



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:30 AM BST

PDB ID : 1KJ2
Title : Murine Alloreactive ScFv TCR-Peptide-MHC Class I Molecule Complex
Authors : Reiser, J.-B.; Gregoire, C.; Darnault, C.; Mosser, T.; Guimezanes, A.; Schmitt-Verhulst, A.-M.; Fontecilla-Camps, J.C.; Mazza, G.; Malissen, B.; Housset, D.
Deposited on : 2001-12-04
Resolution : 2.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

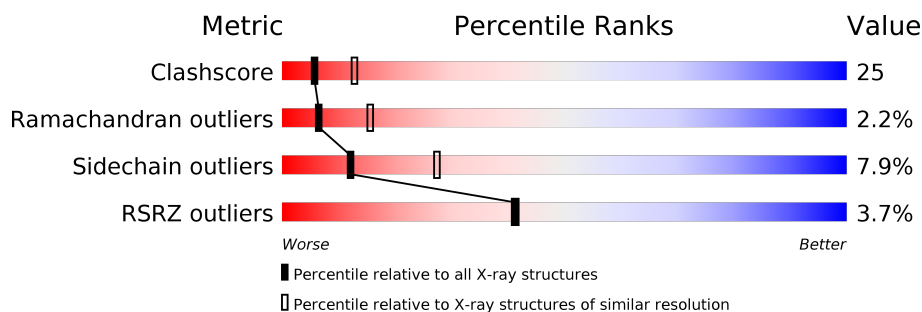
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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))
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on 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	H	277	<div> <div>5%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	I	277	<div> <div>4%</div> <div>61%</div> <div>34%</div> <div>5%</div> </div>
2	P	8	<div> <div>50%</div> <div>38%</div> <div>13%</div> </div>
2	Q	8	<div> <div>25%</div> <div>63%</div> <div>13%</div> </div>
3	L	99	<div> <div>2%</div> <div>59%</div> <div>39%</div> <div>.</div> </div>
3	M	99	<div> <div>4%</div> <div>52%</div> <div>42%</div> <div>6%</div> </div>
4	A	111	<div> <div>2%</div> <div>53%</div> <div>40%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	111	
5	B	117	
5	E	117	
6	C	8	

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
6	MAN	C	3	X	-	-	-
6	MAN	C	8	X	-	-	X
7	NAG	E	401	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10144 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 Allogeneic H-2Kb MHC Class I Molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	276	Total	C	N	O	S	0	0	0
			2247	1418	395	425	9			
1	I	277	Total	C	N	O	S	0	0	0
			2254	1423	396	426	9			

- Molecule 2 is a protein called Naturally processed octapeptide PKB1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	8	Total	C	N	O	0	0	0
			67	46	9	12			
2	Q	8	Total	C	N	O	0	0	0
			67	46	9	12			

- Molecule 3 is a protein called Beta-2 microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
3	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

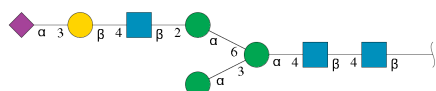
- Molecule 4 is a protein called KB5-C20 T-Cell receptor alpha-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	111	Total	C	N	O	S	0	0	0
			881	560	149	170	2			
4	D	111	Total	C	N	O	S	0	0	0
			881	560	149	170	2			

- Molecule 5 is a protein called KB5-C20 T-Cell receptor beta-chain.

