



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:57 PM UTC

PDB ID : 8W84 / pdb_00008w84
Title : HLA-DQ2.5-alpha2 gliadin peptide in complex with DQN0344AE02
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 : 2.10 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

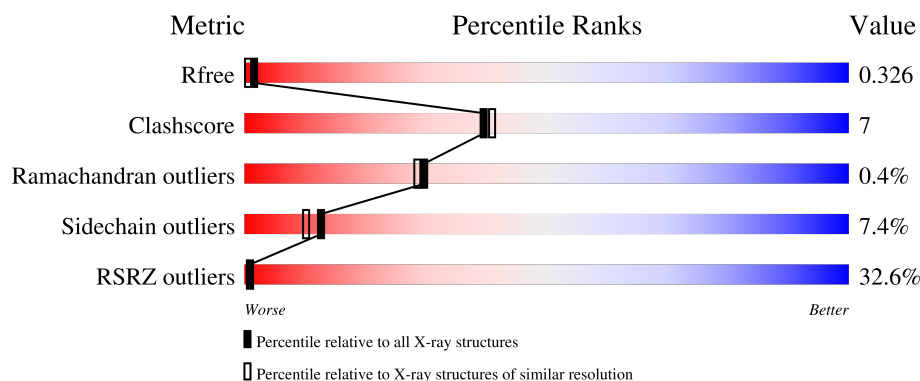
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 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	228	43% 74% 19% 5%
2	B	215	49% 79% 18% ..
3	C	189	21% 83% 14% ..
4	D	226	10% 67% 18% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6415 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 DQN0344AE02 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1594	1009	264	312	9			

- Molecule 2 is a protein called DQN0344AE02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1580	988	258	329	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	188	Total	C	N	O	S	0	0	0
			1460	946	239	273	2			

There are 7 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

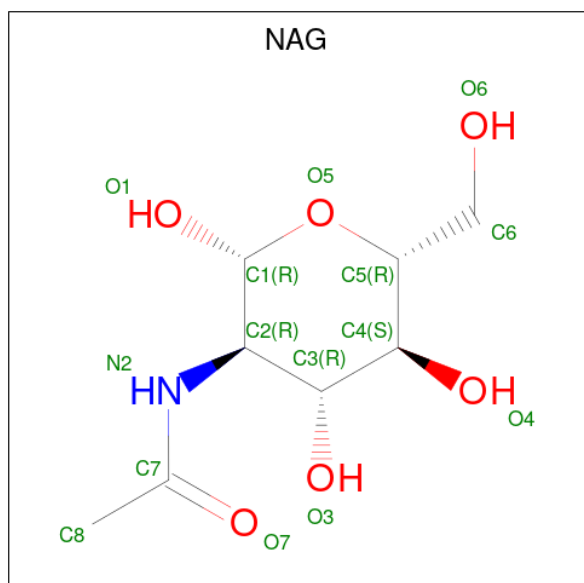
- Molecule 4 is a protein called MHC class II HLA-DQ-beta-1 - alpha2 gliadin peptide chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	0	0
			1586	1011	280	288	7			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	984	GLY	-	linker	PDB ?
D	985	SER	-	linker	PDB ?
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

- 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		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

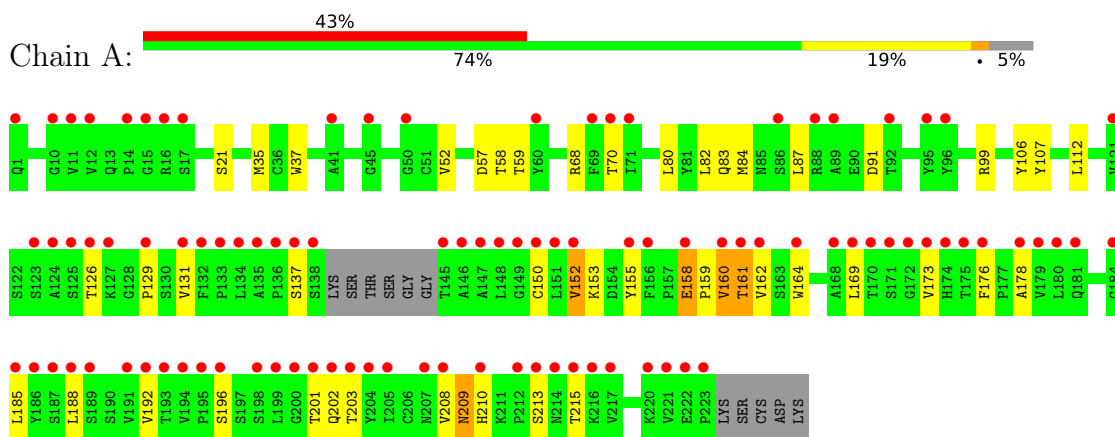
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	30	Total	O	0	0
			30	30		
6	C	42	Total	O	0	0
			42	42		
6	D	64	Total	O	0	0
			64	64		

