



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2017 – 03:18 PM EDT

PDB ID : 4Z7V
Title : L3-12 complex
Authors : Petersen, J.; Rossjohn, J.; Reid, H.H.; Koning, F.
Deposited on : unknown
Resolution : 2.65 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

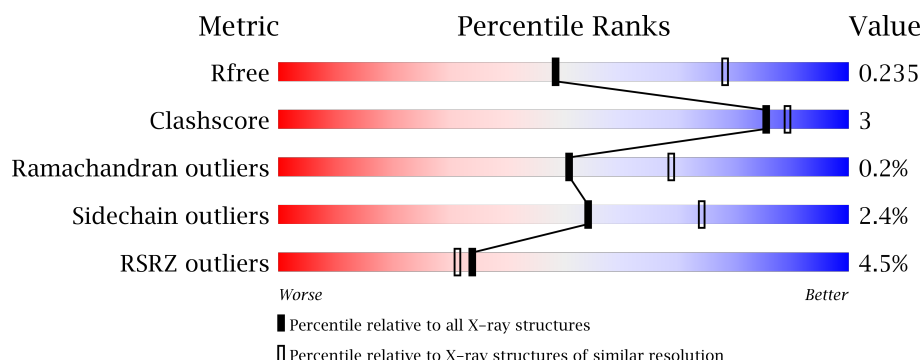
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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 $\leq 5\%$. 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	192	<div> <div>5%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	C	192	<div> <div>7%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	B	213	<div> <div>14%</div> <div>72%</div> <div>8%</div> <div>19%</div> </div>
2	D	213	<div> <div>8%</div> <div>69%</div> <div>12%</div> <div>18%</div> </div>
3	E	204	<div> <div>0%</div> <div>88%</div> <div>9%</div> <div>0%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	204	 <div> <div></div> <div>0%</div> <div>100%</div> </div> 93% 5% 2%
4	F	244	 <div> <div></div> <div>0%</div> <div>100%</div> </div> 95% 5%
4	H	244	 <div> <div></div> <div>0%</div> <div>100%</div> </div> 94% 5% 1%
5	I	18	 <div> <div></div> <div>0%</div> <div>100%</div> </div> 72% 28%
5	J	18	 <div> <div></div> <div>0%</div> <div>100%</div> </div> 67% 6% 28%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13077 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1418	912	236	268	2			
1	C	180	Total	C	N	O	S	0	0	0
			1408	906	232	268	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP Q30069
A	183	SER	-	expression tag	UNP Q30069
A	184	GLY	-	expression tag	UNP Q30069
A	185	ASP	-	expression tag	UNP Q30069
A	186	ASP	-	expression tag	UNP Q30069
A	187	ASP	-	expression tag	UNP Q30069
A	188	ASP	-	expression tag	UNP Q30069
A	189	LYS	-	expression tag	UNP Q30069
C	182	THR	-	expression tag	UNP Q30069
C	183	SER	-	expression tag	UNP Q30069
C	184	GLY	-	expression tag	UNP Q30069
C	185	ASP	-	expression tag	UNP Q30069
C	186	ASP	-	expression tag	UNP Q30069
C	187	ASP	-	expression tag	UNP Q30069
C	188	ASP	-	expression tag	UNP Q30069
C	189	LYS	-	expression tag	UNP Q30069