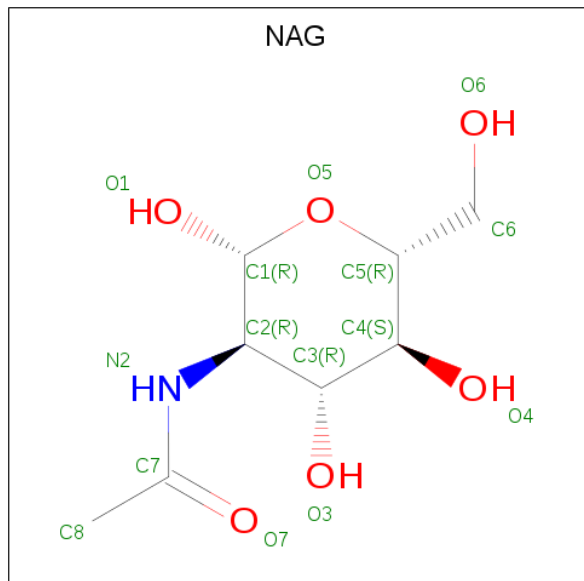
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	117	Total	C	N	O	S	0	0	0
			940	596	167	172	5			
5	E	117	Total	C	N	O	S	0	0	0
			940	596	167	172	5			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	C	8	Total	C	N	O	0	0	0
			106	59	4	43			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

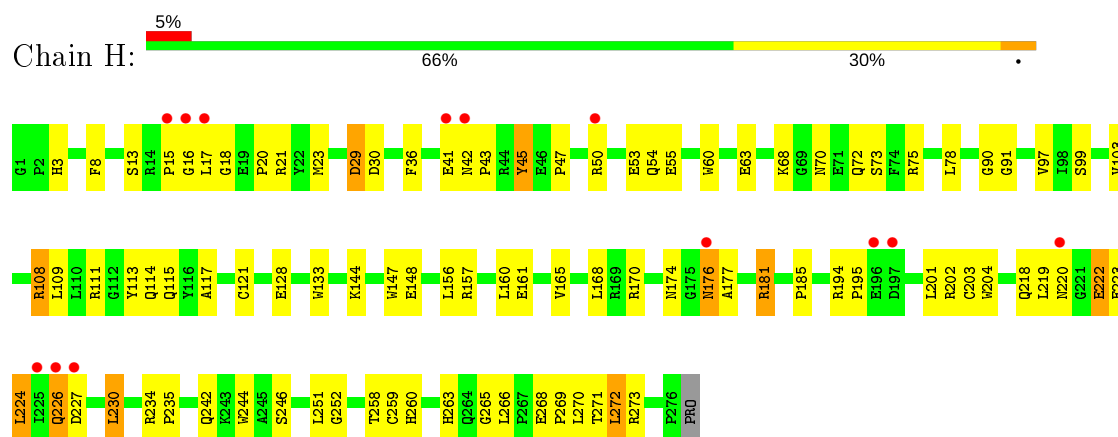
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	22	Total 22	O 22	0	0
8	P	2	Total 2	O 2	0	0
8	L	12	Total 12	O 12	0	0
8	A	5	Total 5	O 5	0	0
8	B	10	Total 10	O 10	0	0
8	I	18	Total 18	O 18	0	0
8	Q	3	Total 3	O 3	0	0
8	M	6	Total 6	O 6	0	0
8	D	6	Total 6	O 6	0	0
8	E	7	Total 7	O 7	0	0

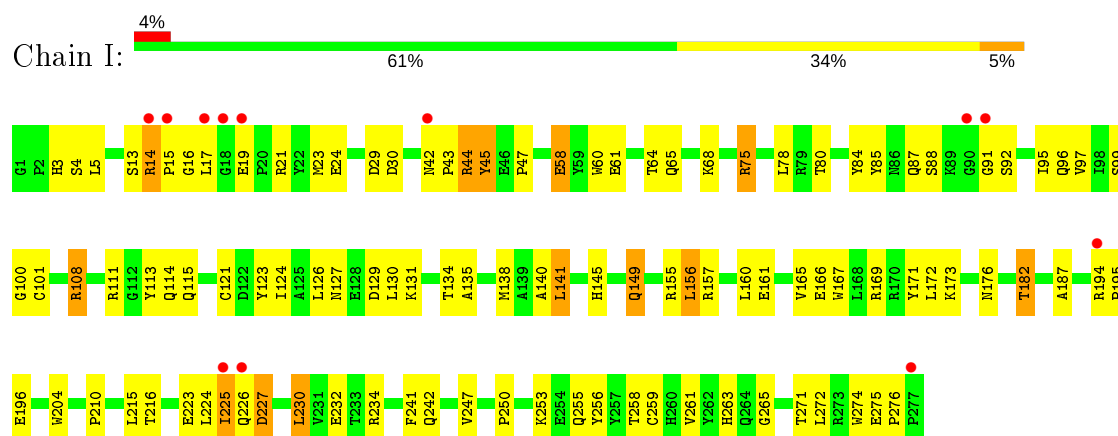
3 Residue-property plots [i](#)

