



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 10:28 PM UTC

PDB ID : 8W85 / pdb_00008w85
Title : HLA-DQ2.5-gamma2 gliadin peptide in complex with DQN0385AE01
Authors : Irie, M.; Tsushima, T.; Teranishi-Ikawa, Y.; Takahashi, N.; Ishii, S.; Okura, Y.; Fukami, T.A.; Torizawa, T.
Deposited on : 2023-08-31
Resolution : 2.77 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 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

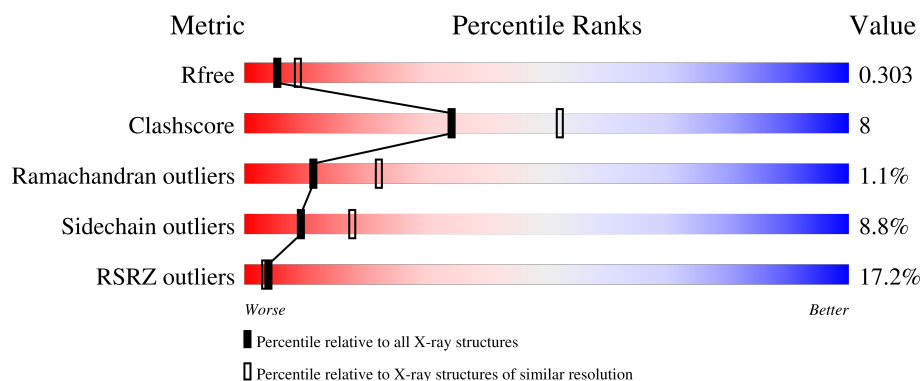
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	223	7% 67% 24% 5%
1	E	223	19% 44% 11% 43%
2	B	213	11% 77% 18% ..
2	F	213	15% 38% 10% 51%
3	C	189	8% 78% 14% 5%

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Mol	Chain	Length	Quality of chain
3	G	189	19% 69% 24% • 5%
4	D	222	10% 68% 15% • 16%
4	H	222	23% 64% 16% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10295 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 DQN0385AE01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1559	988	261	303	7			
1	E	126	Total	C	N	O	S	0	0	0
			875	555	141	174	5			

- Molecule 2 is a protein called DQN0385AE01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1548	973	249	321	5			
2	F	105	Total	C	N	O	S	0	0	0
			736	465	120	148	3			

- Molecule 3 is a protein called HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	180	Total	C	N	O	S	0	0	0
			1383	896	225	260	2			
3	G	179	Total	C	N	O	S	0	0	0
			1379	889	224	264	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	SER	CYS	engineered mutation	UNP P01909
C	184	LEU	-	expression tag	UNP P01909
C	185	GLU	-	expression tag	UNP P01909
C	186	VAL	-	expression tag	UNP P01909
C	187	LEU	-	expression tag	UNP P01909
C	188	PHE	-	expression tag	UNP P01909
C	189	GLN	-	expression tag	UNP P01909
G	47	SER	CYS	engineered mutation	UNP P01909

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Chain	Residue	Modelled	Actual	Comment	Reference
G	184	LEU	-	expression tag	UNP P01909
G	185	GLU	-	expression tag	UNP P01909
G	186	VAL	-	expression tag	UNP P01909
G	187	LEU	-	expression tag	UNP P01909
G	188	PHE	-	expression tag	UNP P01909
G	189	GLN	-	expression tag	UNP P01909

- Molecule 4 is a protein called MHC class II HLA-DQ-beta-1 - gamma2 gliadin peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	186	Total	C	N	O	S	0	0	0
			1427	909	247	264	7			
4	H	178	Total	C	N	O	S	0	0	0
			1360	869	231	253	7			

There are 42 discrepancies between the modelled and reference sequences:

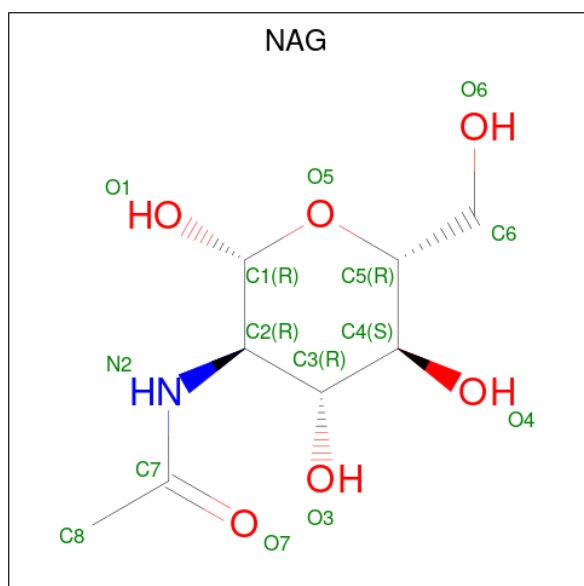
Chain	Residue	Modelled	Actual	Comment	Reference
D	986	GLY	-	linker	PDB ?
D	987	GLY	-	linker	PDB ?
D	988	GLY	-	linker	PDB ?
D	989	GLY	-	linker	PDB ?
D	990	SER	-	linker	PDB ?
D	991	ILE	-	linker	PDB ?
D	992	GLU	-	linker	PDB ?
D	993	GLY	-	linker	PDB ?
D	994	ARG	-	linker	PDB ?
D	995	GLY	-	linker	PDB ?
D	996	SER	-	linker	PDB ?
D	997	GLY	-	linker	PDB ?
D	998	GLY	-	linker	PDB ?
D	999	GLY	-	linker	PDB ?
D	1000	SER	-	linker	PDB ?
D	1191	LEU	-	expression tag	UNP O19712
D	1192	GLU	-	expression tag	UNP O19712
D	1193	VAL	-	expression tag	UNP O19712
D	1194	LEU	-	expression tag	UNP O19712
D	1195	PHE	-	expression tag	UNP O19712
D	1196	GLN	-	expression tag	UNP O19712
H	986	GLY	-	linker	PDB ?
H	987	GLY	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
H	988	GLY	-	linker	PDB ?
H	989	GLY	-	linker	PDB ?
H	990	SER	-	linker	PDB ?
H	991	ILE	-	linker	PDB ?
H	992	GLU	-	linker	PDB ?
H	993	GLY	-	linker	PDB ?
H	994	ARG	-	linker	PDB ?
H	995	GLY	-	linker	PDB ?
H	996	SER	-	linker	PDB ?
H	997	GLY	-	linker	PDB ?
H	998	GLY	-	linker	PDB ?
H	999	GLY	-	linker	PDB ?
H	1000	SER	-	linker	PDB ?
H	1191	LEU	-	expression tag	UNP O19712
H	1192	GLU	-	expression tag	UNP O19712
H	1193	VAL	-	expression tag	UNP O19712
H	1194	LEU	-	expression tag	UNP O19712
H	1195	PHE	-	expression tag	UNP O19712
H	1196	GLN	-	expression tag	UNP O19712

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

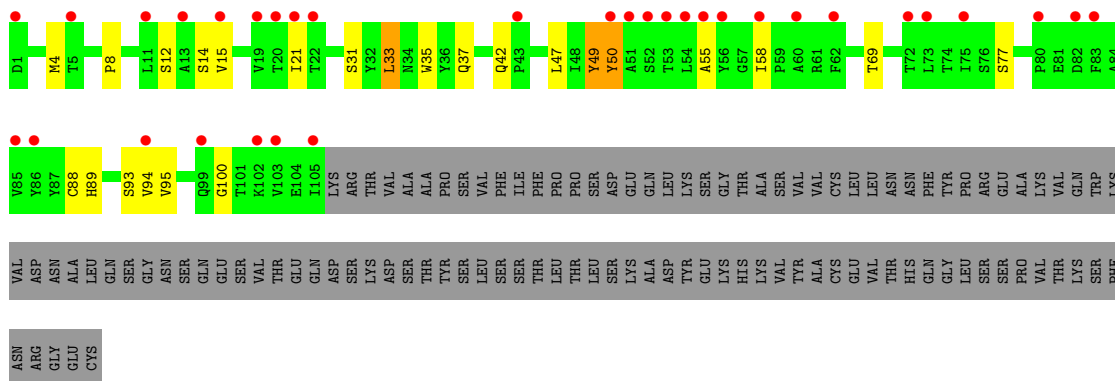
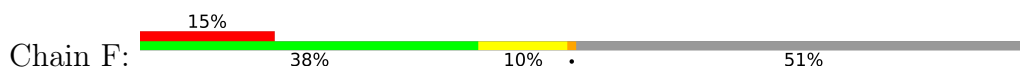
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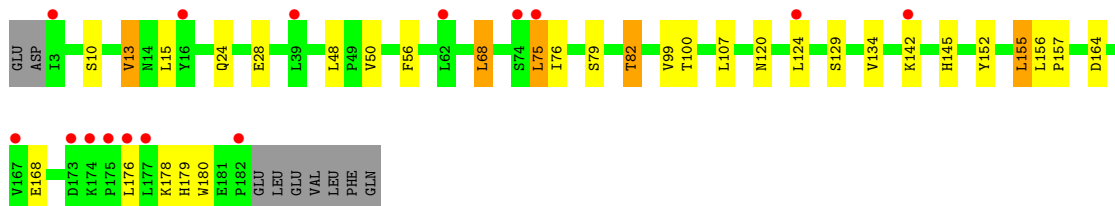
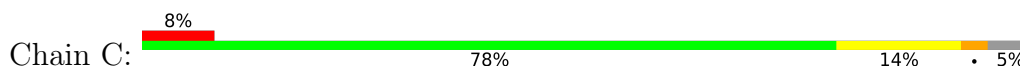
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		



