



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:44 pm GMT

PDB ID : 4HSA
Title : Structure of interleukin 17a in complex with il17ra receptor
Authors : Liu, S.
Deposited on : 2012-10-29
Resolution : 3.15 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 : trunk28620
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) : recalc28949

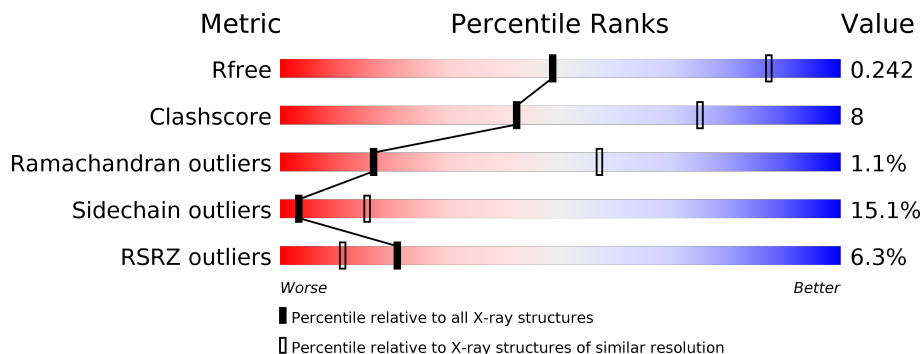
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	122	<div> <div>59%</div> <div>24%</div> <div>• •</div> <div>15%</div> </div>
1	B	122	<div>2%</div> <div>53%</div> <div>31%</div> <div>• •</div> <div>11%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FUC	C	608	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8031 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-17A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			848	532	157	153	6			
1	B	109	Total	C	N	O	S	0	0	0
			885	547	168	164	6			
1	D	100	Total	C	N	O	S	0	0	0
			816	511	152	147	6			
1	E	109	Total	C	N	O	S	0	0	0
			885	547	168	164	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASP	ASN	ENGINEERED MUTATION	UNP Q16552
A	106	SER	CYS	ENGINEERED MUTATION	UNP Q16552
B	45	ASP	ASN	ENGINEERED MUTATION	UNP Q16552
B	106	SER	CYS	ENGINEERED MUTATION	UNP Q16552
D	45	ASP	ASN	ENGINEERED MUTATION	UNP Q16552
D	106	SER	CYS	ENGINEERED MUTATION	UNP Q16552
E	45	ASP	ASN	ENGINEERED MUTATION	UNP Q16552
E	106	SER	CYS	ENGINEERED MUTATION	UNP Q16552

- Molecule 2 is a protein called Interleukin-17 receptor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	272	Total	C	N	O	S	0	0	0
			2203	1388	402	397	16			
2	F	271	Total	C	N	O	S	0	0	0
			2193	1380	401	396	16			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	175	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
C	234	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
C	287	LEU	-	EXPRESSION TAG	UNP Q96F46
C	288	VAL	-	EXPRESSION TAG	UNP Q96F46
C	289	PRO	-	EXPRESSION TAG	UNP Q96F46
C	290	ARG	-	EXPRESSION TAG	UNP Q96F46
C	291	GLY	-	EXPRESSION TAG	UNP Q96F46
C	292	SER	-	EXPRESSION TAG	UNP Q96F46
C	293	ASP	-	EXPRESSION TAG	UNP Q96F46
C	294	TYR	-	EXPRESSION TAG	UNP Q96F46
C	295	LYS	-	EXPRESSION TAG	UNP Q96F46
C	296	ASP	-	EXPRESSION TAG	UNP Q96F46
C	297	ASP	-	EXPRESSION TAG	UNP Q96F46
C	298	ASP	-	EXPRESSION TAG	UNP Q96F46
C	299	ASP	-	EXPRESSION TAG	UNP Q96F46
C	300	LYS	-	EXPRESSION TAG	UNP Q96F46
C	301	GLY	-	EXPRESSION TAG	UNP Q96F46
F	175	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
F	234	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
F	287	LEU	-	EXPRESSION TAG	UNP Q96F46
F	288	VAL	-	EXPRESSION TAG	UNP Q96F46
F	289	PRO	-	EXPRESSION TAG	UNP Q96F46
F	290	ARG	-	EXPRESSION TAG	UNP Q96F46
F	291	GLY	-	EXPRESSION TAG	UNP Q96F46
F	292	SER	-	EXPRESSION TAG	UNP Q96F46
F	293	ASP	-	EXPRESSION TAG	UNP Q96F46
F	294	TYR	-	EXPRESSION TAG	UNP Q96F46
F	295	LYS	-	EXPRESSION TAG	UNP Q96F46
F	296	ASP	-	EXPRESSION TAG	UNP Q96F46
F	297	ASP	-	EXPRESSION TAG	UNP Q96F46
F	298	ASP	-	EXPRESSION TAG	UNP Q96F46
F	299	ASP	-	EXPRESSION TAG	UNP Q96F46
F	300	LYS	-	EXPRESSION TAG	UNP Q96F46
F	301	GLY	-	EXPRESSION TAG	UNP Q96F46