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

- Molecule 1: Allogeneic H-2Kb MHC Class I Molecule



- Molecule 1: Allogeneic H-2Kb MHC Class I Molecule



- Molecule 2: Naturally processed octapeptide PKB1



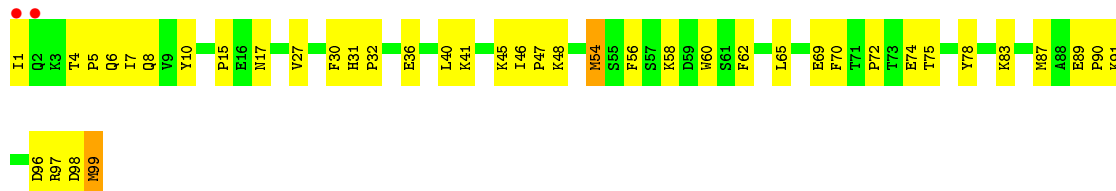
- Molecule 2: Naturally processed octapeptide PKB1

Chain Q: 



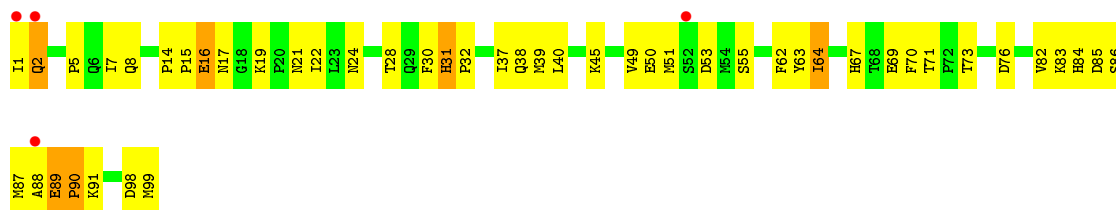
- Molecule 3: Beta-2 microglobulin

Chain L: 



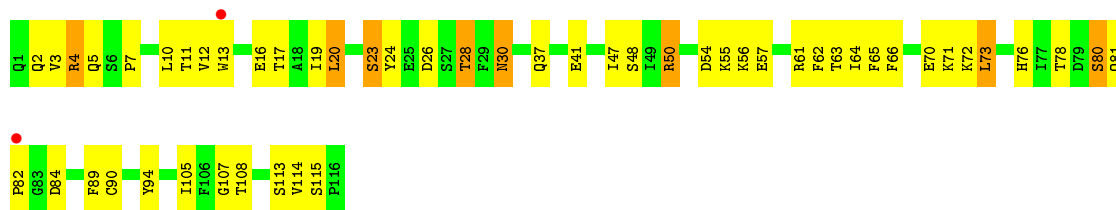
- Molecule 3: Beta-2 microglobulin

Chain M: 



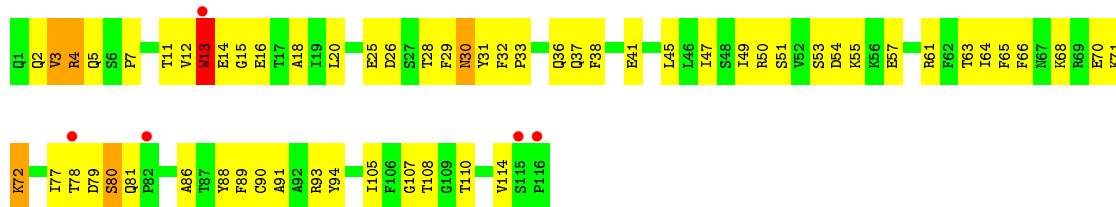
- Molecule 4: KB5-C20 T-Cell receptor alpha-chain