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1338	857	225	249	7			
2	D	175	Total	C	N	O	S	0	0	0
			1361	870	231	253	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP O19707
B	-11	GLY	-	expression tag	UNP O19707
B	-10	SER	-	expression tag	UNP O19707
B	-9	ILE	-	expression tag	UNP O19707
B	-8	GLU	-	expression tag	UNP O19707
B	-7	GLY	-	expression tag	UNP O19707
B	-6	ARG	-	expression tag	UNP O19707
B	-5	GLY	-	expression tag	UNP O19707
B	-4	GLY	-	expression tag	UNP O19707
B	-3	SER	-	expression tag	UNP O19707
B	-2	GLY	-	expression tag	UNP O19707
B	-1	ALA	-	expression tag	UNP O19707
B	0	SER	-	expression tag	UNP O19707
B	193	THR	-	expression tag	UNP O19707
B	194	GLY	-	expression tag	UNP O19707
B	195	GLY	-	expression tag	UNP O19707
B	196	ASP	-	expression tag	UNP O19707
B	197	ASP	-	expression tag	UNP O19707
B	198	ASP	-	expression tag	UNP O19707
B	199	ASP	-	expression tag	UNP O19707
B	200	LYS	-	expression tag	UNP O19707
D	-12	GLY	-	expression tag	UNP O19707
D	-11	GLY	-	expression tag	UNP O19707
D	-10	SER	-	expression tag	UNP O19707
D	-9	ILE	-	expression tag	UNP O19707
D	-8	GLU	-	expression tag	UNP O19707
D	-7	GLY	-	expression tag	UNP O19707
D	-6	ARG	-	expression tag	UNP O19707
D	-5	GLY	-	expression tag	UNP O19707
D	-4	GLY	-	expression tag	UNP O19707
D	-3	SER	-	expression tag	UNP O19707
D	-2	GLY	-	expression tag	UNP O19707
D	-1	ALA	-	expression tag	UNP O19707
D	0	SER	-	expression tag	UNP O19707
D	193	THR	-	expression tag	UNP O19707
D	194	GLY	-	expression tag	UNP O19707
D	195	GLY	-	expression tag	UNP O19707
D	196	ASP	-	expression tag	UNP O19707
D	197	ASP	-	expression tag	UNP O19707
D	198	ASP	-	expression tag	UNP O19707
D	199	ASP	-	expression tag	UNP O19707
D	200	LYS	-	expression tag	UNP O19707

- Molecule 3 is a protein called T-CELL RECEPTOR, L3-12 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	199	Total	C	N	O	S	0	0	0
			1534	954	268	303	9			
3	G	198	Total	C	N	O	S	0	0	0
			1524	949	266	300	9			

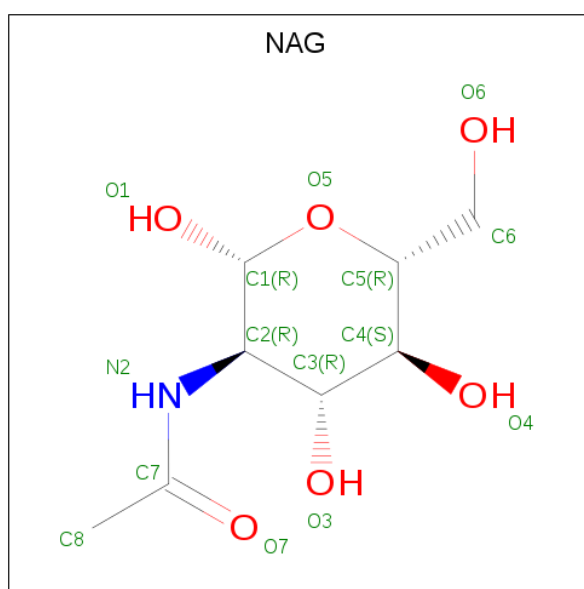
- Molecule 4 is a protein called T-CELL RECEPTOR, L3-12 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	243	Total	C	N	O	S	0	0	0
			1916	1206	332	373	5			
4	H	242	Total	C	N	O	S	0	0	0
			1907	1202	332	368	5			

- Molecule 5 is a protein called deamidated DQ8-glia-alpha1 peptide.