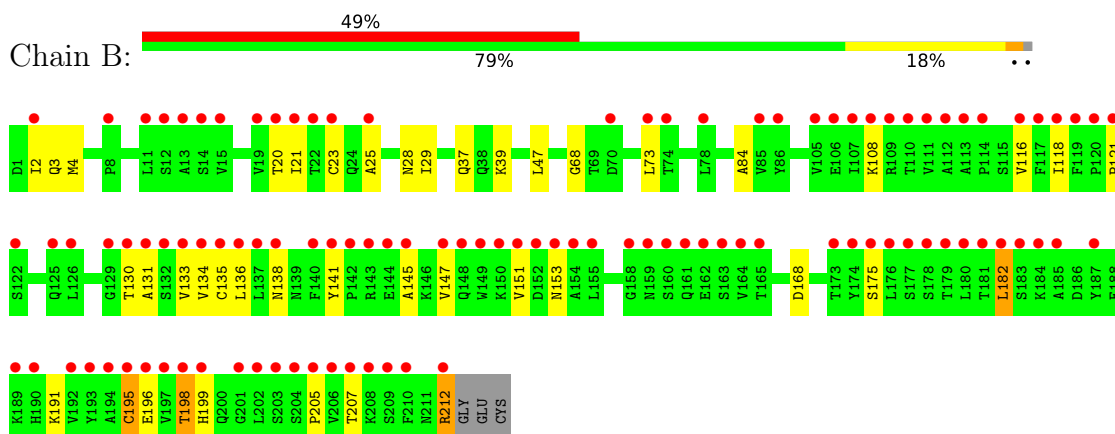
3 Residue-property plots [i](#)

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.

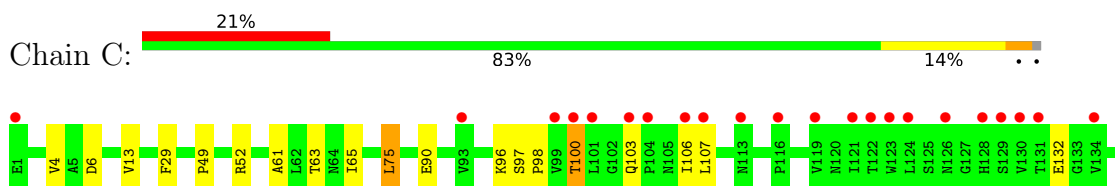
- Molecule 1: DQN0344AE02 Fab heavy chain

