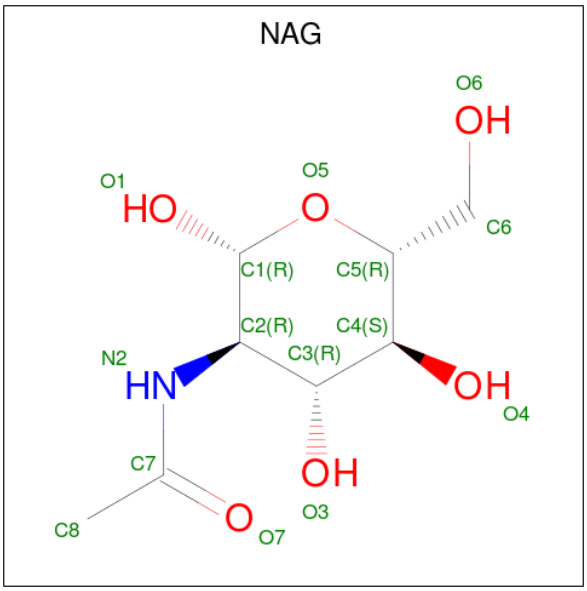
- Molecule 3 is a protein called h44H10-V22 Antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1655	1048	273	327	7			
3	G	221	Total	C	N	O	S	0	0	0
			1642	1042	271	323	6			

- Molecule 4 is a protein called h44H10-V22 Antibody, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	211	Total	C	N	O	S	0	0	0
			1631	1025	272	329	5			
4	H	211	Total	C	N	O	S	0	0	0
			1631	1025	272	329	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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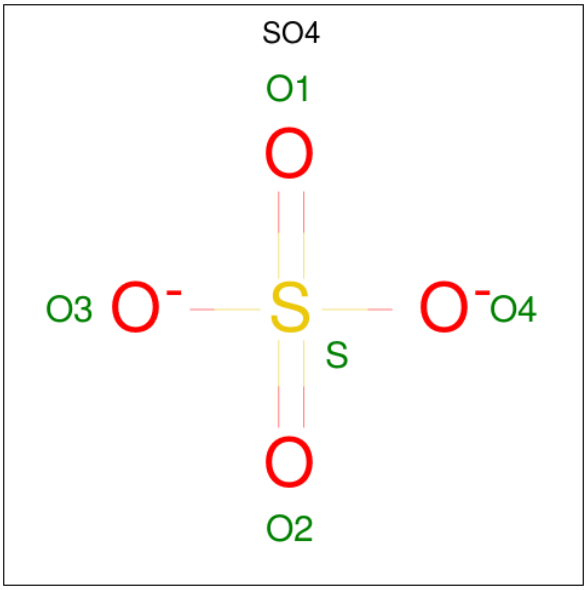
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	E	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



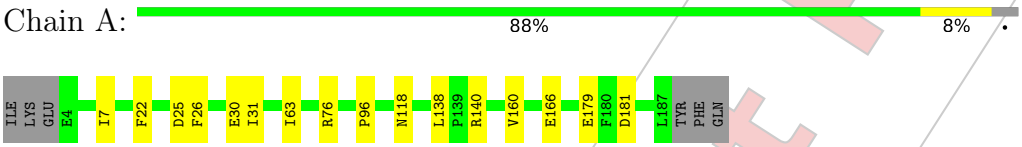
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0

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.

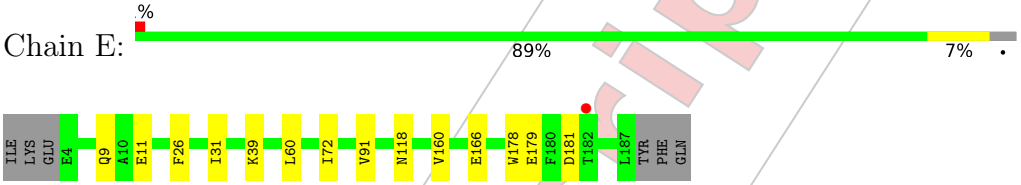
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



