



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:36 AM 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 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/ValidationPDFNotes.html>

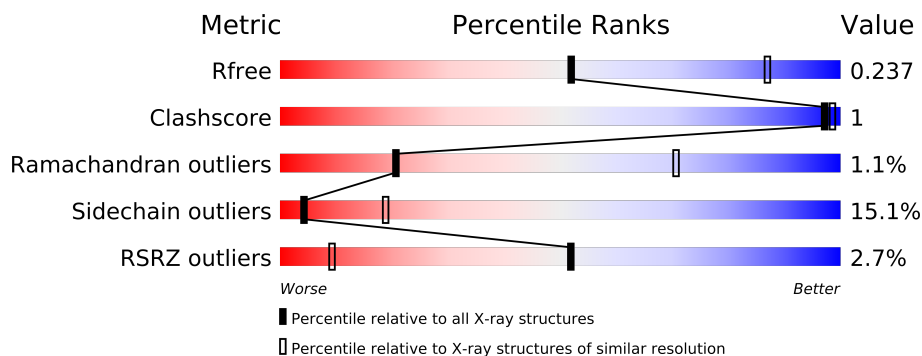
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	122	
1	B	122	
1	D	122	
1	E	122	
2	C	301	
2	F	301	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8031 atoms, of which 0 are hydrogen and 0 are deuterium.

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		

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 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		

There are 17 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

- 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		

There are 17 discrepancies between the modelled and reference sequences:

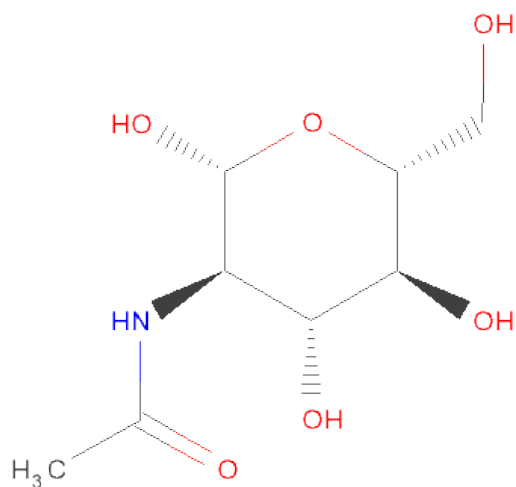
Chain	Residue	Modelled	Actual	Comment	Reference
C	175	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
C	234	ASP	ASN	ENGINEERED MUTATION	UNP Q96F46
C	287	LEU	-	EXPRESSION TAG	UNP Q96F46
C	288	VAL	-	EXPRESSION TAG	UNP Q96F46
C	289	PRO	-	EXPRESSION TAG	UNP Q96F46
C	290	ARG	-	EXPRESSION TAG	UNP Q96F46
C	291	GLY	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	301	GLY	-	EXPRESSION TAG	UNP Q96F46

- 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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Interleukin-17A

Chain A: 



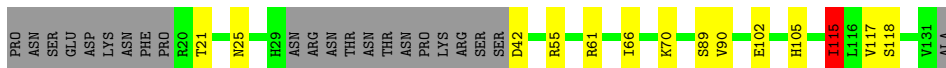
- Molecule 1: Interleukin-17A

Chain B: 



- Molecule 1: Interleukin-17A

Chain D: 



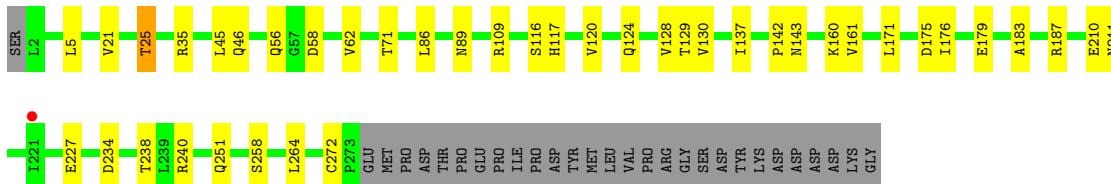
- Molecule 1: Interleukin-17A

Chain E: 