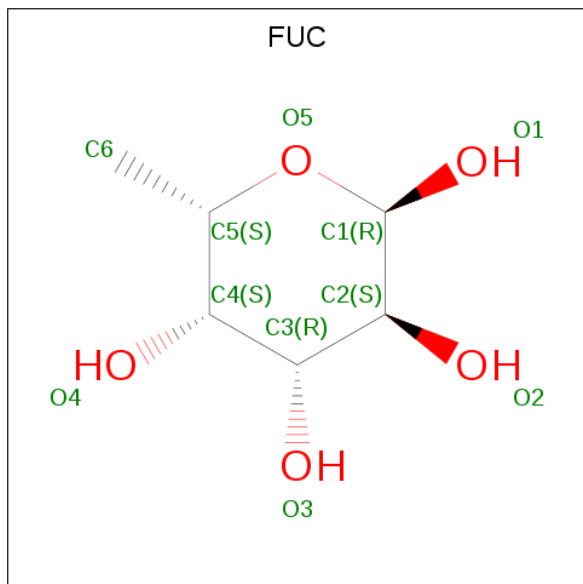
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	13	Total	C	N	O	0	0	0
			95	56	16	23			
5	J	13	Total	C	N	O	0	0	0
			95	56	16	23			

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



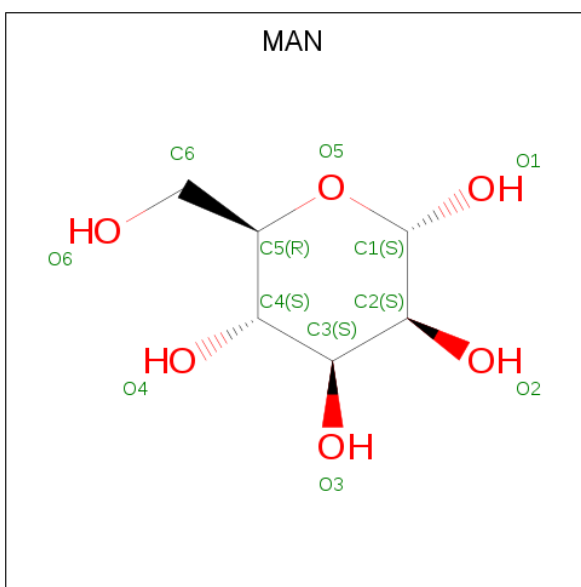
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		

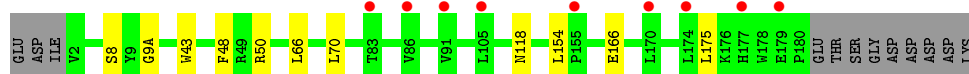
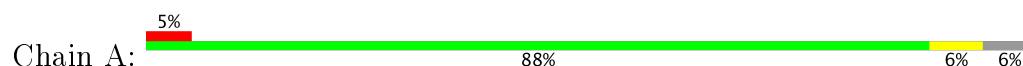
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	12	Total	O	0	0
			12	12		
9	B	7	Total	O	0	0
			7	7		
9	C	17	Total	O	0	0
			17	17		
9	D	10	Total	O	0	0
			10	10		
9	E	63	Total	O	0	0
			63	63		
9	F	79	Total	O	0	0
			79	79		
9	G	59	Total	O	0	0
			59	59		
9	H	84	Total	O	0	0
			84	84		
9	I	2	Total	O	0	0
			2	2		
9	J	2	Total	O	0	0
			2	2		

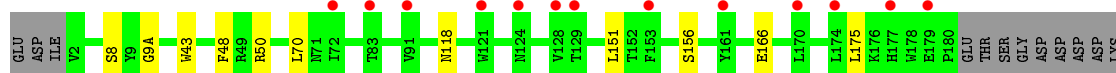
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

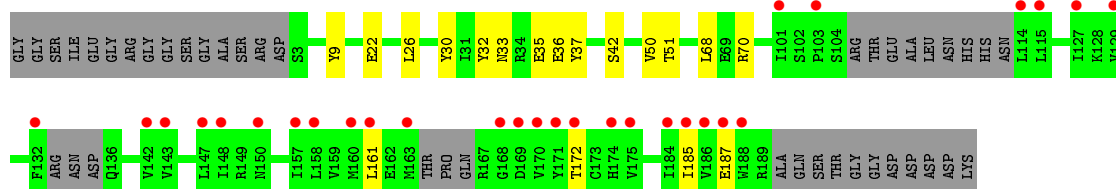
- Molecule 1: MHC class II HLA-DQ-alpha chain