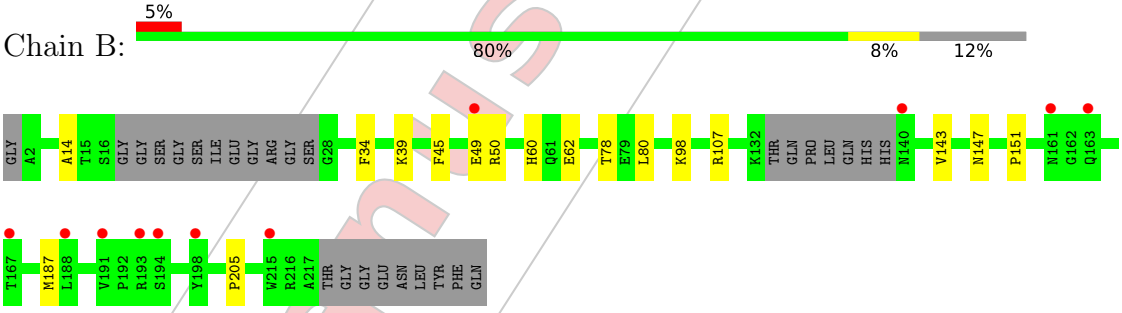
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain E:



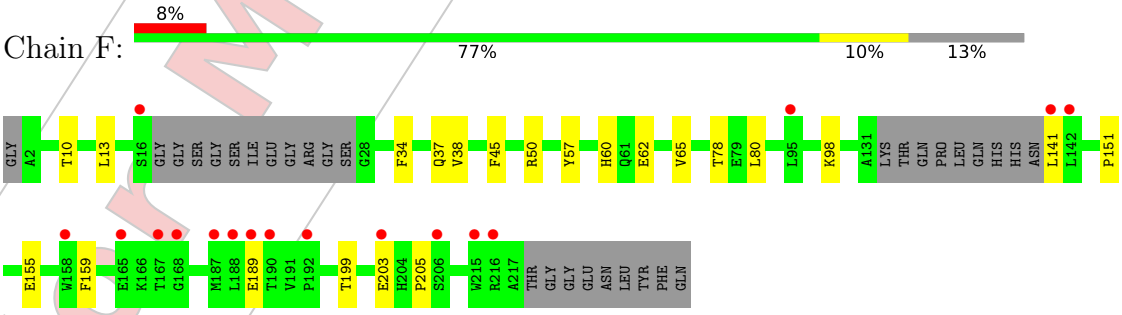
• Molecule 2: Hemagglutinin HA1 chain, HLA class II histocompatibility antigen DR beta chain

Chain B:



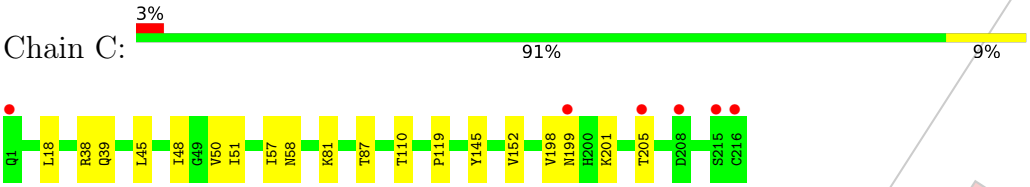
• Molecule 2: Hemagglutinin HA1 chain, HLA class II histocompatibility antigen DR beta chain

Chain F:



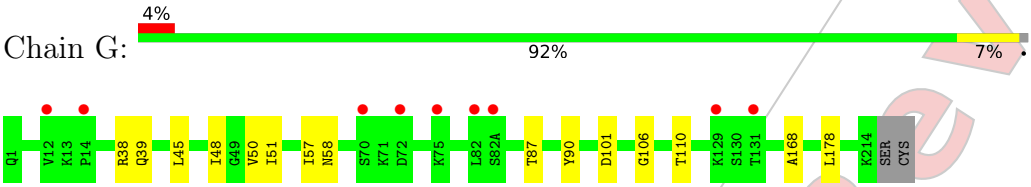
• Molecule 3: h44H10-V22 Antibody, heavy chain

