



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:02 AM UTC

PDB ID : 4OZF / pdb_00004ozf
Title : JR5.1 protein complex
Authors : Petersen, J.; Reid, H.H.; Rossjohn, J.
Deposited on : 2014-02-15
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

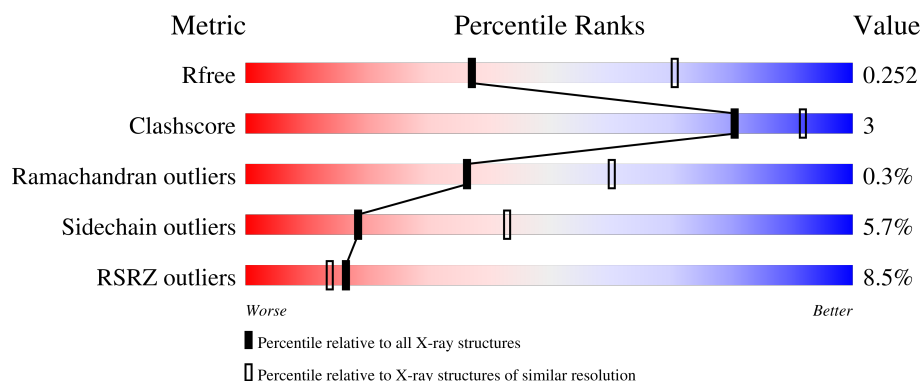
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	191	82% 12% 5%
2	B	213	73% 8% 15%
3	G	202	24% 82% 12% ..
4	H	244	6% 89% 10% .
5	J	13	15% 77% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6624 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, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1445	931	236	275	3			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1480	935	264	274	7			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP Q5Y7D3
B	-11	GLY	-	expression tag	UNP Q5Y7D3
B	-10	SER	-	expression tag	UNP Q5Y7D3
B	-9	ILE	-	expression tag	UNP Q5Y7D3
B	-8	GLU	-	expression tag	UNP Q5Y7D3
B	-7	GLY	-	expression tag	UNP Q5Y7D3
B	-6	ARG	-	expression tag	UNP Q5Y7D3
B	-5	GLY	-	expression tag	UNP Q5Y7D3
B	-4	GLY	-	expression tag	UNP Q5Y7D3
B	-3	SER	-	expression tag	UNP Q5Y7D3
B	-2	GLY	-	expression tag	UNP Q5Y7D3
B	-1	ALA	-	expression tag	UNP Q5Y7D3
B	0	SER	-	expression tag	UNP Q5Y7D3
B	193	THR	-	expression tag	UNP Q5Y7D3
B	194	GLY	-	expression tag	UNP Q5Y7D3
B	195	GLY	-	expression tag	UNP Q5Y7D3
B	196	ASP	-	expression tag	UNP Q5Y7D3
B	197	ASP	-	expression tag	UNP Q5Y7D3
B	198	ASP	-	expression tag	UNP Q5Y7D3
B	199	ASP	-	expression tag	UNP Q5Y7D3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	200	LYS	-	expression tag	UNP Q5Y7D3

- Molecule 3 is a protein called T-CELL RECEPTOR, JR5.1 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	193	Total	C	N	O	S	0	0	0
			1471	920	253	288	10			

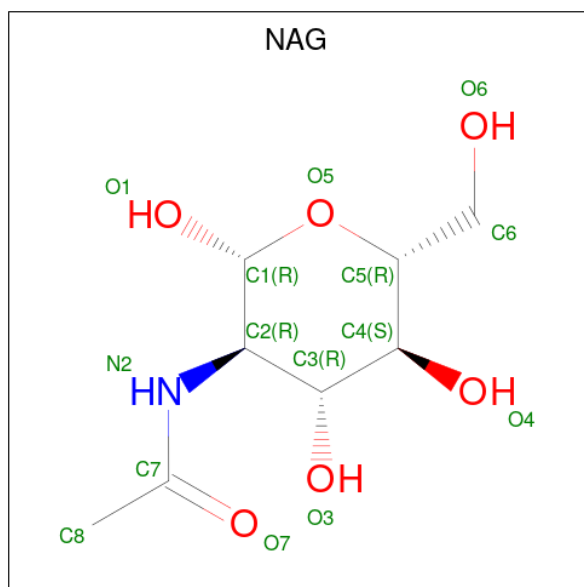
- Molecule 4 is a protein called T-CELL RECEPTOR, JR5.1 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	242	Total	C	N	O	S	0	0	0
			1871	1179	325	362	5			