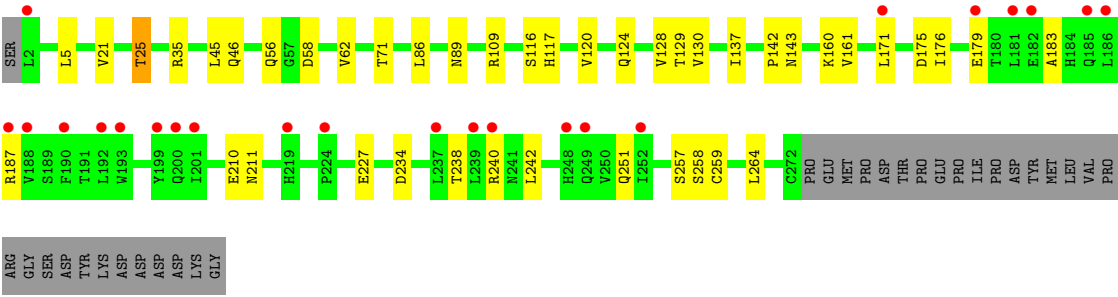
- Molecule 2: Interleukin-17 receptor A

Chain C: 



- Molecule 2: Interleukin-17 receptor A

Chain F: 



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) 99.9 (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 0.201 , 0.237	Depositor DCC
R_{free} test set	1773 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 35006 reflections	Xtriage
F_o, F_c correlation	0.92	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.

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	0.63	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	848	0	0	3	0
1	B	885	0	0	0	0
1	D	816	0	0	3	0
1	E	885	0	0	1	0
2	C	2203	0	0	0	0
2	F	2193	0	0	0	0
3	C	60	0	0	0	0
3	F	60	0	0	0	0
4	C	38	0	0	0	0
5	C	24	0	0	0	0
6	F	14	0	0	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	0	7	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:66:ILE:CG1	1:D:66:ILE:CD1	1.75	1.65
1:A:66:ILE:CG1	1:A:66:ILE:CD1	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:CG1	1:A:115:ILE:CD1	1.91	1.47
1:D:66:ILE:CB	1:D:66:ILE:CD1	2.80	0.49
1:A:42:ASP:OD1	1:A:43:TYR:N	2.45	0.49

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%)	8	44
1	D	96/122 (79%)	94 (98%)	2 (2%)	0	100	100
1	E	107/122 (88%)	99 (92%)	5 (5%)	3 (3%)	8	44
2	C	270/301 (90%)	251 (93%)	17 (6%)	2 (1%)	30	79
2	F	269/301 (89%)	253 (94%)	14 (5%)	2 (1%)	30	79
All	All	949/1090 (87%)	888 (94%)	51 (5%)	10 (1%)	21	70

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%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	104/116 (90%)	85 (82%)	19 (18%)	2	11
1	D	95/116 (82%)	82 (86%)	13 (14%)	5	24
1	E	104/116 (90%)	90 (86%)	14 (14%)	6	25
2	C	251/284 (88%)	212 (84%)	39 (16%)	4	17
2	F	249/284 (88%)	208 (84%)	41 (16%)	3	14
All	All	902/1032 (87%)	766 (85%)	136 (15%)	4	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.27	0	15,19,21	0.57	0
3	NAG	C	602	3	12,14,15	0.31	0	15,19,21	0.45	0
3	MAN	C	603	3	10,11,12	0.35	0	11,15,17	0.43	0
3	MAN	C	604	3	10,11,12	0.36	0	11,15,17	0.46	0
3	FUC	C	605	3	9,10,11	0.36	0	10,14,16	0.43	0
4	NAG	C	606	2,4	12,14,15	0.32	0	15,19,21	0.63	0
4	NAG	C	607	4	12,14,15	0.26	0	15,19,21	0.54	0
4	FUC	C	608	4	9,10,11	0.35	0	10,14,16	0.39	0
5	NAG	C	609	2,5	12,14,15	0.27	0	15,19,21	0.52	0
5	FUC	C	610	5	9,10,11	0.36	0	10,14,16	0.51	0
3	NAG	F	601	3,2	12,14,15	0.26	0	15,19,21	0.57	0
3	NAG	F	602	3	12,14,15	0.30	0	15,19,21	0.49	0
3	MAN	F	603	3	10,11,12	0.33	0	11,15,17	0.35	0
3	MAN	F	604	3	10,11,12	0.36	0	11,15,17	0.44	0
3	FUC	F	605	3	9,10,11	0.37	0	10,14,16	0.44	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
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	0/1/1/1
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	0/1/1/1
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.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