Chain C:



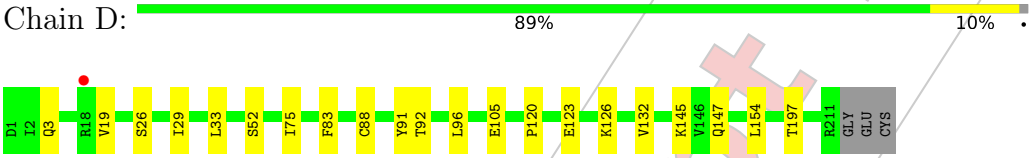
• Molecule 3: h44H10-V22 Antibody, heavy chain

Chain G:



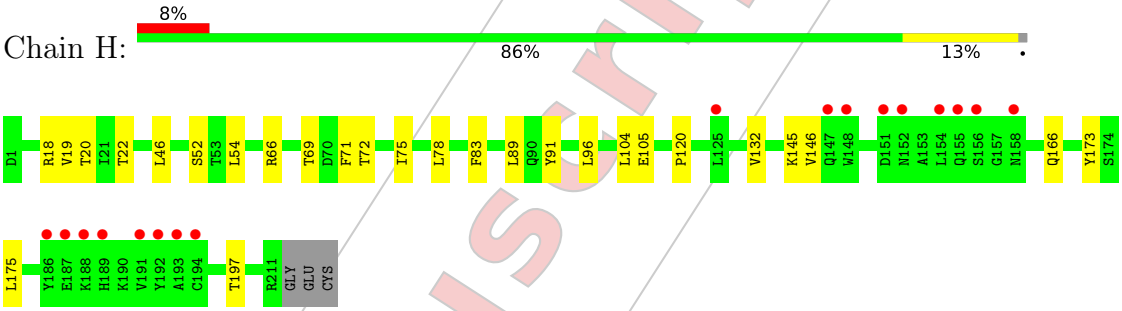
• Molecule 4: h44H10-V22 Antibody, light chain

Chain D:



• Molecule 4: h44H10-V22 Antibody, light chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.59Å 178.80Å 178.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 3.08 47.56 – 3.08	Depositor EDS
% Data completeness (in resolution range)	58.8 (47.56-3.08) 54.6 (47.56-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.237 0.201 , 0.235	Depositor DCC
R_{free} test set	1496 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.031 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12878	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: NAG, SO4

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	0.29	0/1551	0.58	0/2115
1	E	0.29	0/1551	0.59	0/2115
2	B	0.27	0/1670	0.58	0/2265
2	F	0.30	0/1653	0.62	0/2243
3	C	0.27	0/1696	0.55	0/2316
3	G	0.27	0/1683	0.55	0/2300
4	D	0.28	0/1665	0.59	0/2261
4	H	0.28	0/1665	0.59	0/2261
All	All	0.28	0/13134	0.58	0/17876