Chain A: 

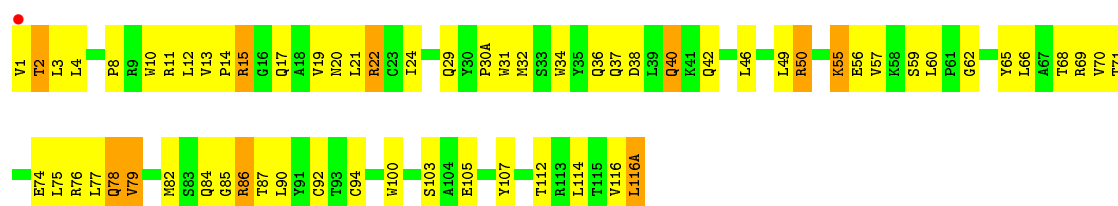
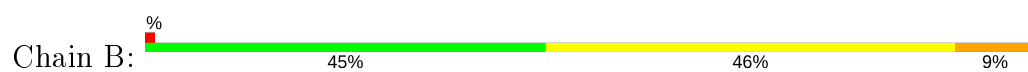


- Molecule 4: KB5-C20 T-Cell receptor alpha-chain

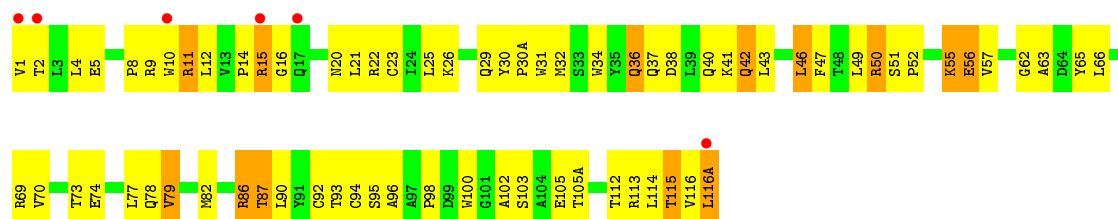
Chain D: 



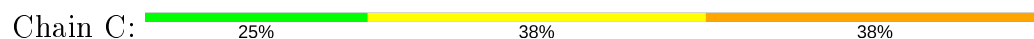
- Molecule 5: KB5-C20 T-Cell receptor beta-chain



- Molecule 5: KB5-C20 T-Cell receptor beta-chain



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)] alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.20Å 77.92Å 132.96Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	12.00 – 2.71 14.99 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (12.00-2.71) 95.5 (14.99-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.73Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.220 , 0.278 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10144	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9477e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SIA, GAL, 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	H	0.45	0/2309	0.71	0/3137
1	I	0.45	0/2317	0.70	0/3149
2	P	0.68	0/67	0.81	0/88
2	Q	0.62	0/67	0.79	0/88
3	L	0.45	0/847	0.73	0/1148
3	M	0.41	0/847	0.71	1/1148 (0.1%)
4	A	0.43	0/904	0.66	0/1225
4	D	0.41	0/904	0.67	0/1225
5	B	0.43	0/962	0.80	0/1310
5	E	0.43	0/962	0.77	0/1310
All	All	0.44	0/10186	0.72	1/13828 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	GLN	N-CA-C	-5.46	96.26	111.00

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	H	2247	0	2136	81	0
1	I	2254	0	2143	99	0
2	P	67	0	77	3	0
2	Q	67	0	77	5	0
3	L	821	0	796	32	0
3	M	821	0	796	44	0
4	A	881	0	844	53	0
4	D	881	0	845	74	0
5	B	940	0	936	70	0
5	E	940	0	936	77	0
6	C	106	0	89	7	0
7	B	14	0	13	0	0
7	E	14	0	13	0	0
8	A	5	0	0	1	0
8	B	10	0	0	1	0
8	D	6	0	0	2	0
8	E	7	0	0	4	0
8	H	22	0	0	2	0
8	I	18	0	0	3	0
8	L	12	0	0	0	0
8	M	6	0	0	0	0
8	P	2	0	0	0	0
8	Q	3	0	0	0	0
All	All	10144	0	9701	502	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 25.