- Molecule 5 is a protein called deamidated Gliadin-alpha2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	13	Total	C	N	O	0	0	0
			97	63	15	19			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

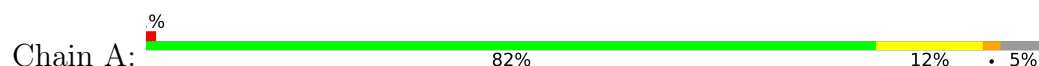
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	78	Total	O	0	0
			78	78		
7	B	68	Total	O	0	0
			68	68		
7	G	43	Total	O	0	0
			43	43		
7	H	40	Total	O	0	0
			40	40		
7	J	3	Total	O	0	0
			3	3		

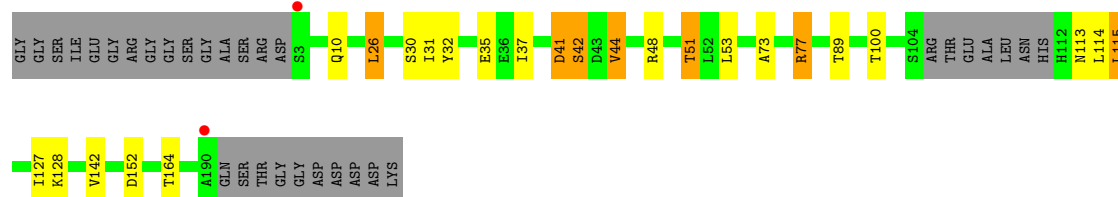
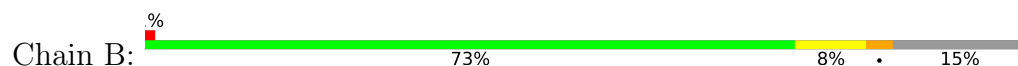
3 Residue-property plots [i](#)

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.

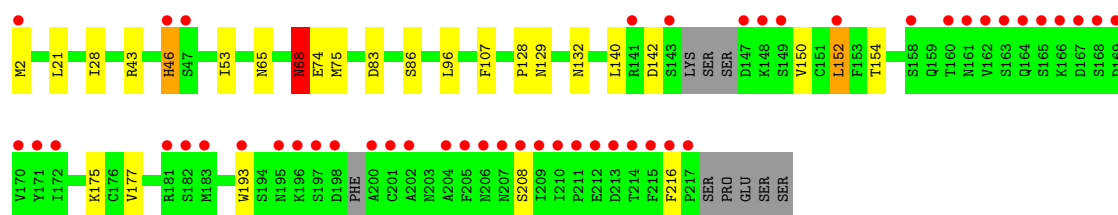
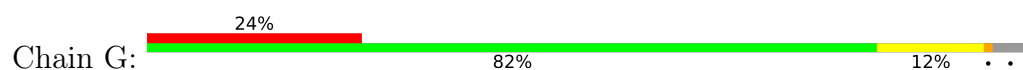
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



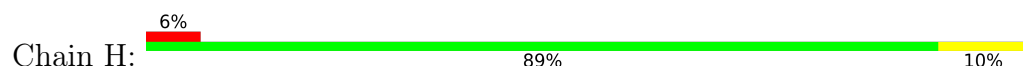
- Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain