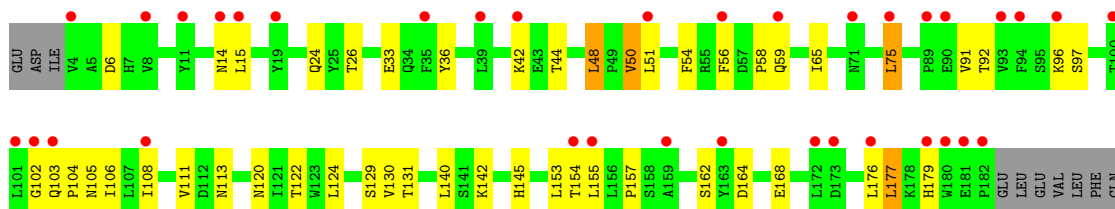
• Molecule 2: DQN0385AE01 Fab light chain



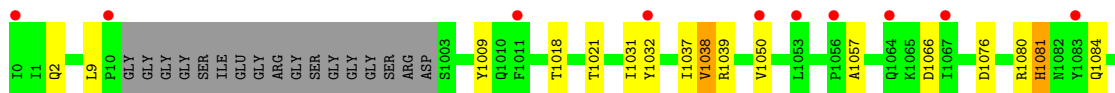
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

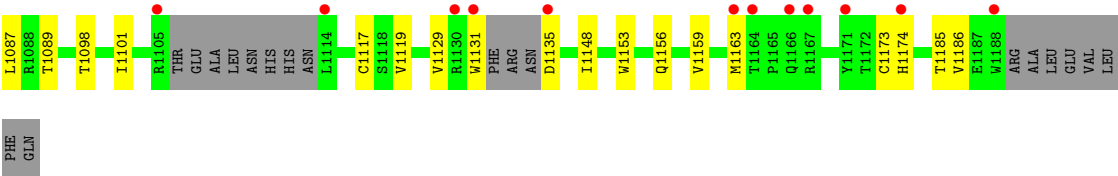


• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

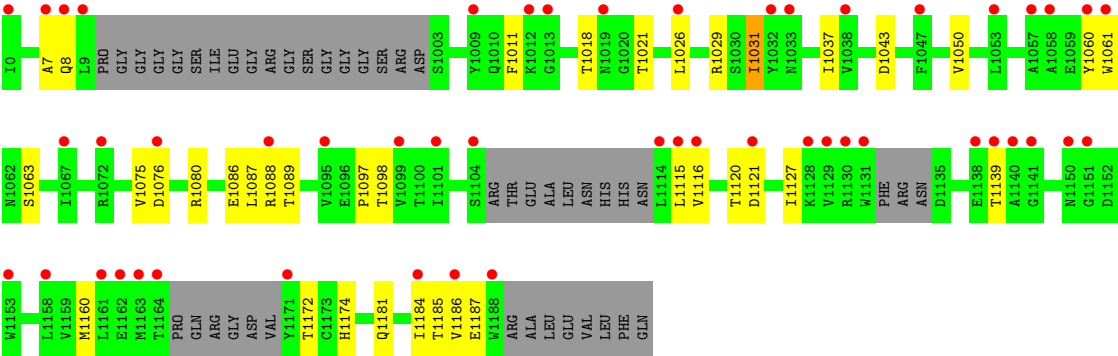


• Molecule 4: MHC class II HLA-DQ-beta-1 - gamma2 gliadin peptide chimeric protein





● Molecule 4: MHC class II HLA-DQ-beta-1 - gamma2 gliadin peptide chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.53Å 243.91Å 136.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.47 – 2.77 50.47 – 2.77	Depositor EDS
% Data completeness (in resolution range)	65.3 (50.47-2.77) 65.3 (50.47-2.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.253 , 0.300 0.251 , 0.303	Depositor DCC
R_{free} test set	2093 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10295	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	0/1601	1.13	5/2197 (0.2%)
1	E	0.73	0/898	1.02	0/1237
2	B	0.86	1/1584 (0.1%)	1.22	10/2172 (0.5%)
2	F	0.82	0/755	1.07	5/1036 (0.5%)
3	C	0.75	0/1425	1.12	3/1956 (0.2%)
3	G	0.69	0/1421	1.09	1/1951 (0.1%)
4	D	0.83	1/1459 (0.1%)	1.12	1/1996 (0.1%)
4	H	0.78	0/1389	1.08	5/1900 (0.3%)
All	All	0.79	2/10532 (0.0%)	1.12	30/14445 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MET	SD-CE	-6.57	1.63	1.79
4	D	1018	THR	CA-C	5.41	1.59	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	TYR	CA-C-N	7.67	136.19	121.54
2	B	50	TYR	C-N-CA	7.67	136.19	121.54
2	B	94	VAL	CB-CA-C	7.42	118.73	111.23
2	B	94	VAL	N-CA-CB	6.92	119.57	112.65
2	F	94	VAL	CA-C-N	6.49	130.25	120.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1559	0	1462	29	0
1	E	875	0	750	19	0
2	B	1548	0	1419	25	0
2	F	736	0	639	12	0
3	C	1383	0	1299	23	0
3	G	1379	0	1280	28	0
4	D	1427	0	1344	26	0
4	H	1360	0	1270	19	0
5	C	14	0	13	1	0
5	G	14	0	13	0	0
All	All	10295	0	9489	151	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.