The worst 5 of 502 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:I:14:ARG:HB3	1:I:15:PRO:HD2	1.33	1.09
4:D:108:THR:HA	5:E:42:GLN:HE22	1.22	1.02
4:D:13:TRP:HB2	4:D:16:GLU:HG3	1.46	0.96
1:I:138:MET:HA	1:I:141:LEU:HD12	1.45	0.95
5:E:36:GLN:HB3	5:E:46:LEU:HD11	1.49	0.93

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	H	274/277 (99%)	247 (90%)	21 (8%)	6 (2%)	6	15
1	I	275/277 (99%)	248 (90%)	23 (8%)	4 (2%)	10	24
2	P	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	Q	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
3	L	97/99 (98%)	90 (93%)	5 (5%)	2 (2%)	7	16
3	M	97/99 (98%)	81 (84%)	10 (10%)	6 (6%)	1	2
4	A	109/111 (98%)	97 (89%)	11 (10%)	1 (1%)	17	38
4	D	109/111 (98%)	88 (81%)	19 (17%)	2 (2%)	8	20
5	B	115/117 (98%)	106 (92%)	7 (6%)	2 (2%)	9	21
5	E	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	38
All	All	1203/1224 (98%)	1069 (89%)	108 (9%)	26 (2%)	6	15

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	17	LEU
1	H	226	GLN
4	A	80	SER
1	I	225	ILE
3	M	53	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	234/235 (100%)	224 (96%)	10 (4%)	29	55
1	I	235/235 (100%)	219 (93%)	16 (7%)	16	35
2	P	8/8 (100%)	8 (100%)	0	100	100
2	Q	8/8 (100%)	8 (100%)	0	100	100
3	L	94/94 (100%)	88 (94%)	6 (6%)	17	37
3	M	94/94 (100%)	89 (95%)	5 (5%)	22	46
4	A	96/96 (100%)	86 (90%)	10 (10%)	7	15
4	D	96/96 (100%)	90 (94%)	6 (6%)	18	38
5	B	102/102 (100%)	90 (88%)	12 (12%)	5	11
5	E	102/102 (100%)	83 (81%)	19 (19%)	1	3
All	All	1069/1070 (100%)	985 (92%)	84 (8%)	12	27

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	116(A)	LEU
1	I	149	GLN
5	E	70	VAL
1	I	44	ARG
1	I	65	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	29	GLN
5	B	44	GLN
4	D	37	GLN
5	B	37	GLN
5	B	78	GLN

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 ⓘ

8 monosaccharides 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	C	1	4,6	14,14,15	0.63	0	17,19,21	0.76	1 (5%)
6	NAG	C	2	6	14,14,15	0.70	0	17,19,21	0.70	0
6	MAN	C	3	6	11,11,12	0.60	0	15,15,17	1.64	2 (13%)
6	MAN	C	4	6	11,11,12	0.79	0	15,15,17	0.66	0
6	NAG	C	5	6	14,14,15	0.66	0	17,19,21	1.18	1 (5%)
6	GAL	C	6	6	11,11,12	0.67	0	15,15,17	0.44	0
6	SIA	C	7	6	17,20,21	0.60	0	21,28,31	0.69	0
6	MAN	C	8	6	11,11,12	0.62	0	15,15,17	1.47	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	C	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	MAN	C	3	6	1/1/4/5	1/2/19/22	0/1/1/1
6	MAN	C	4	6	-	1/2/19/22	0/1/1/1
6	NAG	C	5	6	-	4/6/23/26	0/1/1/1
6	GAL	C	6	6	-	2/2/19/22	0/1/1/1
6	SIA	C	7	6	-	2/14/34/38	0/1/1/1
6	MAN	C	8	6	1/1/4/5	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3	MAN	C1-C2-C3	5.45	116.37	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	8	MAN	C1-C2-C3	3.80	114.34	109.67
6	C	8	MAN	C1-O5-C5	3.62	117.10	112.19
6	C	5	NAG	C4-C3-C2	3.24	115.76	111.02
6	C	1	NAG	C2-N2-C7	-2.37	119.52	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	3	MAN	C1
6	C	8	MAN	C1