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	5	Total	C	N	O	0	0
			60	34	2	24		
3	F	5	Total	C	N	O	0	0
			60	34	2	24		

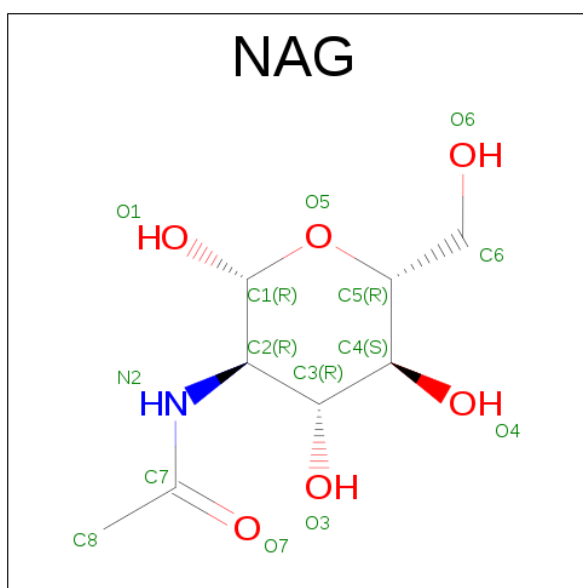
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			24	14	1	9		

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



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

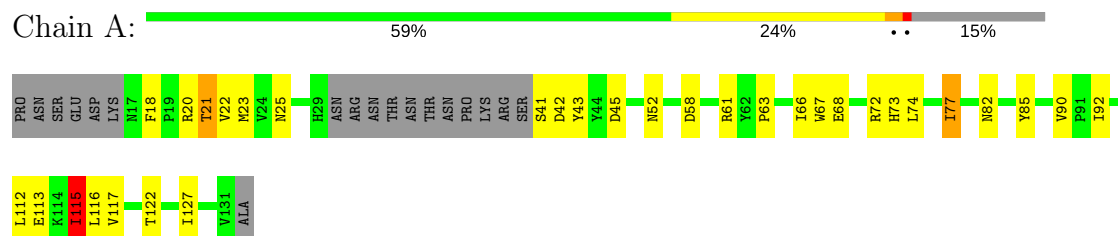
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	O	0	0
			2	2		
7	C	1	Total	O	0	0
			1	1		
7	E	2	Total	O	0	0
			2	2		

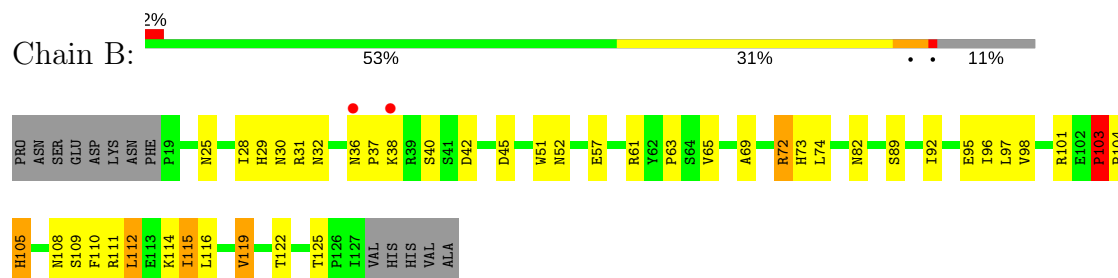
3 Residue-property plots [i](#)

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.