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 (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	1506	0	1438	11	0
1	E	1506	0	1438	8	0
2	B	1629	0	1552	12	0
2	F	1612	0	1533	14	0
3	C	1655	0	1638	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1642	0	1628	9	0
4	D	1631	0	1606	12	0
4	H	1631	0	1606	18	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	D	5	0	0	1	0
6	H	5	0	0	2	0
All	All	12878	0	12491	86	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 (86) 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:160:VAL:HG12	1:A:179:GLU:HB3	1.82	0.62
2:F:34:PHE:HA	2:F:60:HIS:HE1	1.64	0.61
1:A:118:ASN:HB2	1:A:166:GLU:HB3	1.82	0.61
4:D:145:LYS:HB3	4:D:197:THR:HB	1.86	0.58
4:H:120:PRO:HD3	4:H:132:VAL:HG22	1.85	0.58
3:C:38:ARG:HB3	3:C:48:ILE:HD11	1.85	0.57
1:E:9:GLN:NE2	1:E:11:GLU:OE2	2.40	0.55
1:A:76:ARG:NH2	2:B:80:LEU:O	2.37	0.55
4:H:145:LYS:HB3	4:H:197:THR:HB	1.89	0.55
1:E:181:ASP:N	1:E:181:ASP:OD1	2.40	0.54
3:G:101:ASP:HA	4:H:46:LEU:HD22	1.89	0.54
2:F:141:LEU:HD22	2:F:189:GLU:HA	1.89	0.54
2:F:62:GLU:HB2	4:H:52:SER:HB2	1.90	0.54
2:F:45:PHE:HB2	2:F:50:ARG:HB2	1.90	0.53
3:G:168:ALA:HA	3:G:178:LEU:HB3	1.92	0.52
1:A:181:ASP:N	1:A:181:ASP:OD1	2.42	0.51
1:E:39:LYS:HG2	1:E:60:LEU:HD11	1.93	0.51
3:G:38:ARG:HB3	3:G:48:ILE:HD11	1.93	0.51
4:D:91:TYR:HA	4:D:96:LEU:HD22	1.93	0.51
1:E:118:ASN:HB2	1:E:166:GLU:HB3	1.94	0.50
4:D:120:PRO:HD3	4:D:132:VAL:HG22	1.93	0.50
4:H:83:PHE:HD1	4:H:105:GLU:HA	1.77	0.50
2:F:78:THR:HG23	2:F:80:LEU:H	1.76	0.49
4:H:22:THR:HA	4:H:71:PHE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:ILE:N	6:D:301:SO4:O4	2.46	0.49
1:E:72:ILE:HD12	2:F:13:LEU:HB3	1.95	0.49
4:H:91:TYR:HA	4:H:96:LEU:HD22	1.94	0.49
2:F:151:PRO:HD2	2:F:205:PRO:HG2	1.94	0.48
4:H:89:LEU:HD11	4:H:96:LEU:HB3	1.96	0.48
3:C:199:ASN:OD1	3:C:201:LYS:NZ	2.36	0.48
3:C:39:GLN:HB2	3:C:45:LEU:HD23	1.96	0.48
2:B:151:PRO:HD2	2:B:205:PRO:HG2	1.95	0.48
1:E:160:VAL:HG12	1:E:179:GLU:HB3	1.96	0.48
2:F:37:GLN:NE2	2:F:60:HIS:O	2.44	0.47
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.97	0.47
2:B:45:PHE:HB2	2:B:50:ARG:HB2	1.97	0.47
3:C:51:ILE:HD13	3:C:57:ILE:HG12	1.96	0.46
4:D:83:PHE:HD1	4:D:105:GLU:HA	1.80	0.46
2:B:78:THR:HG23	2:B:80:LEU:H	1.81	0.46
1:E:26:PHE:HB2	1:E:31:ILE:HD11	1.97	0.46
2:B:49:GLU:O	2:B:107:ARG:NH2	2.49	0.45
3:C:119:PRO:HB3	3:C:145:TYR:HB3	1.98	0.45
4:H:66:ARG:NH1	6:H:301:SO4:O4	2.48	0.45
1:A:7:ILE:HA	1:A:25:ASP:O	2.16	0.45
3:C:87:THR:HG23	3:C:110:THR:HA	1.98	0.45
4:D:19:VAL:HG22	4:D:75:ILE:HB	1.98	0.45
2:F:34:PHE:HA	2:F:60:HIS:CE1	2.49	0.45