- Molecule 3: T-CELL RECEPTOR, JR5.1 ALPHA CHAIN

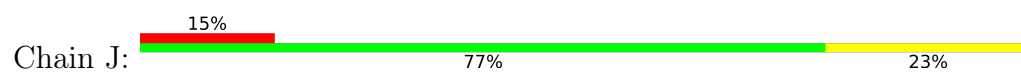


- Molecule 4: T-CELL RECEPTOR, JR5.1 BETA CHAIN





- Molecule 5: deamidated Gliadin-alpha2 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.93Å 84.84Å 109.68Å 90.00° 92.99° 90.00°	Depositor
Resolution (Å)	60.47 – 2.70 60.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (60.47-2.70) 97.8 (60.47-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.184 , 0.238 0.197 , 0.252	Depositor DCC
R_{free} test set	1636 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	0/1487	1.26	7/2031 (0.3%)
2	B	0.87	1/1513 (0.1%)	1.25	8/2056 (0.4%)
3	G	0.84	0/1502	1.29	8/2045 (0.4%)
4	H	0.76	0/1920	1.18	2/2617 (0.1%)
5	J	0.92	0/102	1.25	0/142
All	All	0.82	1/6524 (0.0%)	1.24	25/8891 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	89	THR	CA-C	12.34	1.58	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLY	CA-C-N	8.24	132.46	120.51
1	A	100	GLY	C-N-CA	8.24	132.46	120.51
2	B	32	TYR	CA-C-N	8.03	136.14	121.70
2	B	32	TYR	C-N-CA	8.03	136.14	121.70
4	H	74	ASP	CA-CB-CG	7.28	119.88	112.60
3	G	216	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	113	PHE	CA-CB-CG	-7.01	106.79	113.80
3	G	83	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	118	ASN	CA-CB-CG	6.31	118.91	112.60
3	G	107	PHE	CA-CB-CG	6.19	119.99	113.80
2	B	164	THR	CB-CA-C	5.65	119.66	111.02
3	G	208	SER	CA-C-N	5.64	131.86	121.70
3	G	208	SER	C-N-CA	5.64	131.86	121.70
4	H	108	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	101	GLN	N-CA-C	5.49	115.91	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	152	ASP	CA-CB-CG	5.46	118.06	112.60
3	G	68	ASN	CA-CB-CG	5.42	118.02	112.60
3	G	74	GLU	N-CA-C	-5.37	106.73	113.28
2	B	73	ALA	CA-C-N	5.28	127.88	120.28
2	B	73	ALA	C-N-CA	5.28	127.88	120.28
2	B	41	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	113	ASN	CA-CB-CG	5.13	117.73	112.60
3	G	142	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	140	LYS	CA-C-N	5.04	127.54	120.28
1	A	140	LYS	C-N-CA	5.04	127.54	120.28