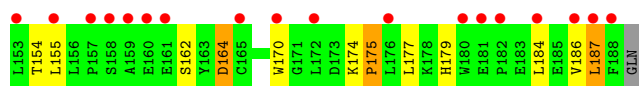


- Molecule 2: DQN0344AE02 Fab light chain

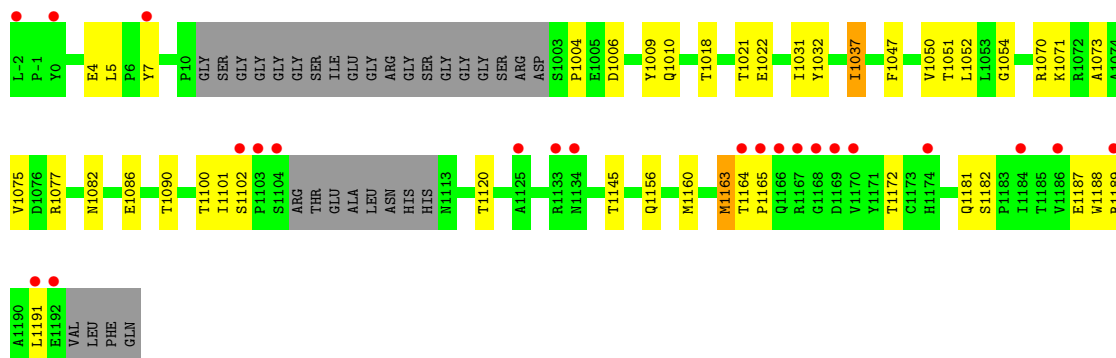


- Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain





- Molecule 4: MHC class II HLA-DQ-beta-1 - alpha2 gliadin peptide chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.86Å 138.71Å 201.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.33 – 2.10 114.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	58.1 (114.33-2.10) 58.1 (114.33-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.260 , 0.325 0.253 , 0.326	Depositor DCC
R_{free} test set	1916 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.6	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	0.92	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.72	0/1638	1.00	0/2246
2	B	0.82	0/1615	1.08	0/2207
3	C	0.76	0/1503	1.11	2/2059 (0.1%)
4	D	0.81	1/1626 (0.1%)	1.06	4/2216 (0.2%)
All	All	0.78	1/6382 (0.0%)	1.06	6/8728 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1163	MET	SD-CE	-5.05	1.67	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1164	THR	CB-CA-C	5.96	116.41	110.33
3	C	6	ASP	CA-CB-CG	5.69	118.29	112.60
3	C	13	VAL	N-CA-CB	5.41	118.18	111.41
4	D	5	LEU	N-CA-C	5.21	117.77	109.64
4	D	1051	THR	CA-C-N	5.13	127.41	120.38
4	D	1051	THR	C-N-CA	5.13	127.41	120.38

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	1594	0	1465	30	0
2	B	1580	0	1459	16	0
3	C	1460	0	1386	24	0
4	D	1586	0	1549	22	0
5	C	14	0	13	4	0
5	D	14	0	13	0	0
6	A	31	0	0	0	0
6	B	30	0	0	0	0
6	C	42	0	0	0	0
6	D	64	0	0	0	0
All	All	6415	0	5885	81	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 7.

