



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:29 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 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:

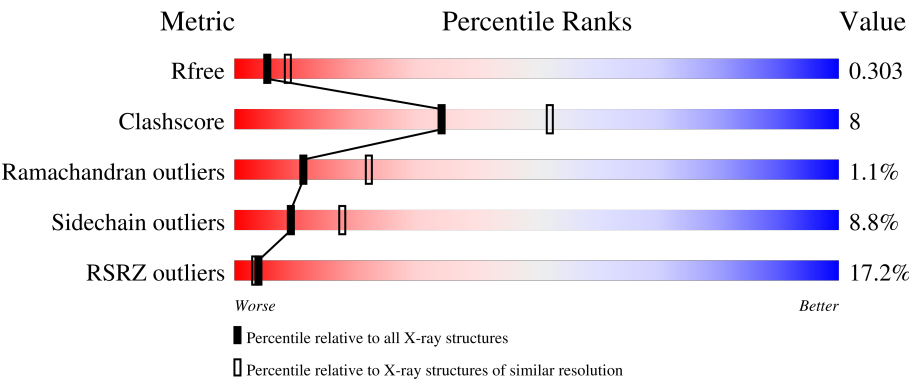
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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:

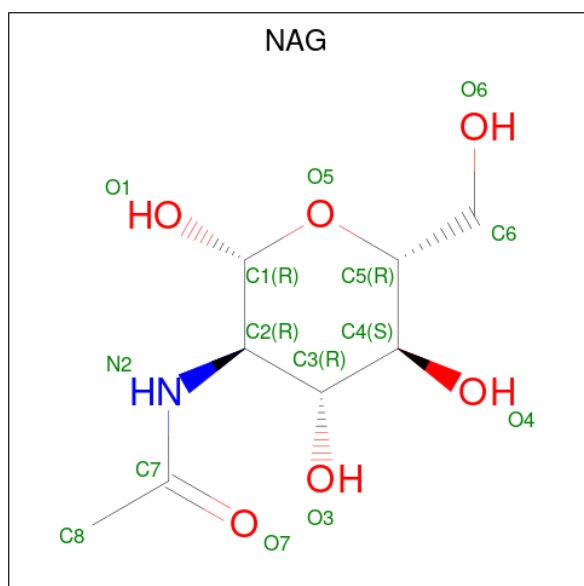
Chain	Residue	Modelled	Actual	Comment	Reference
D	986	GLY	-	linker	PDB ?
D	987	GLY	-	linker	PDB ?
D	988	GLY	-	linker	PDB ?
D	989	GLY	-	linker	PDB ?
D	990	SER	-	linker	PDB ?
D	991	ILE	-	linker	PDB ?
D	992	GLU	-	linker	PDB ?
D	993	GLY	-	linker	PDB ?
D	994	ARG	-	linker	PDB ?
D	995	GLY	-	linker	PDB ?
D	996	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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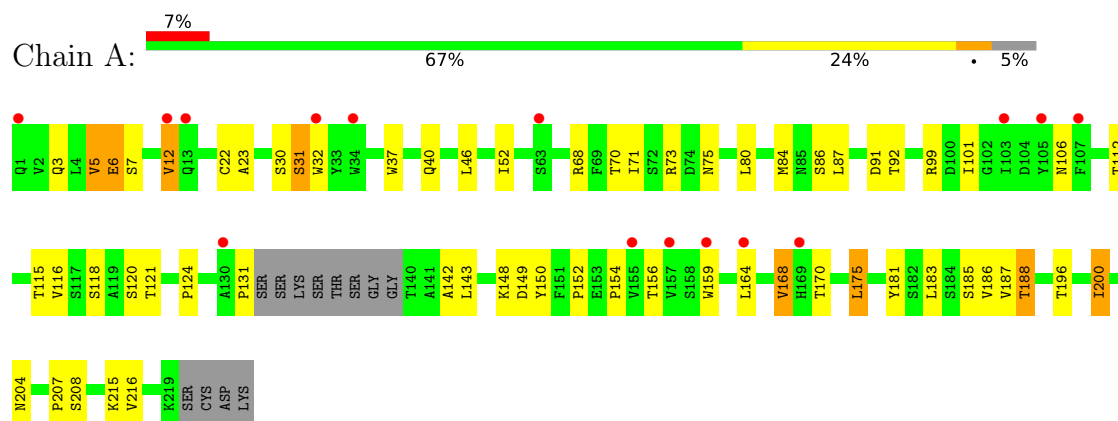
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