The worst 5 of 151 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:E:17:SER:HB3	1:E:85:ASN:HA	1.52	0.89
1:A:92:THR:HG23	1:A:115:THR:HA	1.62	0.80
3:G:113:ASN:H	3:G:142:LYS:NZ	1.80	0.78
1:A:6:GLU:HB3	1:A:112:THR:HB	1.67	0.77
3:C:75:LEU:HD21	4:D:1037:ILE:HD13	1.70	0.73

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	207/223 (93%)	187 (90%)	17 (8%)	3 (1%)	9	17
1	E	122/223 (55%)	106 (87%)	16 (13%)	0	100	100
2	B	209/213 (98%)	185 (88%)	20 (10%)	4 (2%)	6	12
2	F	103/213 (48%)	83 (81%)	17 (16%)	3 (3%)	3	6
3	C	178/189 (94%)	166 (93%)	12 (7%)	0	100	100
3	G	177/189 (94%)	164 (93%)	9 (5%)	4 (2%)	5	9
4	D	178/222 (80%)	169 (95%)	9 (5%)	0	100	100
4	H	168/222 (76%)	153 (91%)	14 (8%)	1 (1%)	21	38
All	All	1342/1694 (79%)	1213 (90%)	114 (8%)	15 (1%)	11	22

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	TRP
2	B	51	ALA
2	B	100	GLY
2	B	137	ASN
1	A	149	ASP

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	168/188 (89%)	150 (89%)	18 (11%)	6	12
1	E	82/188 (44%)	72 (88%)	10 (12%)	5	8
2	B	168/187 (90%)	154 (92%)	14 (8%)	10	19
2	F	71/187 (38%)	62 (87%)	9 (13%)	4	8
3	C	151/173 (87%)	141 (93%)	10 (7%)	15	29
3	G	151/173 (87%)	137 (91%)	14 (9%)	8	16
4	D	150/196 (76%)	144 (96%)	6 (4%)	28	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	142/196 (72%)	128 (90%)	14 (10%)	7	15
All	All	1083/1488 (73%)	988 (91%)	95 (9%)	9	18

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	PHE
3	G	75	LEU
2	F	12	SER
2	F	69	THR
3	G	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	145	HIS
4	H	1156	GLN
4	H	8	GLN
3	C	179	HIS
3	G	17	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	$\# Z > 2$
5	NAG	G	1000	-	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	C	1000	-	14,14,15	0.34	0	17,19,21	1.28	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
5	NAG	G	1000	-	-	1/6/23/26	0/1/1/1
5	NAG	C	1000	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1000	NAG	O5-C1-C2	-4.90	103.70	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1000	NAG	C4-C5-C6-O6
5	C	1000	NAG	O5-C5-C6-O6
5	G	1000	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1000	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	211/223 (94%)	0.58	15 (7%) 22 22	44, 69, 91, 104	0
1	E	126/223 (56%)	1.67	42 (33%) 1 0	94, 115, 133, 144	0
2	B	211/213 (99%)	0.80	24 (11%) 10 8	52, 79, 102, 107	0
2	F	105/213 (49%)	1.84	33 (31%) 1 1	100, 121, 137, 141	0
3	C	180/189 (95%)	0.60	15 (8%) 17 18	46, 66, 88, 99	0
3	G	179/189 (94%)	1.33	35 (19%) 3 2	72, 93, 122, 139	0
4	D	186/222 (83%)	0.76	22 (11%) 9 7	50, 71, 94, 111	0
4	H	178/222 (80%)	1.44	50 (28%) 1 1	74, 95, 108, 116	0
All	All	1376/1694 (81%)	1.05	236 (17%) 4 3	44, 84, 124, 144	0

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	1105	ARG	6.0
4	H	1061	TRP	5.8
2	F	62	PHE	5.7
3	G	182	PRO	5.6
2	F	75	ILE	5.5

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
5	NAG	G	1000	14/15	0.65	0.17	170,170,171,171	0
5	NAG	C	1000	14/15	0.81	0.18	108,109,109,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.