All (81) 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:D:1172:THR:HG22	4:D:1187:GLU:HG2	1.69	0.73
1:A:52:VAL:HG23	1:A:59:THR:HG22	1.71	0.72
4:D:1073:ALA:HB1	4:D:1077:ARG:HE	1.55	0.70
3:C:100:THR:HB	3:C:103:GLN:CB	2.25	0.66
3:C:170:TRP:CD1	5:C:1000:NAG:H83	2.31	0.65
4:D:1163:MET:HE2	4:D:1165:PRO:HG3	1.79	0.64
3:C:107:LEU:HD13	3:C:155:LEU:HD21	1.80	0.62
3:C:75:LEU:HD13	4:D:1009:TYR:HE2	1.65	0.62
3:C:162:SER:HB2	3:C:179:HIS:HE1	1.64	0.61
1:A:160:VAL:HG23	1:A:210:HIS:HD2	1.66	0.61
3:C:170:TRP:NE1	5:C:1000:NAG:H83	2.16	0.60
1:A:70:THR:HB	1:A:83:GLN:HB2	1.82	0.60
1:A:178:ALA:HB2	1:A:188:LEU:HD23	1.84	0.58
3:C:106:ILE:HG12	3:C:154:THR:HG22	1.87	0.56
1:A:84:MET:HB3	1:A:87:LEU:HD21	1.86	0.56
3:C:164:ASP:HB3	3:C:177:LEU:HD12	1.88	0.55
4:D:1070:ARG:HH12	4:D:1077:ARG:CZ	2.20	0.55
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.90	0.54
2:B:198:THR:HG23	2:B:205:PRO:HG3	1.89	0.54
1:A:164:TRP:HD1	1:A:173:VAL:HG11	1.73	0.54
2:B:191:LYS:O	2:B:212:ARG:HB2	2.08	0.54
3:C:187:LEU:HG	4:D:1145:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:TRP:HB3	1:A:169:LEU:HD23	1.90	0.53
3:C:187:LEU:HG	4:D:1145:THR:CG2	2.38	0.53
1:A:160:VAL:CG2	1:A:210:HIS:HD2	2.21	0.53
1:A:129:PRO:HB3	1:A:155:TYR:HB3	1.92	0.52
2:B:121:PRO:HD3	2:B:133:VAL:HG22	1.92	0.52
1:A:160:VAL:CG2	1:A:210:HIS:CD2	2.93	0.52
1:A:99:ARG:HB3	1:A:112:LEU:HB3	1.93	0.51
3:C:170:TRP:CD1	5:C:1000:NAG:C8	2.94	0.51
1:A:107:TYR:O	4:D:1070:ARG:HD3	2.12	0.50
3:C:49:PRO:HA	3:C:52:ARG:HD2	1.92	0.50
2:B:2:ILE:HD13	2:B:29:ILE:HG22	1.94	0.50
2:B:21:ILE:HD12	2:B:73:LEU:HD23	1.92	0.50
3:C:174:LYS:O	3:C:175:PRO:O	2.30	0.49
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.94	0.49
3:C:184:LEU:HD12	3:C:187:LEU:HB2	1.93	0.49
2:B:145:ALA:HB2	2:B:199:HIS:HD2	1.77	0.49
1:A:37:TRP:CE2	1:A:82:LEU:HB2	2.48	0.49
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.95	0.49
1:A:210:HIS:HB3	1:A:215:THR:HB	1.94	0.48
4:D:1082:ASN:O	4:D:1086:GLU:HG2	2.14	0.48
4:D:1047:PHE:CZ	4:D:1071:LYS:HG3	2.49	0.47
1:A:202:GLN:HG3	1:A:203:THR:N	2.30	0.47
3:C:187:LEU:HD13	4:D:1160:MET:HE3	1.97	0.46
4:D:1037:ILE:O	4:D:1054:GLY:HA3	2.16	0.46
1:A:106:TYR:O	4:D:1077:ARG:HD3	2.16	0.46
2:B:28:ASN:OD1	2:B:68:GLY:HA2	2.16	0.46
2:B:131:ALA:HB3	2:B:182:LEU:HD12	1.99	0.45
1:A:160:VAL:HG23	1:A:210:HIS:CD2	2.48	0.45
1:A:131:VAL:HG22	1:A:152:VAL:HG12	1.99	0.44
4:D:1189:ARG:HH21	4:D:1191:LEU:HD21	1.82	0.44
3:C:170:TRP:HZ3	4:D:1006:ASP:HB2	1.82	0.44
3:C:96:LYS:HD3	3:C:106:ILE:HD12	2.00	0.44
3:C:162:SER:HB2	3:C:179:HIS:CE1	2.50	0.44
4:D:1101:ILE:HG21	4:D:1188:TRP:HB2	1.99	0.43
4:D:1010:GLN:HB2	4:D:1031:ILE:HB	2.01	0.43
1:A:153:LYS:HZ2	1:A:153:LYS:HG2	1.59	0.43
1:A:35:MET:HB3	1:A:80:LEU:HD22	2.01	0.43
2:B:4:MET:HE3	2:B:23:CYS:SG	2.59	0.43
1:A:164:TRP:CD1	1:A:173:VAL:CG1	3.02	0.42
2:B:108:LYS:HA	2:B:141:TYR:OH	2.18	0.42
1:A:158:GLU:HG2	1:A:159:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:ALA:O	3:C:65:ILE:HG12	2.19	0.42
3:C:170:TRP:HE1	5:C:1000:NAG:H83	1.80	0.42
1:A:164:TRP:HD1	1:A:173:VAL:CG1	2.32	0.41
1:A:57:ASP:O	1:A:59:THR:HG23	2.21	0.41
3:C:29:PHE:CD2	4:D:1090:THR:HG21	2.56	0.41
4:D:1120:THR:HG22	4:D:1156:GLN:HB2	2.02	0.41
1:A:160:VAL:HG22	1:A:210:HIS:HA	2.02	0.41
3:C:75:LEU:HD22	4:D:1032:TYR:HB2	2.03	0.41
2:B:116:VAL:HA	2:B:136:LEU:O	2.20	0.41
1:A:68:ARG:NH2	1:A:91:ASP:OD2	2.54	0.41
3:C:170:TRP:CE2	4:D:1004:PRO:HD2	2.56	0.41
4:D:7:TYR:CE1	4:D:1071:LYS:HE2	2.56	0.41
1:A:161:THR:HG22	1:A:209:ASN:HB2	2.03	0.41
1:A:176:PHE:HE1	2:B:175:SER:O	2.04	0.40
2:B:118:ILE:HD12	2:B:195:CYS:HB2	2.02	0.40
3:C:97:SER:HB2	3:C:98:PRO:HD2	2.03	0.40
1:A:210:HIS:ND1	1:A:213:SER:OG	2.39	0.40
2:B:4:MET:HE1	2:B:25:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/228 (93%)	199 (93%)	12 (6%)	2 (1%)	14	10
2	B	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
3	C	186/189 (98%)	178 (96%)	7 (4%)	1 (0%)	24	22
4	D	189/226 (84%)	179 (95%)	10 (5%)	0	100	100
All	All	798/858 (93%)	752 (94%)	43 (5%)	3 (0%)	30	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	175	PRO
1	A	137	SER
1	A	58	THR