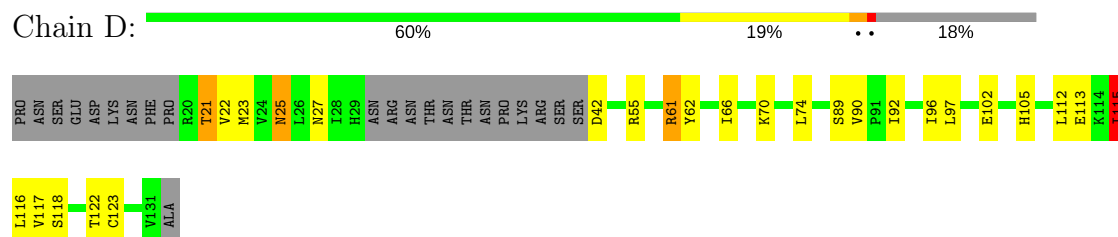
• Molecule 1: Interleukin-17A



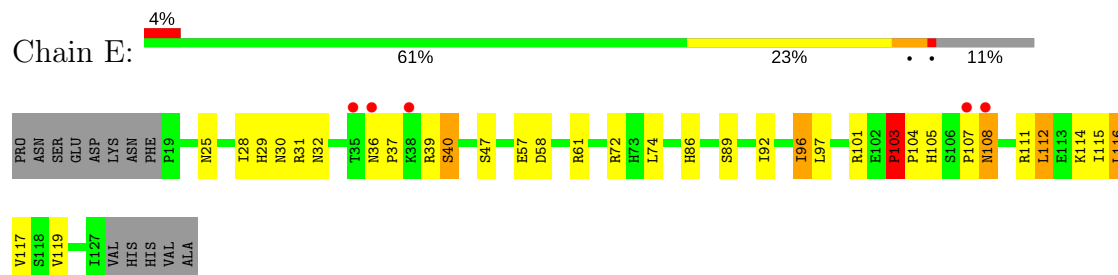
• Molecule 1: Interleukin-17A



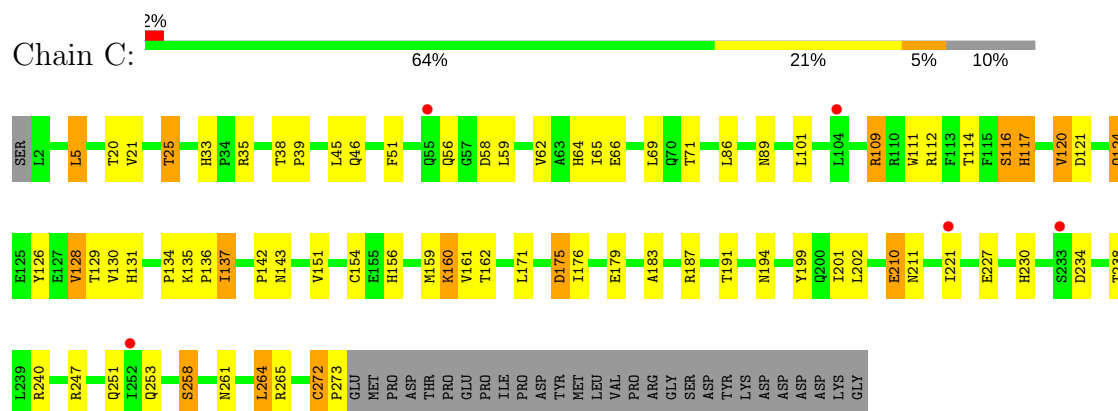
• Molecule 1: Interleukin-17A



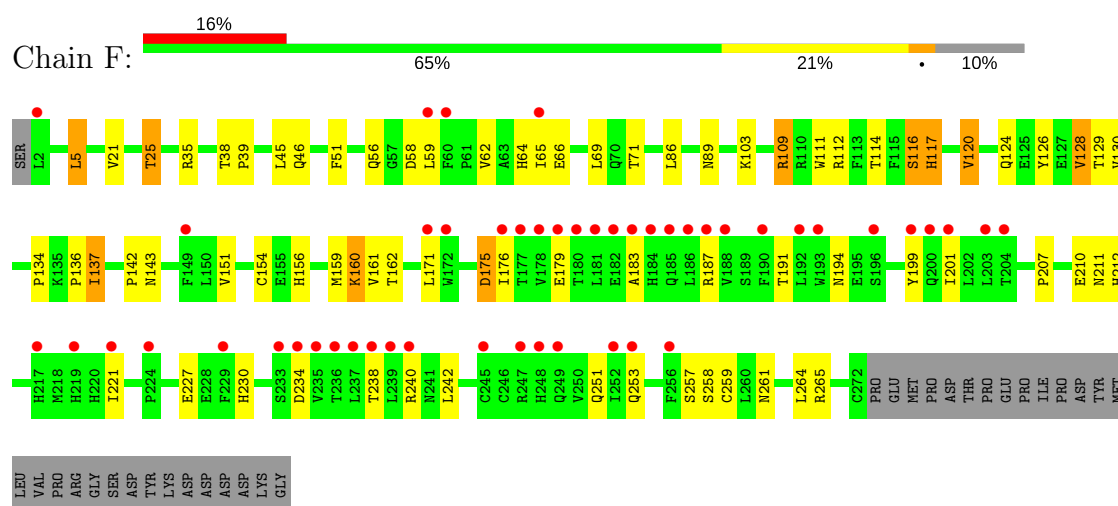
• Molecule 1: Interleukin-17A



• Molecule 2: Interleukin-17 receptor A



• Molecule 2: Interleukin-17 receptor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.71Å 138.71Å 179.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.14 – 3.15 99.76 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.14-3.15) 100.0 (99.76-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.187 , 0.232 0.205 , 0.242	Depositor DCC
R_{free} test set	1776 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8031	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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

5.1 Standard geometry

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	0.63	1/872 (0.1%)	0.83	0/1190
1	B	0.58	0/908	0.91	3/1238 (0.2%)
1	D	0.54	1/838 (0.1%)	0.77	0/1143
1	E	0.55	0/908	0.91	3/1238 (0.2%)
2	C	0.52	0/2271	0.77	1/3098 (0.0%)
2	F	0.47	0/2260	0.76	1/3082 (0.0%)
All	All	0.53	2/8057 (0.0%)	0.81	8/10989 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	ILE	CG1-CD1	5.95	1.91	1.50
1	D	115	ILE	CG1-CD1	5.02	1.85	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	PRO	CA-C-N	6.01	133.94	117.10
1	B	104	PRO	C-N-CA	5.98	136.65	121.70
1	B	119	VAL	N-CA-CB	-5.87	98.59	111.50
2	F	25	THR	N-CA-C	-5.68	95.65	111.00
2	C	25	THR	N-CA-C	-5.41	96.38	111.00
1	E	39	ARG	C-N-CA	5.33	135.01	121.70
1	E	104	PRO	C-N-CA	5.18	134.66	121.70
1	B	103	PRO	CA-C-N	5.16	131.55	117.10

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	848	0	814	27	0
1	B	885	0	858	19	0
1	D	816	0	787	22	0
1	E	885	0	858	20	0
2	C	2203	0	2081	34	0
2	F	2193	0	2066	25	0
3	C	60	0	52	0	0
3	F	60	0	52	0	0
4	C	38	0	34	2	0
5	C	24	0	22	0	0
6	F	14	0	13	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	2	0	0	0	0
All	All	8031	0	7637	124	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 8.