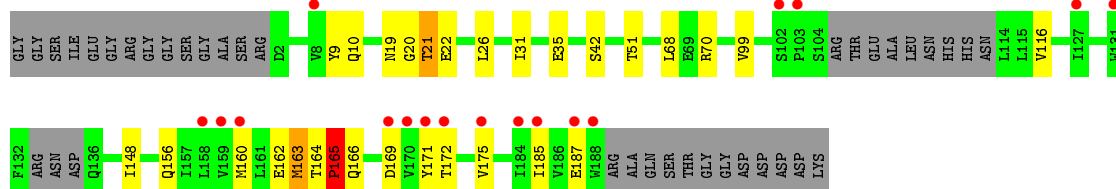
- Molecule 1: MHC class II HLA-DQ-alpha chain



- Molecule 2: MHC class II HLA-DQ-beta-1



- Molecule 2: MHC class II HLA-DQ-beta-1



- Molecule 3: T-CELL RECEPTOR, L3-12 ALPHA CHAIN





- Molecule 3: T-CELL RECEPTOR, L3-12 ALPHA CHAIN



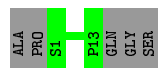
- Molecule 4: T-CELL RECEPTOR, L3-12 BETA CHAIN



- Molecule 4: T-CELL RECEPTOR, L3-12 BETA CHAIN



- Molecule 5: deamidated DQ8-glia-alpha1 peptide



- Molecule 5: deamidated DQ8-glia-alpha1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.51Å 76.96Å 132.28Å 93.87° 89.47° 105.09°	Depositor
Resolution (Å)	74.14 – 2.65 74.14 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (74.14-2.65) 96.1 (74.14-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.187 , 0.226 0.198 , 0.235	Depositor DCC
R_{free} test set	3114 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13077	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FUC, NAG, MAN

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	0.39	0/1462	0.57	0/2002
1	C	0.40	0/1451	0.57	0/1987
2	B	0.45	0/1371	0.58	0/1878
2	D	0.53	1/1396 (0.1%)	0.62	1/1913 (0.1%)
3	E	0.39	0/1567	0.62	0/2134
3	G	0.39	0/1557	0.61	0/2122
4	F	0.39	0/1967	0.61	0/2681
4	H	0.38	0/1958	0.60	0/2669
5	I	0.30	0/97	0.52	0/130
5	J	0.31	0/97	0.55	0/130
All	All	0.41	1/12923 (0.0%)	0.60	1/17646 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	165	PRO	N-CD	5.26	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	164	THR	C-N-CD	5.71	140.39	128.40