2:F:155:GLU:HB3	2:F:203:GLU:HB2	1.99	0.45
4:H:66:ARG:HH21	4:H:69:THR:HA	1.82	0.45
3:G:39:GLN:HB2	3:G:45:LEU:HD23	1.97	0.45
4:H:19:VAL:HG22	4:H:75:ILE:HB	1.98	0.45
3:G:87:THR:HG23	3:G:110:THR:HA	1.99	0.44
4:D:147:GLN:HB3	4:D:154:LEU:HD11	1.99	0.44
3:C:119:PRO:HD2	3:C:205:THR:HG21	1.99	0.44
1:A:22:PHE:HB2	1:A:63:ILE:HD11	1.99	0.43
2:F:159:PHE:HB2	2:F:199:THR:HB	2.01	0.43
3:G:51:ILE:HD13	3:G:57:ILE:HG12	1.99	0.43
4:H:66:ARG:NH1	6:H:301:SO4:S	2.92	0.43
2:B:98:LYS:HA	2:B:98:LYS:HD3	1.84	0.43
3:G:168:ALA:HB2	3:G:178:LEU:HD23	2.00	0.43
4:H:166:GLN:HG3	4:H:173:TYR:CZ	2.54	0.43
4:H:146:VAL:HG21	4:H:175:LEU:HD22	2.01	0.43
4:D:3:GLN:HB2	4:D:26:SER:HB3	2.01	0.42
3:C:50:VAL:HG22	3:C:58:ASN:HB2	2.01	0.42
4:D:123:GLU:HA	4:D:126:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:78:LEU:HD11	4:H:104:LEU:HD21	2.01	0.42
3:C:152:VAL:HG22	3:C:198:VAL:HG22	2.02	0.42
3:G:50:VAL:HG22	3:G:58:ASN:HB2	2.01	0.42
4:H:54:LEU:HD23	4:H:54:LEU:HA	1.90	0.42
2:F:57:TYR:HB2	2:F:65:VAL:HG12	2.01	0.42
1:A:96:PRO:HD3	2:B:147:ASN:ND2	2.35	0.41
1:A:140:ARG:O	2:B:39:LYS:NZ	2.53	0.41
2:B:62:GLU:HB2	4:D:52:SER:HB2	2.01	0.41
2:F:10:THR:HG23	2:F:38:VAL:HG11	2.02	0.41
3:G:90:TYR:O	3:G:106:GLY:HA2	2.20	0.41
1:A:76:ARG:NH1	2:B:14:ALA:O	2.54	0.41
2:B:34:PHE:HA	2:B:60:HIS:HE1	1.85	0.41
4:D:33:LEU:HD21	4:D:88:CYS:HB2	2.02	0.41
4:H:18:ARG:HA	4:H:75:ILE:O	2.20	0.41
4:H:20:THR:HG23	4:H:72:THR:HG23	2.02	0.41
3:C:18:LEU:O	3:C:81:LYS:HA	2.19	0.41
1:E:91:VAL:HG11	1:E:178:TRP:HB2	2.03	0.41
2:F:98:LYS:HA	2:F:98:LYS:HD3	1.91	0.41
2:B:143:VAL:HG22	2:B:187:MET:HG2	2.03	0.40
4:D:29:ILE:HA	4:D:92:THR:HG21	2.03	0.40
1:A:30:GLU:HB2	1:A:138:LEU:HD11	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	182/190 (96%)	177 (97%)	5 (3%)	0	100	100
1	E	182/190 (96%)	178 (98%)	4 (2%)	0	100	100
2	B	192/226 (85%)	187 (97%)	5 (3%)	0	100	100
2	F	190/226 (84%)	186 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
3	G	219/223 (98%)	214 (98%)	5 (2%)	0	100	100
4	D	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
4	H	209/214 (98%)	203 (97%)	6 (3%)	0	100	100
All	All	1604/1706 (94%)	1563 (97%)	41 (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	168/174 (97%)	168 (100%)	0	100	100
1	E	168/174 (97%)	168 (100%)	0	100	100
2	B	177/197 (90%)	177 (100%)	0	100	100
2	F	175/197 (89%)	175 (100%)	0	100	100
3	C	189/189 (100%)	189 (100%)	0	100	100
3	G	187/189 (99%)	187 (100%)	0	100	100
4	D	187/189 (99%)	187 (100%)	0	100	100
4	H	187/189 (99%)	187 (100%)	0	100	100
All	All	1438/1498 (96%)	1438 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