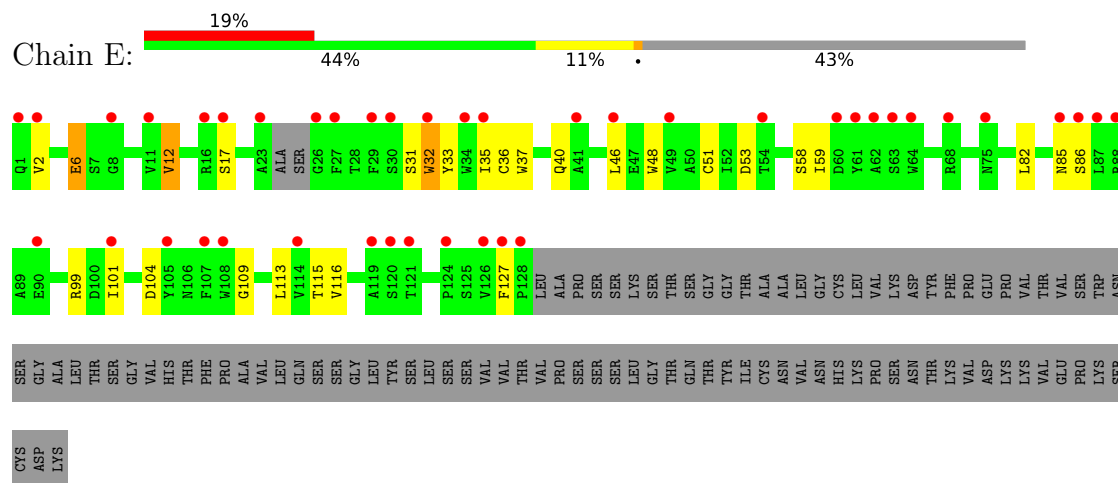
3 Residue-property plots [i](#)

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.

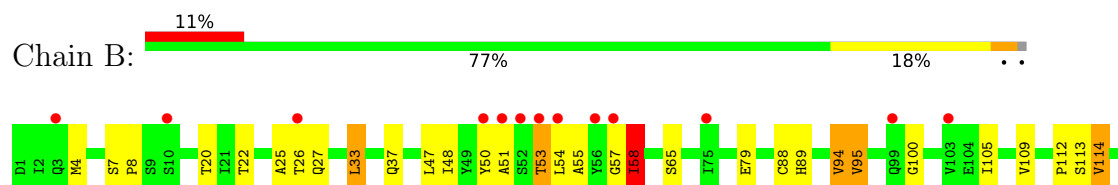
• Molecule 1: DQN0385AE01 Fab heavy chain



• Molecule 1: DQN0385AE01 Fab heavy chain

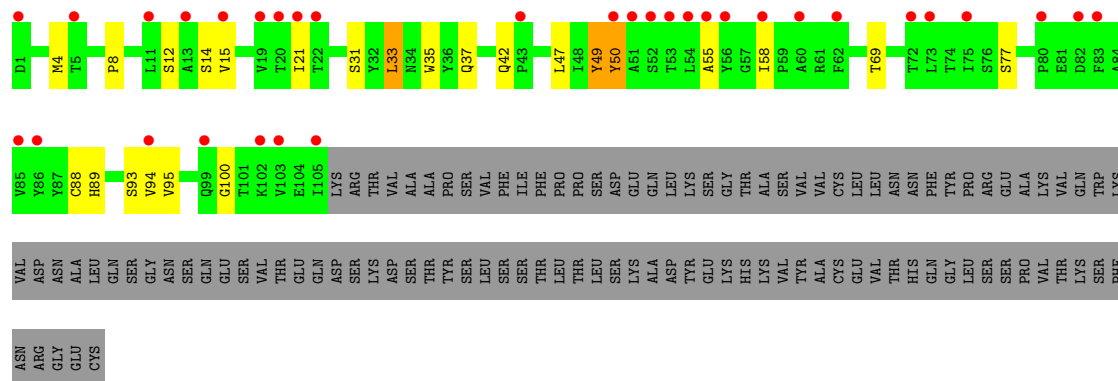
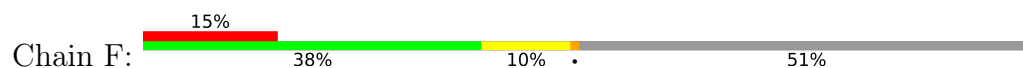