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	1418	0	1311	5	0
1	C	1408	0	1297	5	0
2	B	1338	0	1228	13	0
2	D	1361	0	1243	22	0
3	E	1534	0	1434	9	0
3	G	1524	0	1426	4	0
4	F	1916	0	1795	4	0
4	H	1907	0	1787	6	0
5	I	95	0	80	0	0
5	J	95	0	80	1	0
6	A	14	0	13	0	0
6	B	28	0	22	0	0
6	C	14	0	13	0	0
6	D	28	0	23	4	0
7	B	20	0	20	0	0
7	D	20	0	20	8	0
8	B	22	0	19	0	0
9	A	12	0	0	0	0
9	B	7	0	0	0	0
9	C	17	0	0	0	0
9	D	10	0	0	0	0
9	E	63	0	0	1	0
9	F	79	0	0	0	0
9	G	59	0	0	0	0
9	H	84	0	0	0	0
9	I	2	0	0	0	0
9	J	2	0	0	0	0
All	All	13077	0	11811	64	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 (64) 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:B:35:GLU:OE1	2:B:51:THR:HG21	1.43	1.14
2:D:166:GLN:O	2:D:169:ASP:OD1	1.85	0.95
2:D:35:GLU:OE2	2:D:51:THR:OG1	1.89	0.88
6:D:1000:NAG:O4	6:D:1001:NAG:O7	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:ASN:O	7:D:1003:FUC:O4	1.96	0.82
2:D:162:GLU:HB2	2:D:163:MET:HA	1.62	0.80
6:D:1001:NAG:H61	7:D:1002:FUC:H3	1.70	0.74
3:G:178:LEU:HB3	4:H:184:CYS:HB3	1.70	0.72
2:D:35:GLU:OE2	2:D:51:THR:CB	2.40	0.69
2:B:35:GLU:OE1	2:B:51:THR:CG2	2.32	0.67
2:B:36:GLU:O	2:B:50:VAL:HG23	1.97	0.65
2:D:19:ASN:C	7:D:1003:FUC:HO4	1.99	0.62
1:C:70:LEU:HD13	2:D:9:TYR:HB2	1.82	0.62
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.82	0.61
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.82	0.60
6:D:1001:NAG:O5	7:D:1002:FUC:H5	2.01	0.60
2:D:163:MET:HG3	2:D:171:TYR:CZ	2.36	0.60
4:H:55:GLN:OE1	4:H:110:THR:HG22	2.00	0.59
2:D:99:VAL:HG11	2:D:175:VAL:HG21	1.85	0.59
2:B:70:ARG:HD3	4:H:113:GLU:OE1	2.03	0.58
3:E:178:LEU:HB3	4:F:184:CYS:HB2	1.85	0.57
2:D:21:THR:OG1	7:D:1003:FUC:H3	2.04	0.56
2:D:116:VAL:HG12	2:D:160:MET:HG3	1.88	0.56
1:A:70:LEU:HD13	2:B:9:TYR:HB2	1.88	0.55
2:D:162:GLU:HB2	2:D:163:MET:CA	2.35	0.55
2:B:26:LEU:HG	2:B:42:SER:HB3	1.89	0.54
2:D:26:LEU:HG	2:D:42:SER:HB3	1.90	0.54
2:D:20:GLY:HA3	7:D:1003:FUC:O4	2.08	0.53
2:B:35:GLU:O	2:B:35:GLU:HG3	2.08	0.53
6:D:1001:NAG:C6	7:D:1002:FUC:H3	2.36	0.53
3:E:207:ASN:HA	3:E:210:ILE:HD11	1.91	0.52
2:D:165:PRO:O	2:D:165:PRO:HG2	2.09	0.52