6 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	$\#\|Z\|>2$
6	SO4	D	301	-	4,4,4	0.16	0	6,6,6	0.08	0
6	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	NAG	F	301	2	14,14,15	0.40	0	17,19,21	0.50	0
5	NAG	B	301	2	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
5	NAG	E	201	1	14,14,15	0.45	0	17,19,21	0.47	0
5	NAG	A	201	1	14,14,15	0.47	0	17,19,21	0.55	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	NAG	B	301	2	-	2/6/23/26	0/1/1/1
5	NAG	F	301	2	-	0/6/23/26	0/1/1/1
5	NAG	E	201	1	-	0/6/23/26	0/1/1/1
5	NAG	A	201	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301	NAG	C2-N2-C7	3.05	127.24	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	201	NAG	C8-C7-N2-C2
5	A	201	NAG	O7-C7-N2-C2
5	B	301	NAG	O5-C5-C6-O6
5	B	301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	301	SO4	1	0
6	H	301	SO4	2	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

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	184/190 (96%)	-0.06	0 100 100	37, 66, 97, 124	0
1	E	184/190 (96%)	-0.02	1 (0%) 91 80	43, 63, 100, 123	0
2	B	198/226 (87%)	0.33	11 (5%) 24 11	44, 75, 129, 162	0
2	F	196/226 (86%)	0.54	17 (8%) 10 3	48, 79, 132, 168	0
3	C	223/223 (100%)	0.36	6 (2%) 54 29	45, 75, 101, 142	0
3	G	221/223 (99%)	0.28	9 (4%) 37 18	46, 80, 116, 140	0
4	D	211/214 (98%)	-0.03	1 (0%) 91 80	40, 65, 93, 113	0
4	H	211/214 (98%)	0.45	17 (8%) 12 4	47, 83, 130, 160	0
All	All	1628/1706 (95%)	0.24	62 (3%) 40 20	37, 73, 118, 168	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	GLY	5.1
2	F	192	PRO	4.9
3	C	215	SER	4.3
2	B	163	GLN	4.0
2	F	190	THR	3.8
2	B	188	LEU	3.8
3	C	1	GLN	3.7
3	C	216	CYS	3.6
2	B	161	ASN	3.6
4	H	152	ASN	3.4
4	H	192	TYR	3.4
4	H	188	LYS	3.3
4	H	154	LEU	3.3
2	B	167	THR	3.2
2	B	194	SER	3.0
2	F	167	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	140	ASN	2.9
2	F	16	SER	2.8
2	B	215	TRP	2.8
2	F	189	GLU	2.8
4	H	191	VAL	2.8
2	F	216	ARG	2.7
4	H	194	CYS	2.7
4	H	156	SER	2.7
3	G	82(A)	SER	2.7
2	F	215	TRP	2.6
3	C	199	ASN	2.6
3	C	208	ASP	2.6
4	H	193	ALA	2.5
2	B	193	ARG	2.5
2	F	188	LEU	2.5
4	H	186	TYR	2.5
2	F	142	LEU	2.4
2	F	141	LEU	2.4
4	H	151	ASP	2.4
2	F	187	MET	2.4
2	B	49	GLU	2.3
1	E	182	THR	2.3
3	C	205	THR	2.3
4	H	158	ASN	2.3
4	H	147	GLN	2.3
2	F	206	SER	2.3
3	G	70	SER	2.3
3	G	131	THR	2.3
4	H	187	GLU	2.2
3	G	129	LYS	2.2
2	B	191	VAL	2.2
4	D	18	ARG	2.2
3	G	12	VAL	2.2
4	H	155	GLN	2.1
4	H	125	LEU	2.1
4	H	189	HIS	2.1
3	G	72	ASP	2.1
3	G	82	LEU	2.1
3	G	75	LYS	2.1
2	F	203	GLU	2.1
2	F	95	LEU	2.1
3	G	14	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	148	TRP	2.0
2	F	158	TRP	2.0
2	B	198	TYR	2.0
2	F	165	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	NAG	B	301	14/15	0.74	0.47	128,146,154,158	0
5	NAG	F	301	14/15	0.80	0.48	86,142,163,168	0
5	NAG	E	201	14/15	0.91	0.23	67,81,102,116	0
5	NAG	A	201	14/15	0.94	0.23	53,85,101,106	0
6	SO4	H	301	5/5	0.95	0.26	81,99,142,283	0
6	SO4	D	301	5/5	0.98	0.15	62,70,78,95	0

6.5 Other polymers (i)

There are no such residues in this entry.