All (124) 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:D:66:ILE:CG1	1:D:66:ILE:CD1	1.75	1.65
1:A:66:ILE:CD1	1:A:66:ILE:CG1	1.76	1.58
1:E:96:ILE:CG1	1:E:96:ILE:CD1	1.84	1.52
1:D:115:ILE:CG1	1:D:115:ILE:CD1	1.85	1.51
1:A:115:ILE:CD1	1:A:115:ILE:CG1	1.91	1.47
2:F:156:HIS:HD2	2:F:159:MET:H	1.31	0.78
2:C:156:HIS:HD2	2:C:159:MET:H	1.32	0.75
1:A:115:ILE:HD12	1:A:116:LEU:H	1.51	0.74
1:A:127:ILE:HG22	2:C:264:LEU:HD12	1.72	0.71
1:B:95:GLU:HG2	1:B:114:LYS:HD3	1.73	0.71
1:D:115:ILE:HD12	1:D:116:LEU:H	1.56	0.70
2:C:272:CYS:HB2	2:C:273:PRO:HD3	1.74	0.69
2:C:201:ILE:HG12	2:C:221:ILE:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:ILE:HG12	2:F:221:ILE:HD11	1.76	0.66
1:E:97:LEU:HD22	1:E:112:LEU:CD1	2.27	0.64
1:A:22:VAL:HG22	1:A:23:MET:H	1.64	0.63
1:B:103:PRO:HB3	1:B:105:HIS:CD2	2.35	0.62
1:A:52:ASN:OD1	1:A:72:ARG:HD2	2.00	0.62
2:C:65:ILE:HG12	2:C:128:VAL:HG21	1.82	0.61
2:F:65:ILE:HG12	2:F:128:VAL:HG21	1.83	0.61
2:C:69:LEU:HD22	2:C:111:TRP:HB2	1.82	0.61
2:C:159:MET:O	2:C:162:THR:HG22	2.01	0.61
1:A:92:ILE:HD11	1:A:122:THR:HB	1.83	0.61
2:F:69:LEU:HD22	2:F:111:TRP:HB2	1.83	0.60
1:D:96:ILE:HG13	1:E:96:ILE:CD1	2.31	0.60
2:F:39:PRO:HD3	2:F:134:PRO:HD2	1.83	0.60
1:D:96:ILE:HG13	1:E:96:ILE:HD11	1.83	0.60
2:F:159:MET:O	2:F:162:THR:HG22	2.01	0.60
2:C:39:PRO:HD3	2:C:134:PRO:HD2	1.84	0.59
1:D:66:ILE:HA	1:D:66:ILE:CD1	2.33	0.58
1:A:61:ARG:HH11	1:A:61:ARG:HG2	1.69	0.57
2:C:66:GLU:HB3	2:C:114:THR:HG22	1.87	0.57
2:F:66:GLU:HB3	2:F:114:THR:HG22	1.87	0.56
2:F:51:PHE:HB3	2:F:59:LEU:HD11	1.88	0.56
1:B:97:LEU:HD22	1:B:112:LEU:HD13	1.88	0.56
1:E:58:ASP:HB3	1:E:61:ARG:HG2	1.88	0.55
1:A:42:ASP:CG	1:A:43:TYR:H	2.08	0.55
1:E:36:ASN:HB2	1:E:37:PRO:HD3	1.88	0.55
1:A:20:ARG:HG2	2:C:33:HIS:NE2	2.22	0.54
2:C:20:THR:HG23	2:C:101:LEU:HD11	1.90	0.53
2:C:51:PHE:HB3	2:C:59:LEU:HD11	1.91	0.53
1:A:25:ASN:HB2	1:B:108:ASN:OD1	2.08	0.53
1:B:38:LYS:HB2	2:C:258:SER:HA	1.89	0.53
1:D:97:LEU:HD22	1:D:112:LEU:HD12	1.89	0.53
2:C:175:ASP:H	2:C:191:THR:HG22	1.74	0.52
2:F:120:VAL:HG13	2:F:151:VAL:HG21	1.92	0.52
1:D:66:ILE:HA	1:D:66:ILE:HD12	1.92	0.52
1:A:74:LEU:HD22	2:C:261:ASN:HB3	1.92	0.51
2:F:175:ASP:H	2:F:191:THR:HG22	1.75	0.51
1:A:85:TYR:CB	2:C:202:LEU:HD21	2.41	0.51
2:F:201:ILE:HG12	2:F:221:ILE:CD1	2.41	0.51
1:D:74:LEU:HD22	2:F:261:ASN:HB3	1.93	0.51
1:D:22:VAL:HG22	1:D:23:MET:H	1.75	0.50
2:C:201:ILE:HG12	2:C:221:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:109:ARG:HH12	2:F:112:ARG:HH12	1.58	0.50
2:F:64:HIS:HD2	2:F:116:SER:OG	1.95	0.50
2:C:253:GLN:HG3	2:C:265:ARG:HG2	1.93	0.50
1:B:36:ASN:HB2	1:B:37:PRO:HD3	1.91	0.50
2:C:64:HIS:HD2	2:C:116:SER:OG	1.94	0.50
1:B:30:ASN:HD21	1:B:32:ASN:HB3	1.77	0.49
1:B:63:PRO:HD2	1:B:98:VAL:HG12	1.94	0.49
1:D:66:ILE:CB	1:D:66:ILE:CD1	2.80	0.49
1:B:51:TRP:CD1	1:B:69:ALA:HB1	2.47	0.49
2:C:109:ARG:HH12	2:C:112:ARG:HH12	1.58	0.49
2:F:253:GLN:HG3	2:F:265:ARG:HG2	1.94	0.49
1:D:112:LEU:HG	1:E:28:ILE:HG12	1.95	0.49
1:E:97:LEU:HD22	1:E:112:LEU:HD11	1.94	0.49