2:D:162:GLU:CB	2:D:163:MET:HA	2.31	0.52
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.46	0.51
1:C:43:TRP:CE3	1:C:48:PHE:HB3	2.46	0.51
7:D:1003:FUC:O3	7:D:1003:FUC:H63	2.11	0.50
3:E:94:ALA:HB3	9:E:301:HOH:O	2.12	0.50
2:D:19:ASN:ND2	2:D:22:GLU:OE1	2.45	0.49
2:B:172:THR:HG22	2:B:187:GLU:HG2	1.93	0.49
2:B:32:TYR:O	2:B:33:ASN:HB2	2.13	0.49
2:D:70:ARG:HD3	4:F:113:GLU:OE1	2.12	0.49
2:D:172:THR:HG22	2:D:187:GLU:HG2	1.93	0.48
3:G:109:SER:O	4:H:112:GLY:HA3	2.12	0.48
1:A:8:SER:C	1:A:9(A):GLY:HA2	2.33	0.47
1:C:8:SER:C	1:C:9(A):GLY:HA2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:165:SER:HB2	3:E:172:ILE:HD12	1.97	0.47
2:B:70:ARG:HD2	5:J:7:GLN:NE2	2.29	0.47
2:D:10:GLN:HB2	2:D:31:ILE:HB	1.96	0.46
4:H:40:TYR:HB2	4:H:105:ALA:HB3	1.98	0.45
2:B:37:TYR:HA	2:B:51:THR:HB	1.97	0.45
3:E:206:ASN:HA	3:E:207:ASN:HA	1.61	0.44
3:E:210:ILE:H	3:E:210:ILE:HG13	1.54	0.44
2:D:148:ILE:HB	2:D:156:GLN:HG3	1.99	0.43
1:C:50:ARG:HA	3:G:209:ILE:HD11	2.00	0.43
3:E:40:HIS:CD2	3:E:107:ARG:HB3	2.54	0.42
3:G:165:SER:HB2	3:G:172:ILE:HD12	2.02	0.42
2:D:166:GLN:C	2:D:169:ASP:OD1	2.56	0.41
3:E:39:ILE:O	3:E:55:HIS:HA	2.19	0.41
4:H:136:PRO:HB3	4:H:163:PHE:CD1	2.55	0.41
3:E:128:PRO:HG3	3:E:177:VAL:HG21	2.01	0.41
1:A:66:LEU:HG	2:B:9:TYR:CD1	2.57	0.40
4:F:63:GLY:HA2	4:F:80:GLN:HB3	2.03	0.40
2:B:30:TYR:N	2:B:30:TYR:CD1	2.89	0.40
4:F:25:PRO:HD3	4:F:86:HIS:HA	2.02	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	178/192 (93%)	173 (97%)	5 (3%)	0	100	100
1	C	178/192 (93%)	173 (97%)	5 (3%)	0	100	100
2	B	164/213 (77%)	156 (95%)	8 (5%)	0	100	100
2	D	169/213 (79%)	160 (95%)	9 (5%)	0	100	100
3	E	197/204 (97%)	189 (96%)	5 (2%)	3 (2%)	12	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	194/204 (95%)	185 (95%)	9 (5%)	0	100	100
4	F	241/244 (99%)	234 (97%)	7 (3%)	0	100	100
4	H	240/244 (98%)	234 (98%)	6 (2%)	0	100	100
5	I	11/18 (61%)	11 (100%)	0	0	100	100
5	J	11/18 (61%)	11 (100%)	0	0	100	100
All	All	1583/1742 (91%)	1526 (96%)	54 (3%)	3 (0%)	51	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	64	SER
3	E	145	SER
3	E	209	ILE