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	A	168/193 (87%)	155 (92%)	13 (8%)	12	9
2	B	172/188 (92%)	156 (91%)	16 (9%)	8	6
3	C	160/173 (92%)	151 (94%)	9 (6%)	19	18
4	D	175/200 (88%)	163 (93%)	12 (7%)	14	12
All	All	675/754 (90%)	625 (93%)	50 (7%)	13	10

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	126	THR
1	A	150	CYS
1	A	152	VAL
1	A	158	GLU
1	A	160	VAL
1	A	161	THR
1	A	162	VAL
1	A	185	LEU
1	A	196	SER
1	A	201	THR
1	A	208	VAL
1	A	209	ASN
2	B	3	GLN
2	B	20	THR
2	B	130	THR
2	B	134	VAL
2	B	135	CYS
2	B	138	ASN

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Mol	Chain	Res	Type
2	B	147	VAL
2	B	151	VAL
2	B	153	ASN
2	B	168	ASP
2	B	182	LEU
2	B	195	CYS
2	B	196	GLU
2	B	198	THR
2	B	207	THR
2	B	212	ARG
3	C	4	VAL
3	C	63	THR
3	C	75	LEU
3	C	90	GLU
3	C	100	THR
3	C	132	GLU
3	C	164	ASP
3	C	186	VAL
3	C	187	LEU
4	D	4	GLU
4	D	1018	THR
4	D	1021	THR
4	D	1022	GLU
4	D	1037	ILE
4	D	1050	VAL
4	D	1052	LEU
4	D	1075	VAL
4	D	1100	THR
4	D	1102	SER
4	D	1181	GLN
4	D	1182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	75	ASN
1	A	83	GLN
1	A	85	ASN
1	A	209	ASN
2	B	38	GLN
3	C	59	GLN

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Mol	Chain	Res	Type
4	D	1150	ASN
4	D	1156	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 ⓘ

There are no oligosaccharides in this entry.

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	$\# Z > 2$
5	NAG	C	1000	3	14,14,15	0.26	0	17,19,21	0.60	0
5	NAG	D	2000	4	14,14,15	0.33	0	17,19,21	1.49	3 (17%)

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	C	1000	3	-	0/6/23/26	0/1/1/1
5	NAG	D	2000	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	D	2000	NAG	O5-C1-C2	4.34	118.00	111.29
5	D	2000	NAG	C1-C2-N2	-2.80	106.02	110.43
5	D	2000	NAG	C1-O5-C5	2.55	115.61	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1000	NAG	4	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