• Molecule 2: DQN0385AE01 Fab light chain

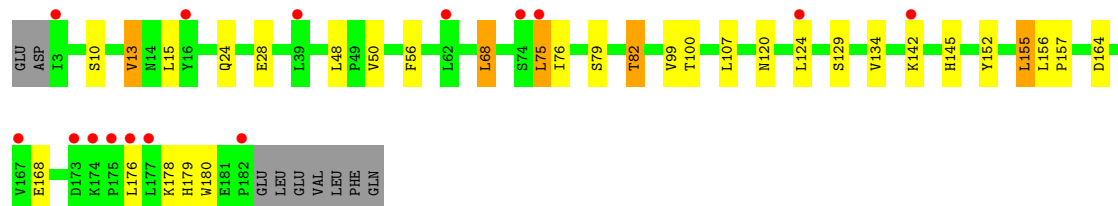
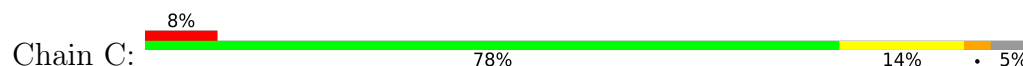




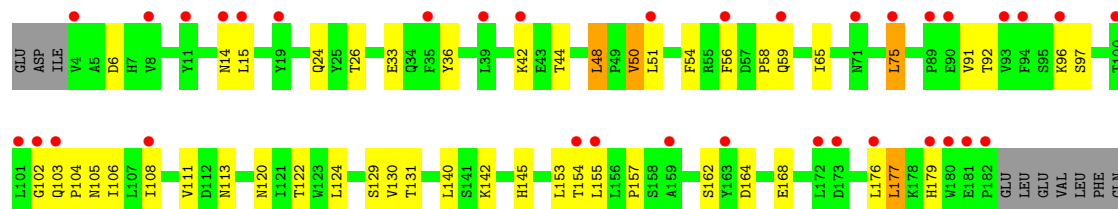
• Molecule 2: DQN0385AE01 Fab light chain



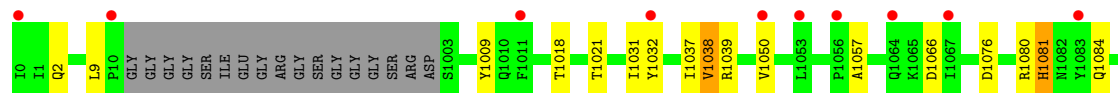
• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