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	7	SIA	C11-C10-N5-C5
6	C	7	SIA	O10-C10-N5-C5
6	C	5	NAG	O5-C5-C6-O6
6	C	5	NAG	C4-C5-C6-O6
6	C	6	GAL	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3	MAN	2	0
6	C	2	NAG	4	0
6	C	5	NAG	4	0
6	C	4	MAN	2	0
6	C	1	NAG	1	0

5.6 Ligand geometry

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
7	NAG	E	401	5	14,14,15	1.14	1 (7%)	17,19,21	1.08	2 (11%)
7	NAG	B	301	5	14,14,15	0.61	0	17,19,21	0.83	1 (5%)

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
7	NAG	B	301	5	-	2/6/23/26	0/1/1/1
7	NAG	E	401	5	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	401	NAG	C1-C2	3.74	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	401	NAG	O5-C1-C2	2.58	115.36	111.29
7	B	301	NAG	C2-N2-C7	-2.44	119.42	122.90
7	E	401	NAG	C3-C4-C5	-2.29	106.15	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	401	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	401	NAG	C8-C7-N2-C2
7	E	401	NAG	O7-C7-N2-C2
7	B	301	NAG	C8-C7-N2-C2
7	B	301	NAG	O7-C7-N2-C2

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	H	276/277 (99%)	-0.24	13 (4%) 31 30	13, 35, 78, 101	7 (2%)
1	I	277/277 (100%)	-0.13	12 (4%) 35 34	23, 40, 76, 102	10 (3%)
2	P	8/8 (100%)	-1.14	0 100 100	16, 19, 29, 31	0
2	Q	8/8 (100%)	-1.08	0 100 100	23, 29, 38, 42	0
3	L	99/99 (100%)	-0.28	2 (2%) 65 67	22, 36, 58, 88	2 (2%)
3	M	99/99 (100%)	0.25	4 (4%) 38 37	26, 55, 86, 98	3 (3%)
4	A	111/111 (100%)	-0.14	2 (1%) 68 70	17, 43, 71, 82	1 (0%)
4	D	111/111 (100%)	0.32	5 (4%) 33 32	23, 58, 89, 104	1 (0%)
5	B	117/117 (100%)	-0.15	1 (0%) 84 85	20, 44, 77, 86	1 (0%)
5	E	117/117 (100%)	-0.08	6 (5%) 28 27	23, 45, 81, 92	3 (2%)
All	All	1223/1224 (99%)	-0.11	45 (3%) 41 41	13, 42, 80, 104	28 (2%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	116	PRO	5.8
1	I	225	ILE	4.8
4	D	13	TRP	4.5
1	I	226	GLN	4.4
3	M	1	ILE	4.4

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 [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(Å ²)	Q<0.9
6	MAN	C	8	11/12	0.77	0.47	102,104,105,106	0
6	MAN	C	3	11/12	0.78	0.25	92,94,96,100	0
6	GAL	C	6	11/12	0.79	0.33	97,101,102,104	0
6	SIA	C	7	20/21	0.81	0.31	99,102,104,104	0
6	MAN	C	4	11/12	0.82	0.35	96,98,99,100	0
6	NAG	C	5	14/15	0.83	0.23	96,98,100,100	0
6	NAG	C	1	14/15	0.86	0.27	62,72,74,76	0
6	NAG	C	2	14/15	0.89	0.26	80,83,85,88	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. 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(Å ²)	Q<0.9
7	NAG	E	401	14/15	0.85	0.29	63,67,70,70	0
7	NAG	B	301	14/15	0.85	0.32	68,70,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.