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	217/228 (95%)	1.86	97 (44%) 0 1	27, 62, 87, 104	0
2	B	212/215 (98%)	2.13	106 (50%) 0 0	31, 59, 89, 93	0
3	C	188/189 (99%)	1.21	40 (21%) 2 2	26, 49, 78, 84	0
4	D	195/226 (86%)	0.73	22 (11%) 10 10	23, 39, 60, 69	0
All	All	812/858 (94%)	1.51	265 (32%) 1 1	23, 51, 84, 104	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	185	ALA	6.4
4	D	1192	GLU	6.3
1	A	221	VAL	5.9
2	B	187	TYR	5.6
2	B	119	PHE	5.4
2	B	134	VAL	5.3
3	C	188	PHE	5.3
1	A	223	PRO	5.3
2	B	194	ALA	5.3
3	C	187	LEU	5.2
2	B	164	VAL	5.2
2	B	181	THR	5.1
4	D	1166	GLN	5.0
1	A	176	PHE	5.0
2	B	193	TYR	5.0
2	B	151	VAL	4.9
3	C	186	VAL	4.9
1	A	135	ALA	4.9
1	A	136	PRO	4.8
4	D	1168	GLY	4.8
2	B	141	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	210	PHE	4.7
1	A	199	LEU	4.7
1	A	124	ALA	4.6
3	C	159	ALA	4.6
2	B	182	LEU	4.5
1	A	184	GLY	4.5
1	A	134	LEU	4.5
2	B	149	TRP	4.5
2	B	180	LEU	4.4
1	A	145	THR	4.3
2	B	140	PHE	4.3
1	A	214	ASN	4.3
2	B	192	VAL	4.2
2	B	206	VAL	4.2
1	A	148	LEU	4.2
2	B	197	VAL	4.2
2	B	165	THR	4.2
3	C	101	LEU	4.2
3	C	121	ILE	4.1
1	A	180	LEU	4.1
2	B	203	SER	4.1
2	B	2	ILE	4.1
2	B	15	VAL	4.0
1	A	138	SER	4.0
1	A	126	THR	4.0
4	D	1167	ARG	4.0
2	B	195	CYS	4.0
3	C	100	THR	3.9
1	A	194	VAL	3.9
2	B	118	ILE	3.9
2	B	11	LEU	3.9
2	B	133	VAL	3.8
2	B	202	LEU	3.8
2	B	147	VAL	3.8
1	A	217	VAL	3.8
2	B	148	GLN	3.8
1	A	186	TYR	3.7
2	B	155	LEU	3.7
1	A	204	TYR	3.7
2	B	137	LEU	3.7
2	B	199	HIS	3.7
1	A	195	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	159	ASN	3.7
1	A	155	TYR	3.7
2	B	201	GLY	3.6
2	B	13	ALA	3.6
2	B	176	LEU	3.6
3	C	134	VAL	3.6
1	A	164	TRP	3.6
2	B	131	ALA	3.6
3	C	181	GLU	3.6
1	A	12	VAL	3.5
1	A	69	PHE	3.5
1	A	151	LEU	3.5
1	A	173	VAL	3.5
2	B	178	SER	3.5
1	A	121	VAL	3.5
2	B	113	ALA	3.5
2	B	120	PRO	3.4
1	A	147	ALA	3.4
1	A	189	SER	3.4
2	B	126	LEU	3.4
1	A	201	THR	3.4
4	D	1165	PRO	3.4
1	A	220	LYS	3.4
2	B	135	CYS	3.4
2	B	111	VAL	3.4
1	A	169	LEU	3.4
1	A	215	THR	3.3
2	B	150	LYS	3.3
3	C	176	LEU	3.3
2	B	179	THR	3.3
2	B	114	PRO	3.3
1	A	185	LEU	3.3
1	A	132	PHE	3.3
2	B	138	ASN	3.3
1	A	162	VAL	3.3
2	B	145	ALA	3.3
1	A	188	LEU	3.3
1	A	192	VAL	3.2
4	D	1186	VAL	3.2
4	D	-2	LEU	3.2
2	B	189	LYS	3.2
1	A	175	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	3.2
1	A	178	ALA	3.2
2	B	21	ILE	3.2
3	C	103	GLN	3.2
3	C	131	THR	3.2
2	B	143	ARG	3.2
4	D	1170	VAL	3.1
3	C	155	LEU	3.1
1	A	222	GLU	3.1
2	B	163	SER	3.1
2	B	142	PRO	3.1
1	A	10	GLY	3.1
1	A	146	ALA	3.1
1	A	156	PHE	3.1
1	A	89	ALA	3.1
3	C	180	TRP	3.0
2	B	109	ARG	3.0
3	C	184	LEU	3.0
1	A	198	SER	3.0
2	B	136	LEU	3.0
2	B	121	PRO	3.0
2	B	112	ALA	3.0