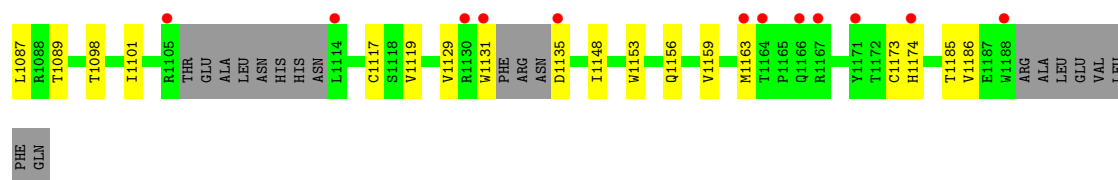


• Molecule 3: HLA class II histocompatibility antigen, DQ alpha 1 chain

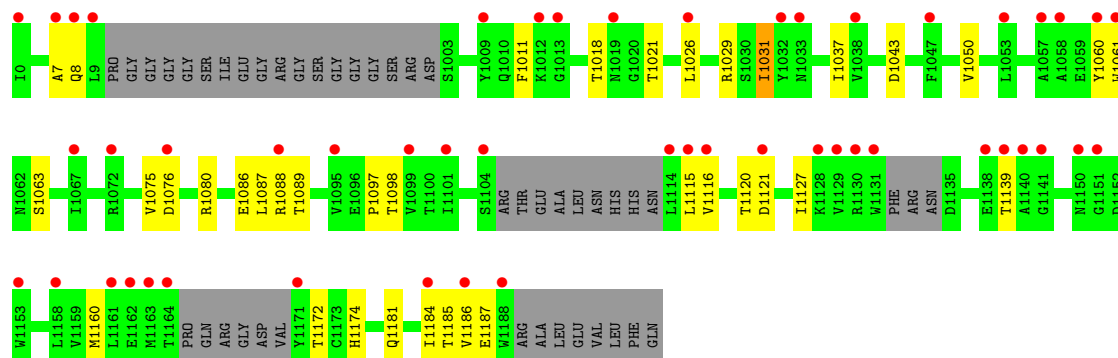


• Molecule 4: MHC class II HLA-DQ-beta-1 - gamma2 gliadin peptide chimeric protein





- 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

All (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
2	F	94	VAL	C-N-CA	6.49	130.25	120.77
2	B	58	ILE	N-CA-CB	6.36	120.11	111.21
4	D	1050	VAL	N-CA-C	-5.83	106.13	111.67
1	A	31	SER	CA-C-N	5.72	132.47	121.54
1	A	31	SER	C-N-CA	5.72	132.47	121.54
4	H	1115	LEU	N-CA-C	5.64	117.92	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	13	VAL	N-CA-CB	5.43	120.19	111.23
4	H	1029	ARG	N-CA-C	5.42	117.50	108.02
2	B	25	ALA	CA-C-N	5.34	129.15	120.60
2	B	25	ALA	C-N-CA	5.34	129.15	120.60
2	B	54	LEU	CA-C-N	5.31	130.92	122.10
2	B	54	LEU	C-N-CA	5.31	130.92	122.10
3	C	76	ILE	N-CA-C	-5.30	105.55	110.53
1	A	87	LEU	N-CA-C	5.20	117.88	110.24
3	G	6	ASP	N-CA-C	-5.20	105.52	111.14
3	C	56	PHE	CA-CB-CG	-5.18	108.61	113.80
1	A	86	SER	CA-C-N	5.14	128.40	121.05
1	A	86	SER	C-N-CA	5.14	128.40	121.05
2	B	95	VAL	N-CA-C	5.14	115.98	108.58
4	H	1181	GLN	N-CA-C	-5.13	105.14	111.40
2	F	95	VAL	N-CA-C	5.07	115.78	108.93
4	H	1098	THR	CA-C-N	5.02	128.09	120.77
4	H	1098	THR	C-N-CA	5.02	128.09	120.77
2	F	50	TYR	CA-C-N	5.01	131.10	121.54
2	F	50	TYR	C-N-CA	5.01	131.10	121.54