1:B:73:HIS:O	1:B:89:SER:HB2	2.12	0.49
1:D:123:CYS:O	1:E:47:SER:HA	2.13	0.49
1:A:42:ASP:OD1	1:A:43:TYR:N	2.45	0.49
1:D:21:THR:HB	1:E:25:ASN:HA	1.95	0.48
4:C:606:NAG:H61	4:C:607:NAG:C7	2.44	0.48
1:B:52:ASN:ND2	1:B:72:ARG:HH11	2.11	0.48
1:E:96:ILE:HG22	1:E:115:ILE:HG13	1.96	0.48
2:F:199:TYR:HB2	2:F:221:ILE:HB	1.96	0.48
2:F:38:THR:HG21	2:F:136:PRO:HA	1.95	0.47
1:A:112:LEU:HD23	1:B:28:ILE:HG12	1.95	0.47
2:C:38:THR:HG21	2:C:136:PRO:HA	1.97	0.47
2:C:137:ILE:HD13	2:C:137:ILE:H	1.80	0.47
1:A:85:TYR:HB3	2:C:202:LEU:HD21	1.97	0.47
2:C:199:TYR:HB2	2:C:221:ILE:HB	1.97	0.46
1:D:113:GLU:HG2	1:E:29:HIS:HB3	1.98	0.46
1:A:61:ARG:HG2	1:A:63:PRO:O	2.17	0.45
1:D:115:ILE:HD12	1:D:116:LEU:N	2.29	0.45
1:A:22:VAL:HG21	1:B:110:PHE:CE1	2.52	0.45
1:A:92:ILE:HD13	1:B:92:ILE:HD12	1.98	0.45
1:A:115:ILE:HD12	1:A:116:LEU:N	2.25	0.45
4:C:606:NAG:H62	4:C:608:FUC:H5	1.98	0.45
1:E:30:ASN:HD21	1:E:32:ASN:HB3	1.81	0.45
1:D:92:ILE:HD12	1:E:92:ILE:HD12	1.99	0.45
1:A:58:ASP:HB3	1:A:61:ARG:HB3	1.98	0.45
1:D:25:ASN:HB2	1:E:108:ASN:HB2	1.98	0.45
2:C:131:HIS:CE1	2:C:135:LYS:HD3	2.53	0.44
2:F:103:LYS:HA	2:F:103:LYS:HD3	1.87	0.44
2:F:137:ILE:HD13	2:F:137:ILE:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:HIS:HB3	2:C:159:MET:HB2	2.00	0.43
2:F:194:ASN:HB3	2:F:230:HIS:NE2	2.33	0.43
2:C:121:ASP:HB2	2:C:124:GLN:HG3	2.00	0.43
2:C:194:ASN:HB3	2:C:230:HIS:NE2	2.34	0.43
1:A:92:ILE:HD13	1:B:92:ILE:CD1	2.48	0.43
2:F:207:PRO:HD3	2:F:212:HIS:O	2.19	0.43
1:B:115:ILE:HD13	1:B:115:ILE:HA	1.77	0.42
1:E:116:LEU:HA	1:E:116:LEU:HD23	1.94	0.42
1:A:113:GLU:HG2	1:B:29:HIS:HB3	2.01	0.42
2:C:120:VAL:HG22	2:C:126:TYR:CE2	2.54	0.42
1:A:73:HIS:CD2	1:A:77:ILE:HD13	2.55	0.42
2:F:156:HIS:HB3	2:F:159:MET:HB2	2.01	0.42
2:C:154:CYS:O	2:C:160:LYS:HB3	2.19	0.42
2:F:154:CYS:O	2:F:160:LYS:HB3	2.19	0.42
1:A:66:ILE:HD12	1:A:67:TRP:H	1.84	0.42
1:B:74:LEU:HD22	1:E:74:LEU:HG	2.03	0.41
1:D:61:ARG:HG3	1:D:62:TYR:N	2.34	0.41
1:A:21:THR:HA	1:B:25:ASN:HA	2.02	0.41
2:C:120:VAL:HG13	2:C:151:VAL:HG21	2.02	0.41
2:C:210:GLU:H	2:C:247:ARG:HH12	1.67	0.41
1:A:66:ILE:HA	1:A:66:ILE:CD1	2.51	0.41
1:E:107:PRO:HA	1:E:108:ASN:HA	1.67	0.41
2:F:5:LEU:HD13	2:F:117:HIS:CE1	2.56	0.41
2:C:272:CYS:CB	2:C:273:PRO:HD3	2.45	0.40
1:D:92:ILE:CG2	1:E:119:VAL:HG12	2.51	0.40
2:C:5:LEU:HD13	2:C:117:HIS:CE1	2.56	0.40
1:D:27:ASN:HD21	1:E:111:ARG:HD2	1.86	0.40
1:D:92:ILE:HD11	1:D:122:THR:HB	2.02	0.40
2:F:120:VAL:HG22	2:F:126:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	100/122 (82%)	93 (93%)	7 (7%)	0	100	100
1	B	107/122 (88%)	98 (92%)	6 (6%)	3 (3%)	6	32
1	D	96/122 (79%)	94 (98%)	2 (2%)	0	100	100
1	E	107/122 (88%)	99 (92%)	5 (5%)	3 (3%)	6	32
2	C	270/301 (90%)	251 (93%)	17 (6%)	2 (1%)	25	67
2	F	269/301 (89%)	253 (94%)	14 (5%)	2 (1%)	25	67
All	All	949/1090 (87%)	888 (94%)	51 (5%)	10 (1%)	17	57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	SER
1	B	103	PRO
1	B	105	HIS
1	E	40	SER
1	E	103	PRO
1	E	105	HIS
2	C	272	CYS
2	F	257	SER
2	C	183	ALA
2	F	183	ALA