3	C	165	CYS	3.0
2	B	107	ILE	3.0
2	B	198	THR	3.0
4	D	1164	THR	3.0
1	A	150	CYS	2.9
1	A	131	VAL	2.9
2	B	152	ASP	2.9
2	B	190	HIS	2.9
1	A	129	PRO	2.9
1	A	191	VAL	2.8
2	B	19	VAL	2.8
1	A	137	SER	2.8
2	B	160	SER	2.8
1	A	196	SER	2.8
2	B	204	SER	2.8
2	B	20	THR	2.8
3	C	124	LEU	2.8
2	B	175	SER	2.7
1	A	216	LYS	2.7
2	B	174	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	193	THR	2.7
3	C	182	PRO	2.7
2	B	161	GLN	2.7
3	C	123	TRP	2.7
1	A	207	ASN	2.7
2	B	153	ASN	2.7
3	C	113	ASN	2.7
3	C	128	HIS	2.7
4	D	1104	SER	2.7
1	A	203	THR	2.7
3	C	104	PRO	2.7
1	A	179	VAL	2.7
2	B	105	VAL	2.7
1	A	210	HIS	2.6
1	A	213	SER	2.6
2	B	14	SER	2.6
2	B	110	THR	2.6
1	A	133	PRO	2.6
3	C	116	PRO	2.6
4	D	1191	LEU	2.6
2	B	183	SER	2.6
2	B	184	LYS	2.6
2	B	208	LYS	2.6
3	C	126	ASN	2.6
2	B	130	THR	2.6
2	B	154	ALA	2.6
1	A	127	LYS	2.6
2	B	78	LEU	2.6
3	C	153	LEU	2.6
1	A	123	SER	2.6
1	A	208	VAL	2.6
1	A	45	GLY	2.6
3	C	93	VAL	2.5
3	C	130	VAL	2.5
2	B	158	GLY	2.5
2	B	73	LEU	2.5
3	C	160	GLU	2.5
4	D	7	TYR	2.5
1	A	17	SER	2.5
2	B	117	PHE	2.5
2	B	116	VAL	2.5
3	C	161	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	12	SER	2.5
1	A	212	PRO	2.5
4	D	1133	ARG	2.5
4	D	1184	ILE	2.5
2	B	125	GLN	2.4
1	A	95	TYR	2.4
2	B	23	CYS	2.4
1	A	170	THR	2.4
2	B	122	SER	2.4
4	D	1103	PRO	2.4
2	B	144	GLU	2.4
4	D	1102	SER	2.4
3	C	99	VAL	2.4
1	A	60	TYR	2.4
2	B	74	THR	2.4
2	B	8	PRO	2.4
1	A	181	GLN	2.4
1	A	205	ILE	2.4
1	A	171	SER	2.4
2	B	132	SER	2.4
1	A	149	GLY	2.3
4	D	1169	ASP	2.3
3	C	129	SER	2.3
1	A	158	GLU	2.3
3	C	170	TRP	2.3
1	A	15	GLY	2.3
1	A	71	ILE	2.3
1	A	11	VAL	2.3
1	A	202	GLN	2.3
1	A	96	TYR	2.3
2	B	212	ARG	2.3
1	A	86	SER	2.3
1	A	174	HIS	2.3
1	A	187	SER	2.3
2	B	196	GLU	2.3
2	B	85	VAL	2.3
2	B	209	SER	2.2
1	A	160	VAL	2.2
3	C	122	THR	2.2
3	C	157	PRO	2.2
1	A	50	GLY	2.2
2	B	129	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	107	LEU	2.2
2	B	162	GLU	2.2
1	A	16	ARG	2.2
4	D	1189	ARG	2.2
1	A	200	GLY	2.2
2	B	25	ALA	2.2
1	A	1	GLN	2.2
1	A	125	SER	2.2
2	B	177	SER	2.2
1	A	14	PRO	2.2
1	A	161	THR	2.2
2	B	70	ASP	2.2
1	A	172	GLY	2.2
1	A	41	ALA	2.2
1	A	168	ALA	2.2
3	C	158	SER	2.2
3	C	1	GLU	2.1
3	C	119	VAL	2.1
2	B	108	LYS	2.1
3	C	106	ILE	2.1
3	C	172	LEU	2.1
4	D	1134	ASN	2.1
2	B	86	TYR	2.1
1	A	70	THR	2.1
2	B	22	THR	2.1
4	D	1125	ALA	2.1
2	B	173	THR	2.1
2	B	205	PRO	2.1
2	B	207	THR	2.1
4	D	0	TYR	2.1
1	A	88	ARG	2.0
4	D	1174	HIS	2.0
2	B	106	GLU	2.0
1	A	92	THR	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 [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	D	2000	14/15	0.74	0.12	75,76,77,77	0
5	NAG	C	1000	14/15	0.78	0.14	76,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.