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:B:53:THR:HG23	2:B:53:THR:O	1.87	0.72
1:A:159:TRP:CD1	1:A:168:VAL:HG11	2.26	0.71
1:A:156:THR:HB	1:A:204:ASN:HB3	1.72	0.70
1:A:200:ILE:HG13	1:A:215:LYS:HA	1.73	0.70
2:B:7:SER:OG	2:B:8:PRO:HD3	1.92	0.69
2:B:89:HIS:NE2	2:B:95:VAL:HG13	2.08	0.69
3:C:10:SER:HB3	3:C:13:VAL:HG23	1.75	0.69
4:H:1172:THR:HG21	4:H:1174:HIS:NE2	2.07	0.69
1:E:17:SER:CB	1:E:85:ASN:HA	2.21	0.68
1:A:68:ARG:NH2	1:A:91:ASP:OD2	2.25	0.67
1:A:101:ILE:HG22	2:B:89:HIS:CE1	2.30	0.66
2:B:105:ILE:H	2:B:165:GLN:HE22	1.44	0.65
3:C:145:HIS:CD2	4:D:1031:ILE:HD12	2.32	0.64
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.80	0.62
1:E:104:ASP:HB2	2:F:49:TYR:CE2	2.35	0.62
3:C:68:LEU:HG	4:D:1009:TYR:HD1	1.66	0.61
3:C:120:ASN:HD21	5:C:1000:NAG:C1	2.14	0.61
3:G:113:ASN:H	3:G:142:LYS:HZ3	1.47	0.60
2:F:55:ALA:HB3	2:F:58:ILE:HB	1.82	0.60
3:G:145:HIS:CE1	4:H:1031:ILE:HD12	2.36	0.60
2:B:53:THR:O	2:B:53:THR:CG2	2.48	0.60
3:C:120:ASN:HB2	3:C:168:GLU:HB2	1.84	0.60
3:G:120:ASN:HB2	3:G:168:GLU:HB2	1.85	0.59
1:A:159:TRP:HD1	1:A:168:VAL:HG11	1.65	0.59
3:C:145:HIS:NE2	4:D:1031:ILE:HD12	2.18	0.59
4:D:1037:ILE:HG13	4:D:1038:VAL:HG23	1.84	0.59
4:D:1119:VAL:HG21	4:D:1129:VAL:HG21	1.85	0.58
1:E:35:ILE:HG12	1:E:99:ARG:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:LEU:HD11	3:G:51:LEU:HD12	1.85	0.57
1:A:37:TRP:HD1	1:A:71:ILE:HD12	1.70	0.57
3:C:48:LEU:HD13	4:D:1153:TRP:CD1	2.40	0.57
3:C:75:LEU:HD23	4:D:1032:TYR:HB2	1.87	0.57
4:D:2:GLN:HG3	4:D:1081:HIS:CD2	2.39	0.57
4:D:1101:ILE:HD11	4:D:1173:CYS:HB2	1.87	0.56
4:H:1021:THR:HB	4:H:1080:ARG:HE	1.71	0.56
1:A:142:ALA:HB2	1:A:188:THR:HG23	1.87	0.56
4:H:7:ALA:HB3	4:H:1061:TRP:CE2	2.40	0.56
1:E:6:GLU:OE2	1:E:109:GLY:HA3	2.06	0.54
2:B:200:LEU:HD13	2:B:204:VAL:HG23	1.89	0.54
3:G:54:PHE:HE2	4:H:1089:THR:HG21	1.73	0.53
2:B:55:ALA:HB2	2:B:58:ILE:HG23	1.91	0.53
2:B:55:ALA:CB	2:B:58:ILE:HG23	2.37	0.53
1:A:175:LEU:HD12	1:A:181:TYR:CE1	2.44	0.53
2:B:48:ILE:HG12	2:B:53:THR:HA	1.89	0.53
3:G:106:ILE:HD12	3:G:154:THR:HG22	1.92	0.52
3:G:50:VAL:HG12	4:H:1089:THR:HG22	1.92	0.52
4:D:1174:HIS:HD2	4:D:1185:THR:HG22	1.74	0.52
1:A:40:GLN:HB2	1:A:46:LEU:HD23	1.92	0.52
1:E:31:SER:HB2	1:E:33:TYR:CE2	2.45	0.51
3:G:33:GLU:HB2	3:G:140:LEU:HD21	1.91	0.51
4:D:1038:VAL:HG12	4:D:1039:ARG:H	1.74	0.51
1:E:104:ASP:HB3	4:H:8:GLN:HE21	1.75	0.51
4:D:1148:ILE:HB	4:D:1156:GLN:HG2	1.92	0.51
3:G:164:ASP:HB3	3:G:177:LEU:HD12	1.92	0.51
3:G:162:SER:HB2	3:G:179:HIS:CE1	2.46	0.51
4:D:1037:ILE:HG13	4:D:1038:VAL:N	2.25	0.51
1:E:58:SER:HB3	3:G:42:LYS:HZ1	1.76	0.50
3:G:162:SER:HB2	3:G:179:HIS:HE1	1.76	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.50
2:F:93:SER:HB3	3:G:59:GLN:HE22	1.77	0.50
1:A:170:THR:HG23	1:A:185:SER:HB2	1.93	0.49
1:A:159:TRP:CD1	1:A:168:VAL:CG1	2.96	0.48
1:A:131:PRO:HB3	1:A:143:LEU:HB3	1.95	0.48
2:B:162:VAL:HG22	2:B:174:LEU:HD12	1.95	0.48
3:C:10:SER:CB	3:C:13:VAL:HG23	2.40	0.48
1:E:58:SER:HB3	3:G:42:LYS:NZ	2.28	0.48
3:G:44:THR:OG1	3:G:56:PHE:O	2.27	0.48
3:C:68:LEU:HG	4:D:1009:TYR:CD1	2.48	0.48
1:A:5:VAL:HG13	1:A:23:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1172:THR:CG2	4:H:1174:HIS:NE2	2.77	0.48
4:D:1101:ILE:HD12	4:D:1186:VAL:HG12	1.96	0.47
4:H:1172:THR:HG22	4:H:1174:HIS:CD2	2.50	0.47
1:A:143:LEU:HB2	1:A:216:VAL:HG11	1.96	0.47