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	99/116 (85%)	89 (90%)	10 (10%)	9	32
1	B	104/116 (90%)	85 (82%)	19 (18%)	2	10
1	D	95/116 (82%)	82 (86%)	13 (14%)	4	19
1	E	104/116 (90%)	90 (86%)	14 (14%)	4	20
2	C	251/284 (88%)	212 (84%)	39 (16%)	3	13
2	F	249/284 (88%)	208 (84%)	41 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	902/1032 (87%)	766 (85%)	136 (15%)	3 15

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	21	THR
1	A	41	SER
1	A	45	ASP
1	A	68	GLU
1	A	77	ILE
1	A	82	ASN
1	A	90	VAL
1	A	115	ILE
1	A	117	VAL
1	B	31	ARG
1	B	42	ASP
1	B	45	ASP
1	B	57	GLU
1	B	61	ARG
1	B	65	VAL
1	B	72	ARG
1	B	82	ASN
1	B	96	ILE
1	B	101	ARG
1	B	103	PRO
1	B	109	SER
1	B	111	ARG
1	B	112	LEU
1	B	115	ILE
1	B	116	LEU
1	B	119	VAL
1	B	122	THR
1	B	125	THR
2	C	5	LEU
2	C	21	VAL
2	C	25	THR
2	C	35	ARG
2	C	45	LEU
2	C	46	GLN
2	C	56	GLN
2	C	58	ASP

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Mol	Chain	Res	Type
2	C	62	VAL
2	C	71	THR
2	C	86	LEU
2	C	89	ASN
2	C	109	ARG
2	C	116	SER
2	C	117	HIS
2	C	120	VAL
2	C	124	GLN
2	C	128	VAL
2	C	129	THR
2	C	130	VAL
2	C	137	ILE
2	C	142	PRO
2	C	143	ASN
2	C	160	LYS
2	C	161	VAL
2	C	171	LEU
2	C	175	ASP
2	C	176	ILE
2	C	179	GLU
2	C	187	ARG
2	C	210	GLU
2	C	211	ASN
2	C	227	GLU
2	C	234	ASP
2	C	238	THR
2	C	240	ARG
2	C	251	GLN
2	C	258	SER
2	C	264	LEU
1	D	21	THR
1	D	25	ASN
1	D	42	ASP
1	D	55	ARG
1	D	61	ARG
1	D	70	LYS
1	D	89	SER
1	D	90	VAL
1	D	102	GLU
1	D	105	HIS
1	D	115	ILE