5.3.2 Protein sidechains ⓘ

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	154/176 (88%)	151 (98%)	3 (2%)	62	80
1	C	152/176 (86%)	149 (98%)	3 (2%)	60	80
2	B	138/189 (73%)	134 (97%)	4 (3%)	48	68
2	D	139/189 (74%)	134 (96%)	5 (4%)	40	59
3	E	168/185 (91%)	164 (98%)	4 (2%)	54	74
3	G	168/185 (91%)	164 (98%)	4 (2%)	54	74
4	F	205/211 (97%)	200 (98%)	5 (2%)	54	74
4	H	203/211 (96%)	198 (98%)	5 (2%)	53	73
5	I	11/14 (79%)	11 (100%)	0	100	100
5	J	11/14 (79%)	11 (100%)	0	100	100
All	All	1349/1550 (87%)	1316 (98%)	33 (2%)	54	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	154	LEU
1	A	175	LEU
2	B	22	GLU
2	B	68	LEU
2	B	161	LEU
2	B	185	ILE
1	C	151	LEU
1	C	156	SER
1	C	175	LEU
2	D	21	THR
2	D	68	LEU
2	D	163	MET
2	D	165	PRO
2	D	185	ILE
3	E	17	GLU
3	E	159	GLN
3	E	176	CYS
3	E	210	ILE
4	F	13	THR
4	F	66	ARG
4	F	177	LYS
4	F	206	ARG
4	F	232	GLU
3	G	17	GLU
3	G	20	HIS
3	G	212	GLU
3	G	218	SER
4	H	13	THR
4	H	66	ARG
4	H	159	LEU
4	H	184	CYS
4	H	232	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	203	ASN
4	F	55	GLN
3	G	67	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	NAG	A	1000	1	14,14,15	0.27	0	15,19,21	0.87	1 (6%)
6	NAG	B	1000	2,7,6	14,14,15	0.29	0	15,19,21	0.80	1 (6%)
6	NAG	B	1001	8,6	14,14,15	0.31	0	15,19,21	1.06	1 (6%)
7	FUC	B	1002	6	9,10,11	0.39	0	13,14,16	0.95	1 (7%)
7	FUC	B	1003	6	9,10,11	0.49	0	13,14,16	1.39	1 (7%)
8	MAN	B	1004	8,6	11,11,12	0.37	0	13,15,17	1.41	1 (7%)
8	MAN	B	1005	8	11,11,12	0.34	0	13,15,17	1.04	1 (7%)
6	NAG	C	1000	1	14,14,15	0.29	0	15,19,21	0.78	1 (6%)
6	NAG	D	1000	2,7,6	14,14,15	1.15	1 (7%)	15,19,21	1.99	4 (26%)
6	NAG	D	1001	6	14,14,15	0.73	0	15,19,21	1.63	2 (13%)
7	FUC	D	1002	6	9,10,11	0.40	0	13,14,16	0.77	0
7	FUC	D	1003	6	9,10,11	0.39	0	13,14,16	2.45	6 (46%)