2:B:7:SER:HB3	2:B:22:THR:OG1	2.15	0.47
3:C:15:LEU:HD23	3:C:24:GLN:HB3	1.96	0.47
1:E:40:GLN:HG3	1:E:46:LEU:HD23	1.97	0.47
2:B:89:HIS:CD2	2:B:95:VAL:HG13	2.49	0.47
3:C:145:HIS:CD2	4:D:1031:ILE:CD1	2.97	0.47
4:D:1119:VAL:HG21	4:D:1129:VAL:CG2	2.45	0.47
3:C:124:LEU:HB2	3:C:164:ASP:HB2	1.95	0.47
4:D:1117:CYS:HB2	4:D:1131:TRP:CZ2	2.50	0.46
1:A:152:PRO:HD2	1:A:207:PRO:CB	2.45	0.46
3:G:14:ASN:HB2	4:H:1011:PHE:HB3	1.97	0.46
1:E:48:TRP:HE1	1:E:51:CYS:HB2	1.80	0.46
1:E:101:ILE:HG22	2:F:89:HIS:NE2	2.29	0.46
3:C:164:ASP:OD1	3:C:179:HIS:HD2	1.99	0.46
2:B:55:ALA:C	2:B:57:GLY:H	2.22	0.46
4:H:1186:VAL:HG12	4:H:1187:GLU:H	1.81	0.46
3:G:113:ASN:H	3:G:142:LYS:HZ1	1.63	0.46
4:D:1131:TRP:HE1	4:D:1159:VAL:HG12	1.82	0.45
4:D:1135:ASP:OD1	4:D:1135:ASP:O	2.34	0.45
2:B:53:THR:OG1	2:B:58:ILE:HD11	2.16	0.45
2:B:188:HIS:O	2:B:210:ARG:NH1	2.44	0.45
1:A:52:ILE:CG2	1:A:80:LEU:HD11	2.47	0.45
3:C:99:VAL:HG21	3:C:180:TRP:HZ2	1.81	0.45
4:H:1076:ASP:HA	4:H:1080:ARG:HB2	1.98	0.45
3:G:97:SER:HA	4:H:1120:THR:HG21	1.99	0.45
3:C:79:SER:O	3:C:82:THR:OG1	2.34	0.44
2:F:33:LEU:HD11	2:F:88:CYS:HB2	1.98	0.44
3:G:26:THR:HG22	3:G:36:TYR:HB3	1.99	0.44
3:C:124:LEU:HD23	3:C:129:SER:HA	1.99	0.44
4:D:1076:ASP:HA	4:D:1080:ARG:HB2	1.99	0.44
2:B:55:ALA:C	2:B:57:GLY:N	2.76	0.44
3:C:134:VAL:HA	3:C:152:TYR:O	2.18	0.44
3:C:145:HIS:NE2	4:D:1031:ILE:CD1	2.80	0.44
1:E:37:TRP:CD1	1:E:82:LEU:HD13	2.52	0.44
1:A:73:ARG:HD3	1:A:75:ASN:OD1	2.18	0.43
3:C:50:VAL:HG22	4:D:1089:THR:HG22	2.00	0.43
3:G:42:LYS:O	3:G:58:PRO:HG2	2.17	0.43
1:A:99:ARG:NH1	1:A:106:ASN:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HG12	1:E:116:VAL:HG22	2.00	0.43
3:G:145:HIS:CE1	4:H:1031:ILE:CD1	3.01	0.43
2:B:114:VAL:HG22	2:B:206:LYS:HG3	2.01	0.43
2:F:33:LEU:CD2	2:F:35:TRP:NE1	2.82	0.43
1:A:124:PRO:HA	1:A:150:TYR:HB3	2.00	0.42
1:A:22:CYS:HB3	1:A:80:LEU:HB3	2.01	0.42
1:A:52:ILE:HG21	1:A:80:LEU:HD11	2.00	0.42
1:E:104:ASP:OD2	2:F:55:ALA:HA	2.19	0.42
3:C:107:LEU:HD23	3:C:107:LEU:HA	1.91	0.42
2:B:119:PRO:HD3	2:B:131:VAL:HG22	2.01	0.42
3:G:130:VAL:HG11	3:G:153:LEU:HD11	2.01	0.42
4:H:1097:PRO:HG2	4:H:1184:ILE:HD12	2.02	0.42
1:A:186:VAL:HG21	2:B:134:LEU:HD13	2.01	0.42
3:C:155:LEU:HD13	3:C:157:PRO:HD3	2.00	0.42
3:G:75:LEU:HD21	4:H:1037:ILE:HD11	2.01	0.42
4:H:1060:TYR:O	4:H:1063:SER:OG	2.37	0.42
2:B:33:LEU:HD11	2:B:88:CYS:HB2	2.02	0.42
2:B:112:PRO:HB3	2:B:138:PHE:CD2	2.55	0.42
2:F:8:PRO:HG2	2:F:21:ILE:HG12	2.02	0.42
3:G:91:VAL:HG22	3:G:111:VAL:HG22	2.02	0.41
1:E:101:ILE:HG22	2:F:89:HIS:CD2	2.55	0.41
2:F:8:PRO:HD2	2:F:21:ILE:HG23	2.02	0.41
4:D:1084:GLN:HA	4:D:1087:LEU:HD12	2.02	0.41
1:E:101:ILE:HG22	2:F:89:HIS:CE1	2.55	0.41
3:G:96:LYS:HG3	3:G:108:ILE:HD11	2.01	0.41
1:A:101:ILE:HG22	2:B:89:HIS:NE2	2.36	0.41
2:B:89:HIS:CD2	2:B:95:VAL:CG1	3.03	0.41
4:D:9:LEU:HD21	4:D:1057:ALA:HB2	2.02	0.41
1:A:121:THR:HG22	1:A:208:SER:HB3	2.03	0.41
3:G:26:THR:HG22	3:G:36:TYR:CB	2.51	0.41
1:A:164:LEU:HD21	1:A:187:VAL:HG21	2.03	0.41
1:E:32:TRP:HZ3	3:G:65:ILE:HG21	1.86	0.41
4:H:1186:VAL:HG12	4:H:1187:GLU:N	2.36	0.41
1:E:53:ASP:HB3	1:E:58:SER:H	1.86	0.41
1:A:12:VAL:HG13	1:A:116:VAL:HG22	2.03	0.40
4:H:1172:THR:CG2	4:H:1174:HIS:CD2	3.04	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	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