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Mol	Chain	Res	Type
1	D	117	VAL
1	D	118	SER
1	E	31	ARG
1	E	40	SER
1	E	57	GLU
1	E	72	ARG
1	E	86	HIS
1	E	89	SER
1	E	96	ILE
1	E	101	ARG
1	E	103	PRO
1	E	108	ASN
1	E	112	LEU
1	E	114	LYS
1	E	116	LEU
1	E	117	VAL
2	F	5	LEU
2	F	21	VAL
2	F	25	THR
2	F	35	ARG
2	F	45	LEU
2	F	46	GLN
2	F	56	GLN
2	F	58	ASP
2	F	62	VAL
2	F	71	THR
2	F	86	LEU
2	F	89	ASN
2	F	109	ARG
2	F	116	SER
2	F	117	HIS
2	F	120	VAL
2	F	124	GLN
2	F	128	VAL
2	F	129	THR
2	F	130	VAL
2	F	137	ILE
2	F	142	PRO
2	F	143	ASN
2	F	160	LYS
2	F	161	VAL
2	F	171	LEU

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Mol	Chain	Res	Type
2	F	175	ASP
2	F	176	ILE
2	F	179	GLU
2	F	187	ARG
2	F	210	GLU
2	F	211	ASN
2	F	227	GLU
2	F	234	ASP
2	F	238	THR
2	F	240	ARG
2	F	242	LEU
2	F	251	GLN
2	F	258	SER
2	F	259	CYS
2	F	264	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	86	HIS
1	B	30	ASN
1	B	52	ASN
1	B	94	GLN
2	C	7	HIS
2	C	50	HIS
2	C	64	HIS
2	C	87	GLN
2	C	106	HIS
2	C	107	HIS
2	C	117	HIS
2	C	131	HIS
2	C	156	HIS
2	C	219	HIS
1	D	27	ASN
1	D	105	HIS
1	D	108	ASN
1	E	30	ASN
1	E	52	ASN
2	F	64	HIS
2	F	87	GLN
2	F	106	HIS

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Mol	Chain	Res	Type
2	F	107	HIS
2	F	117	HIS
2	F	131	HIS
2	F	156	HIS
2	F	219	HIS

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 ⓘ

15 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	$\# Z > 2$
3	NAG	C	601	3,2	14,14,15	0.30	0	15,19,21	0.72	1 (6%)
3	NAG	C	602	3	14,14,15	0.30	0	15,19,21	0.61	0
3	MAN	C	603	3	11,11,12	0.32	0	13,15,17	0.91	1 (7%)
3	MAN	C	604	3	11,11,12	0.39	0	13,15,17	0.98	2 (15%)
3	FUC	C	605	3	9,10,11	0.38	0	13,14,16	0.80	1 (7%)
4	NAG	C	606	2,4	14,14,15	0.41	0	15,19,21	1.56	2 (13%)
4	NAG	C	607	4	14,14,15	0.32	0	15,19,21	0.95	2 (13%)
4	FUC	C	608	4	9,10,11	0.55	0	13,14,16	1.43	2 (15%)
5	NAG	C	609	2,5	14,14,15	0.32	0	15,19,21	0.84	1 (6%)
5	FUC	C	610	5	9,10,11	0.42	0	13,14,16	1.20	1 (7%)
3	NAG	F	601	3,2	14,14,15	0.31	0	15,19,21	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	602	3	14,14,15	0.30	0	15,19,21	0.69	0
3	MAN	F	603	3	11,11,12	0.33	0	13,15,17	0.86	1 (7%)
3	MAN	F	604	3	11,11,12	0.42	0	13,15,17	0.98	2 (15%)
3	FUC	F	605	3	9,10,11	0.39	0	13,14,16	0.73	1 (7%)

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	C	601	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	602	3	-	0/6/23/26	0/1/1/1
3	MAN	C	603	3	-	0/2/19/22	1/1/1/1
3	MAN	C	604	3	-	0/2/19/22	0/1/1/1
3	FUC	C	605	3	-	0/0/17/20	0/1/1/1
4	NAG	C	606	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	607	4	-	0/6/23/26	0/1/1/1
4	FUC	C	608	4	-	0/0/17/20	0/1/1/1
5	NAG	C	609	2,5	-	0/6/23/26	0/1/1/1
5	FUC	C	610	5	-	0/0/17/20	0/1/1/1
3	NAG	F	601	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	602	3	-	0/6/23/26	0/1/1/1
3	MAN	F	603	3	-	0/2/19/22	1/1/1/1
3	MAN	F	604	3	-	0/2/19/22	0/1/1/1
3	FUC	F	605	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	MAN	C1-C2-C3	2.00	112.19	109.65
4	C	607	NAG	C1-C2-N2	2.02	113.94	110.49
3	F	604	MAN	C1-C2-C3	2.04	112.24	109.65
3	F	605	FUC	C1-O5-C5	2.12	117.09	112.39
3	C	601	NAG	C1-O5-C5	2.15	115.13	112.17
4	C	608	FUC	O2-C2-C1	2.24	113.74	109.18
3	C	605	FUC	C1-O5-C5	2.33	117.55	112.39
3	F	601	NAG	C1-O5-C5	2.52	115.65	112.17
5	C	609	NAG	C1-O5-C5	2.56	115.69	112.17
3	F	604	MAN	C1-O5-C5	2.61	115.77	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	MAN	C1-O5-C5	2.63	115.79	112.17
4	C	607	NAG	C1-O5-C5	2.67	115.84	112.17
3	F	603	MAN	C1-O5-C5	2.80	116.03	112.17
3	C	603	MAN	C1-O5-C5	2.85	116.10	112.17
4	C	606	NAG	C1-C2-N2	3.35	116.21	110.49
5	C	610	FUC	C1-O5-C5	3.36	119.83	112.39
4	C	608	FUC	C1-O5-C5	4.41	122.14	112.39
4	C	606	NAG	C1-O5-C5	4.69	118.63	112.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	603	MAN	C1-C2-C3-C4-C5-O5
3	C	603	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	606	NAG	2	0
4	C	607	NAG	1	0
4	C	608	FUC	1	0