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	12,14,15	0.28	0	15,19,21	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
6	NAG	F	606	2	-	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.

There are no torsion outliers.

There are no ring outliers.

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, 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(Å²)	Q<0.9
1	A	104/122 (85%)	0.16	0	100100	59, 87, 121, 158	0
1	B	109/122 (89%)	0.21	0	100100	59, 79, 146, 172	0
1	D	100/122 (81%)	0.05	0	100100	70, 100, 140, 174	0
1	E	109/122 (89%)	0.26	1 (0%)	8129	58, 83, 139, 183	0
2	C	272/301 (90%)	0.32	1 (0%)	9049	55, 91, 137, 173	0
2	F	271/301 (90%)	0.54	23 (8%)	112	59, 114, 219, 230	0
All	All	965/1090 (88%)	0.32	25 (2%)	529	55, 93, 188, 230	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	38	LYS	4.5
2	F	240	ARG	3.8
2	F	237	LEU	3.3
2	F	171	LEU	3.1
2	F	192	LEU	3.1
2	F	186	LEU	2.9
2	F	239	LEU	2.9
2	F	190	PHE	2.8
2	F	249	GLN	2.7
2	F	252	ILE	2.7
2	F	201	ILE	2.5
2	F	181	LEU	2.5
2	F	193	TRP	2.5
2	F	219	HIS	2.4
2	F	188	VAL	2.4
2	F	179	GLU	2.4
2	F	248	HIS	2.4
2	F	224	PRO	2.3
2	F	182	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	187	ARG	2.1
2	F	200	GLN	2.1
2	F	185	GLN	2.1
2	F	199	TYR	2.0
2	C	221	ILE	2.0
2	F	2	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FUC	C	608	10/11	0.86	9.41	164,170,174,174	0
5	NAG	C	609	14/15	0.39	1.81	149,154,166,166	0
3	NAG	F	601	14/15	0.24	-0.64	198,202,203,203	0
4	NAG	C	606	14/15	0.24	-0.75	132,148,162,168	0
3	NAG	F	602	14/15	0.34	-0.89	196,207,211,214	0
3	NAG	C	602	14/15	0.18	-1.63	170,180,188,192	0
3	NAG	C	601	14/15	0.18	-3.82	150,159,164,168	0
3	MAN	C	603	11/12	0.26	-5.93	194,198,199,201	0
5	FUC	C	610	10/11	0.38	-	166,174,177,177	0
3	FUC	C	605	10/11	0.25	-	162,165,168,171	0
3	FUC	F	605	10/11	0.39	-	203,204,205,206	0
3	MAN	C	604	11/12	0.39	-	197,199,200,200	0
3	MAN	F	603	11/12	0.17	-	213,216,220,223	0
4	NAG	C	607	14/15	0.28	-	151,161,166,167	0
3	MAN	F	604	11/12	0.36	-	225,227,230,231	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	F	606	14/15	0.19	-0.49	155,163,169,173	0

6.5 Other polymers ⓘ

There are no such residues in this entry.