All (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
2	B	109	VAL
2	F	100	GLY
3	G	103	GLN
4	H	1121	ASP
2	F	50	TYR
3	G	102	GLY
2	F	15	VAL
3	G	104	PRO
3	G	157	PRO
1	A	154	PRO

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

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	VAL
1	A	6	GLU
1	A	7	SER
1	A	12	VAL
1	A	30	SER
1	A	31	SER
1	A	70	THR
1	A	84	MET
1	A	118	SER
1	A	120	SER
1	A	148	LYS
1	A	168	VAL
1	A	175	LEU
1	A	183	LEU
1	A	188	THR
1	A	196	THR
1	A	200	ILE
2	B	20	THR

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Mol	Chain	Res	Type
2	B	26	THR
2	B	27	GLN
2	B	33	LEU
2	B	53	THR
2	B	58	ILE
2	B	65	SER
2	B	79	GLU
2	B	94	VAL
2	B	113	SER
2	B	114	VAL
2	B	153	LEU
2	B	165	GLN
2	B	180	LEU
3	C	28	GLU
3	C	68	LEU
3	C	75	LEU
3	C	82	THR
3	C	100	THR
3	C	142	LYS
3	C	155	LEU
3	C	156	LEU
3	C	176	LEU
3	C	178	LYS
4	D	1021	THR
4	D	1038	VAL
4	D	1066	ASP
4	D	1081	HIS
4	D	1098	THR
4	D	1163	MET
1	E	2	VAL
1	E	6	GLU
1	E	12	VAL
1	E	32	TRP
1	E	36	CYS
1	E	59	ILE
1	E	86	SER
1	E	113	LEU
1	E	115	THR
1	E	127	PHE
2	F	4	MET
2	F	12	SER
2	F	14	SER