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	1445	0	1396	10	0
2	B	1480	0	1443	9	0
3	G	1471	0	1361	8	0
4	H	1871	0	1765	9	0
5	J	97	0	89	2	0
6	A	28	0	26	0	0
7	A	78	0	0	0	0
7	B	68	0	0	0	0
7	G	43	0	0	0	0
7	H	40	0	0	0	0
7	J	3	0	0	0	0
All	All	6624	0	6080	32	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 (32) 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)
4:H:109:ARG:HH21	5:J:8:PRO:HD2	1.47	0.78
2:B:41:ASP:HB3	2:B:44:VAL:HG13	1.70	0.72
4:H:21:LEU:HD22	4:H:122:THR:HG21	1.79	0.65
2:B:35:GLU:OE1	2:B:51:THR:HG21	1.96	0.64
1:A:62:ASN:OD1	4:H:109:ARG:NH2	2.33	0.61
2:B:77:ARG:NH2	5:J:5:PRO:O	2.35	0.60
2:B:51:THR:HG22	2:B:53:LEU:H	1.69	0.57
3:G:68:ASN:HB3	3:G:75:MET:H	1.76	0.50
3:G:150:VAL:HG12	3:G:193:TRP:HB3	1.94	0.49
1:A:97:VAL:HG21	1:A:178:TRP:HZ2	1.78	0.49
4:H:83:GLY:HA3	4:H:85:SER:H	1.78	0.48
1:A:7:ALA:HB2	1:A:26:PHE:HD1	1.79	0.47
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.96	0.47
1:A:132:VAL:HA	1:A:150:TYR:O	2.14	0.47
3:G:43:ARG:HB3	3:G:53:ILE:HD11	1.96	0.46
4:H:145:GLU:HA	4:H:148:ILE:HD12	2.00	0.44
3:G:152:LEU:HD22	3:G:154:THR:HB	2.00	0.44
1:A:105:LEU:HG	1:A:153:LEU:HD22	1.98	0.44
2:B:10:GLN:HB2	2:B:31:ILE:HB	2.00	0.43
2:B:37:ILE:HA	2:B:51:THR:HB	2.01	0.43
2:B:26:LEU:H	2:B:42:SER:HB3	1.83	0.42
2:B:115:LEU:HD12	2:B:115:LEU:HA	1.89	0.42
1:A:76:ARG:HG2	2:B:53:LEU:HD22	2.01	0.42
3:G:46:HIS:HD2	4:H:187:PRO:HB2	1.84	0.42
3:G:2:MET:CB	3:G:28:ILE:HA	2.50	0.42
4:H:46:LEU:HD23	4:H:47:GLY:HA2	2.02	0.41
4:H:6:GLN:HB2	4:H:120:PRO:HD2	2.01	0.41
1:A:7:ALA:HB2	1:A:26:PHE:CD1	2.56	0.41
3:G:140:LEU:HB3	4:H:141:PHE:HB3	2.03	0.41
1:A:117:VAL:HG23	1:A:167:HIS:HB2	2.03	0.41
1:A:122:LEU:HD11	1:A:164:LYS:HD3	2.03	0.41
3:G:128:PRO:HG3	3:G:177:VAL:HG21	2.02	0.41

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	179/191 (94%)	174 (97%)	5 (3%)	0	100	100
2	B	177/213 (83%)	168 (95%)	9 (5%)	0	100	100
3	G	187/202 (93%)	177 (95%)	9 (5%)	1 (0%)	24	48
4	H	240/244 (98%)	226 (94%)	13 (5%)	1 (0%)	30	54
5	J	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
All	All	794/863 (92%)	754 (95%)	38 (5%)	2 (0%)	36	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	83	GLY
3	G	46	HIS

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	165/174 (95%)	158 (96%)	7 (4%)	26	55
2	B	164/188 (87%)	151 (92%)	13 (8%)	11	28
3	G	157/181 (87%)	148 (94%)	9 (6%)	18	43
4	H	199/209 (95%)	189 (95%)	10 (5%)	22	48
5	J	11/11 (100%)	10 (91%)	1 (9%)	9	22
All	All	696/763 (91%)	656 (94%)	40 (6%)	18	43

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	128	VAL
1	A	129	THR

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Mol	Chain	Res	Type
1	A	132	VAL
1	A	153	LEU
1	A	156	SER
1	A	158	GLU
2	B	26	LEU
2	B	30	SER
2	B	42	SER
2	B	44	VAL
2	B	48	ARG
2	B	51	THR
2	B	77	ARG
2	B	100	THR
2	B	114	LEU
2	B	115	LEU
2	B	127	ILE
2	B	128	LYS
2	B	142	VAL
3	G	21	LEU
3	G	65	ASN
3	G	68	ASN
3	G	86	SER
3	G	96	LEU
3	G	129	ASN
3	G	132	ASN
3	G	152	LEU
3	G	175	LYS
4	H	7	SER
4	H	45	SER
4	H	48	GLN
4	H	79	GLU
4	H	89	LEU
4	H	111	LEU
4	H	127	LEU
4	H	156	LEU
4	H	204	SER
4	H	212	THR
5	J	6	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN

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Mol	Chain	Res	Type
2	B	19	ASN
2	B	92	GLN
3	G	44	GLN
3	G	195	ASN
4	H	29	HIS
4	H	44	GLN
4	H	63	ASN
4	H	95	GLN
4	H	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	1001	1	14,14,15	0.39	0	17,19,21	1.57	2 (11%)
6	NAG	A	1000	1	14,14,15	0.31	0	17,19,21	1.10	2 (11%)

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	1001	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1000	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1001	NAG	C1-C2-N2	5.29	118.77	110.43
6	A	1000	NAG	C1-O5-C5	3.57	116.97	112.19
6	A	1001	NAG	C2-N2-C7	2.06	125.66	122.90
6	A	1000	NAG	O5-C1-C2	-2.01	108.19	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	NAG	C1-C2-N2-C7

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	181/191 (94%)	-0.35	2 (1%) 78 76	14, 27, 47, 84	0
2	B	181/213 (84%)	-0.21	2 (1%) 78 76	11, 28, 60, 90	0
3	G	193/202 (95%)	0.92	48 (24%) 2 1	16, 49, 112, 140	0
4	H	242/244 (99%)	0.45	15 (6%) 26 23	17, 49, 88, 106	0
5	J	13/13 (100%)	0.18	2 (15%) 5 4	15, 22, 47, 64	0
All	All	810/863 (93%)	0.23	69 (8%) 16 14	11, 35, 94, 140	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	143	SER	7.4
4	H	256	ALA	6.1
2	B	190	ALA	5.5
3	G	217	PRO	5.3
3	G	168	SER	5.2
3	G	167	ASP	5.2
3	G	198	ASP	4.6
3	G	200	ALA	4.4
3	G	169	ASP	3.7
3	G	211	PRO	3.6
3	G	210	ILE	3.6
3	G	170	VAL	3.5
4	H	47	GLY	3.4
3	G	165	SER	3.4
3	G	205	PHE	3.4
3	G	214	THR	3.3
3	G	207	ASN	3.3
3	G	2	MET	3.3
3	G	197	SER	3.3
3	G	208	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	G	213	ASP	3.2
3	G	141	ARG	3.2
3	G	216	PHE	3.1
4	H	240	ARG	3.1
3	G	161	ASN	3.0
3	G	162	VAL	3.0
3	G	181	ARG	3.0
3	G	160	THR	3.0
3	G	215	PHE	3.0
3	G	212	GLU	3.0
3	G	46	HIS	2.9
4	H	197	ASN	2.9
3	G	172	ILE	2.9
3	G	149	SER	2.8
1	A	1	ILE	2.8
3	G	166	LYS	2.8
3	G	209	ILE	2.8
1	A	181	GLU	2.8
3	G	206	ASN	2.7
2	B	3	SER	2.7
3	G	193	TRP	2.7
5	J	2	ALA	2.6
3	G	171	TYR	2.6
3	G	182	SER	2.5
3	G	152	LEU	2.5
3	G	148	LYS	2.5
3	G	163	SER	2.5
3	G	204	ALA	2.5
3	G	47	SER	2.4
4	H	46	LEU	2.3
5	J	13	GLY	2.3
4	H	217	PRO	2.3
4	H	48	GLN	2.2
4	H	195	ALA	2.2
4	H	132	ASN	2.2
3	G	202	ALA	2.1
4	H	255	ARG	2.1
4	H	212	THR	2.1
3	G	195	ASN	2.1
3	G	147	ASP	2.1
3	G	158	SER	2.1
4	H	96	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	196	LYS	2.1
3	G	201	CYS	2.1
4	H	149	SER	2.0
4	H	236	TRP	2.0
4	H	198	ASP	2.0
3	G	183	MET	2.0
3	G	164	GLN	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	1001	14/15	0.54	0.20	77,84,86,86	0
6	NAG	A	1000	14/15	0.87	0.11	36,48,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.