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
6	NAG	A	1000	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1000	2,7,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1001	8,6	-	0/6/23/26	0/1/1/1
7	FUC	B	1002	6	-	0/0/17/20	0/1/1/1
7	FUC	B	1003	6	-	0/0/17/20	0/1/1/1
8	MAN	B	1004	8,6	-	0/2/19/22	1/1/1/1
8	MAN	B	1005	8	-	0/2/19/22	1/1/1/1
6	NAG	C	1000	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1000	2,7,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1001	6	-	0/6/23/26	0/1/1/1
7	FUC	D	1002	6	-	0/0/17/20	0/1/1/1
7	FUC	D	1003	6	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1000	NAG	C1-C2	3.44	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1001	NAG	C2-N2-C7	-4.98	115.67	122.94
7	D	1003	FUC	O5-C1-C2	-4.48	103.77	110.79
6	B	1001	NAG	O5-C1-C2	-3.08	107.19	111.47
6	D	1000	NAG	C6-C5-C4	-3.04	105.89	113.00
6	D	1001	NAG	O5-C1-C2	-2.81	107.56	111.47
6	D	1000	NAG	C2-N2-C7	-2.30	119.59	122.94
6	D	1000	NAG	O3-C3-C2	-2.16	104.76	109.39
7	D	1003	FUC	C3-C4-C5	-2.04	106.48	109.68
6	B	1000	NAG	C1-O5-C5	2.23	115.24	112.17
6	C	1000	NAG	C1-O5-C5	2.33	115.37	112.17
7	D	1003	FUC	C2-C3-C4	2.41	115.08	110.88
6	A	1000	NAG	C1-O5-C5	2.68	115.86	112.17
7	B	1002	FUC	C1-O5-C5	2.89	118.79	112.39
7	D	1003	FUC	C1-O5-C5	3.25	119.59	112.39
7	D	1003	FUC	O5-C5-C4	3.27	115.02	109.62
8	B	1005	MAN	C1-O5-C5	3.37	116.81	112.17
7	B	1003	FUC	C1-O5-C5	3.87	120.95	112.39
7	D	1003	FUC	C1-C2-C3	4.41	115.24	109.65
8	B	1004	MAN	C1-O5-C5	4.58	118.47	112.17
6	D	1000	NAG	C1-O5-C5	5.14	119.25	112.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1005	MAN	C1-C2-C3-C4-C5-O5
8	B	1004	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1000	NAG	1	0
6	D	1001	NAG	4	0
7	D	1002	FUC	3	0
7	D	1003	FUC	5	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, 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	180/192 (93%)	0.41	9 (5%) 30 27	36, 79, 113, 127	0
1	C	180/192 (93%)	0.40	13 (7%) 16 14	40, 79, 118, 138	0
2	B	172/213 (80%)	0.76	29 (16%) 2 1	42, 82, 148, 164	0
2	D	175/213 (82%)	0.48	17 (9%) 8 6	41, 76, 148, 176	0
3	E	199/204 (97%)	-0.09	2 (1%) 82 82	26, 44, 85, 100	0
3	G	198/204 (97%)	-0.14	2 (1%) 82 82	28, 44, 80, 99	0
4	F	243/244 (99%)	-0.23	0 100 100	27, 41, 65, 80	0
4	H	242/244 (99%)	-0.20	0 100 100	29, 42, 61, 83	0
5	I	13/18 (72%)	-0.05	0 100 100	40, 45, 70, 73	0
5	J	13/18 (72%)	-0.09	0 100 100	44, 48, 76, 85	0
All	All	1615/1742 (92%)	0.13	72 (4%) 34 31	26, 54, 115, 176	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	184	ILE	5.3
1	C	174	LEU	5.2
2	B	188	TRP	5.2
2	D	185	ILE	5.1
2	B	170	VAL	5.1
2	B	185	ILE	4.6
2	B	168	GLY	4.3
3	E	207	ASN	4.3
2	D	188	TRP	4.2
2	B	161	LEU	4.0
2	D	172	THR	3.9
2	B	171	TYR	3.8
2	D	171	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	132	PHE	3.7
2	B	169	ASP	3.5
1	A	174	LEU	3.4
2	B	127	ILE	3.4
2	B	115	LEU	3.4
2	B	175	VAL	3.3
2	D	170	VAL	3.3
2	B	186	VAL	3.2
2	B	172	THR	3.2
2	B	114	LEU	3.1
2	D	103	PRO	3.1
1	C	177	HIS	3.1
2	B	174	HIS	3.1
2	B	101	ILE	3.1
2	B	148	ILE	3.1
1	C	121	TRP	3.0
2	B	142	VAL	2.9
2	D	187	GLU	2.9
2	B	150	ASN	2.8
1	A	91	VAL	2.8
2	D	102	SER	2.8
2	B	143	VAL	2.8
1	C	179	GLU	2.7
2	B	158	LEU	2.7
1	A	86	VAL	2.7
1	C	170	LEU	2.7
2	B	187	GLU	2.6
2	D	159	VAL	2.6
1	C	153	PHE	2.6
1	C	161	TYR	2.5
3	G	3	ALA	2.5
3	G	143	SER	2.5
1	A	170	LEU	2.5
1	A	179	GLU	2.5
3	E	209	ILE	2.4
1	C	72	ILE	2.4
1	C	128	VAL	2.3
2	B	147	LEU	2.3
2	D	169	ASP	2.3
1	A	83	THR	2.3
2	D	184	ILE	2.3
2	D	8	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	158	LEU	2.3
2	D	127	ILE	2.2
1	A	177	HIS	2.2
1	C	124	ASN	2.2
2	B	129	VAL	2.2
1	A	155	PRO	2.2
2	D	131	TRP	2.2
2	B	160	MET	2.2
1	C	129	THR	2.2
2	D	160	MET	2.2
2	B	157	ILE	2.2
2	D	175	VAL	2.1
2	B	103	PRO	2.1
1	C	83	THR	2.1
1	A	105	LEU	2.1
2	B	163	MET	2.0
1	C	91	VAL	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 carbohydrates 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. 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(\AA^2)	Q<0.9
6	NAG	A	1000	14/15	0.82	0.23	0.77	113,117,123,123	0
6	NAG	C	1000	14/15	0.87	0.18	-0.94	114,118,122,122	0
7	FUC	D	1002	10/11	0.83	0.21	-	107,110,115,115	0
6	NAG	D	1000	14/15	0.87	0.18	-	95,100,105,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	D	1001	14/15	0.87	0.20	-	114,117,123,124	0
6	NAG	B	1001	14/15	0.91	0.16	-	124,131,137,138	0
7	FUC	B	1002	10/11	0.89	0.17	-	127,131,136,137	0
8	MAN	B	1004	11/12	0.78	0.26	-	141,144,149,149	0
7	FUC	D	1003	10/11	0.89	0.18	-	99,102,104,106	0
8	MAN	B	1005	11/12	0.72	0.37	-	145,150,157,159	0
7	FUC	B	1003	10/11	0.84	0.21	-	120,124,127,128	0
6	NAG	B	1000	14/15	0.88	0.13	-	114,117,124,125	0

6.5 Other polymers

There are no such residues in this entry.