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	$\# Z > 2$
6	NAG	F	606	2	14,14,15	0.37	0	15,19,21	1.40	2 (13%)

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	F	606	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	606	NAG	C1-C2-N2	3.36	116.22	110.49
6	F	606	NAG	C1-O5-C5	3.98	117.65	112.17

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	104/122 (85%)	0.40	0 100 100	59, 87, 121, 158	0
1	B	109/122 (89%)	0.51	2 (1%) 69 53	59, 79, 146, 172	0
1	D	100/122 (81%)	0.21	0 100 100	70, 100, 140, 174	0
1	E	109/122 (89%)	0.59	5 (4%) 33 19	58, 83, 139, 183	0
2	C	272/301 (90%)	0.54	5 (1%) 69 53	55, 91, 137, 173	0
2	F	271/301 (90%)	1.06	49 (18%) 1 1	59, 114, 219, 230	0
All	All	965/1090 (88%)	0.64	61 (6%) 21 11	55, 93, 188, 230	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	38	LYS	6.4
2	F	190	PHE	5.2
2	F	171	LEU	5.1
2	F	249	GLN	5.1
2	F	193	TRP	5.1
2	F	192	LEU	5.0
2	F	237	LEU	4.9
2	F	239	LEU	4.8
2	F	240	ARG	4.7
2	F	188	VAL	4.6
2	F	248	HIS	4.4
2	F	181	LEU	4.4
2	F	186	LEU	4.3
2	F	252	ILE	4.2
2	F	185	GLN	4.0
2	F	236	THR	3.8
2	F	201	ILE	3.8
2	F	179	GLU	3.7
2	F	233	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	224	PRO	3.5
1	B	36	ASN	3.4
2	F	187	ARG	3.2
2	F	219	HIS	3.2
1	E	108	ASN	3.2
2	F	176	ILE	3.2
2	F	2	LEU	3.2
2	F	200	GLN	3.0
2	F	203	LEU	2.9
2	F	199	TYR	2.9
2	C	104	LEU	2.9
2	F	182	GLU	2.8
2	F	204	THR	2.7
2	F	238	THR	2.7
1	E	107	PRO	2.6
1	B	38	LYS	2.5
1	E	35	THR	2.5
2	F	149	PHE	2.4
2	F	172	TRP	2.4
2	C	55	GLN	2.4
2	C	221	ILE	2.4
2	F	59	LEU	2.3
2	F	60	PHE	2.3
2	F	234	ASP	2.3
2	F	245	CYS	2.3
2	F	229	PHE	2.3
2	F	178	VAL	2.3
2	F	256	PHE	2.2
2	F	184	HIS	2.2
2	C	252	ILE	2.2
2	F	65	ILE	2.1
2	F	196	SER	2.1
2	C	233	SER	2.1
2	F	183	ALA	2.1
2	F	221	ILE	2.1
2	F	180	THR	2.0
2	F	253	GLN	2.0
2	F	177	THR	2.0
2	F	217	HIS	2.0
2	F	247	ARG	2.0
1	E	36	ASN	2.0
2	F	235	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](#)

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	FUC	C	608	10/11	0.78	0.90	11.11	164,170,174,174	0
3	NAG	C	601	14/15	0.91	0.16	-	150,159,164,168	0
3	MAN	F	603	11/12	0.79	0.17	-	213,216,220,223	0
5	FUC	C	610	10/11	0.76	0.34	-	166,174,177,177	0
3	FUC	C	605	10/11	0.92	0.26	-	162,165,168,171	0
3	FUC	F	605	10/11	0.78	0.39	-	203,204,205,206	0
5	NAG	C	609	14/15	0.83	0.40	-	149,154,166,166	0
4	NAG	C	607	14/15	0.77	0.27	-	151,161,166,167	0
3	MAN	C	603	11/12	0.80	0.24	-	194,198,199,201	0
4	NAG	C	606	14/15	0.44	0.24	-	132,148,162,168	0
3	NAG	F	602	14/15	0.76	0.35	-	196,207,211,214	0
3	MAN	C	604	11/12	0.73	0.35	-	197,199,200,200	0
3	NAG	F	601	14/15	0.81	0.26	-	198,202,203,203	0
3	NAG	C	602	14/15	0.91	0.19	-	170,180,188,192	0
3	MAN	F	604	11/12	0.77	0.44	-	225,227,230,231	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
6	NAG	F	606	14/15	0.66	0.19	-	155,163,169,173	0

6.5 Other polymers [i](#)

There are no such residues in this entry.