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Mol	Chain	Res	Type
2	F	31	SER
2	F	33	LEU
2	F	42	GLN
2	F	49	TYR
2	F	69	THR
2	F	77	SER
3	G	15	LEU
3	G	24	GLN
3	G	48	LEU
3	G	50	VAL
3	G	75	LEU
3	G	92	THR
3	G	105	ASN
3	G	122	THR
3	G	124	LEU
3	G	129	SER
3	G	131	THR
3	G	155	LEU
3	G	176	LEU
3	G	177	LEU
4	H	1018	THR
4	H	1026	LEU
4	H	1031	ILE
4	H	1043	ASP
4	H	1050	VAL
4	H	1075	VAL
4	H	1086	GLU
4	H	1087	LEU
4	H	1088	ARG
4	H	1116	VAL
4	H	1127	ILE
4	H	1139	THR
4	H	1160	MET
4	H	1185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	159	GLN
2	B	198	GLN
2	B	209	ASN
3	C	14	ASN

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Mol	Chain	Res	Type
3	C	17	GLN
3	C	53	GLN
3	C	64	ASN
3	C	120	ASN
3	C	179	HIS
4	D	1019	ASN
4	D	1092	GLN
4	D	1174	HIS
3	G	7	HIS
3	G	17	GLN
3	G	145	HIS
3	G	179	HIS
4	H	8	GLN
4	H	1156	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(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

All (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
2	F	1	ASP	5.4
2	B	56	TYR	5.1
1	E	60	ASP	5.1
2	B	211	GLY	5.0
3	G	75	LEU	4.9
1	A	34	TRP	4.9
2	F	19	VAL	4.8
1	E	127	PHE	4.7
3	C	39	LEU	4.7
1	E	17	SER	4.6
4	D	1167	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
3	C	173	ASP	4.5
3	G	101	LEU	4.4
4	H	1047	PHE	4.4
3	G	90	GLU	4.3
4	H	1060	TYR	4.2
2	B	180	LEU	4.2
1	E	46	LEU	4.2
4	H	9	LEU	4.2
4	H	1076	ASP	4.0
2	F	99	GLN	4.0
4	H	1038	VAL	4.0
2	F	5	THR	4.0
4	D	1188	TRP	4.0
1	E	49	VAL	4.0
4	H	1032	TYR	3.9
1	E	2	VAL	3.9
4	D	1171	TYR	3.9
3	G	176	LEU	3.9
3	C	182	PRO	3.8
2	B	129	ALA	3.8
2	F	73	LEU	3.8
4	H	1162	GLU	3.7
2	F	80	PRO	3.7
4	D	10	PRO	3.7
3	C	3	ILE	3.7
3	G	159	ALA	3.6
2	F	21	ILE	3.5
2	B	53	THR	3.5
2	F	20	THR	3.5
3	G	71	ASN	3.5
1	A	32	TRP	3.5
3	G	96	LYS	3.5
1	A	107	PHE	3.5
1	E	107	PHE	3.5
4	H	1163	MET	3.5
1	E	32	TRP	3.5
2	F	53	THR	3.4
2	F	54	LEU	3.4
2	F	105	ILE	3.4
3	G	180	TRP	3.4
4	H	1141	GLY	3.4
4	H	1101	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
4	H	1088	ARG	3.3
1	E	105	TYR	3.3
3	G	154	THR	3.3
4	H	1009	TYR	3.3
2	F	22	THR	3.3
4	H	1114	LEU	3.2
3	C	16	TYR	3.2
3	G	14	ASN	3.2
3	G	181	GLU	3.2
1	A	63	SER	3.2
4	H	8	GLN	3.2
3	G	102	GLY	3.2
3	G	4	VAL	3.2
1	E	34	TRP	3.1
2	B	57	GLY	3.1
1	E	108	TRP	3.1
2	B	51	ALA	3.1
4	H	1058	ALA	3.1
3	G	56	PHE	3.1
3	C	75	LEU	3.1
3	G	173	ASP	3.1
2	F	51	ALA	3.1
1	A	155	VAL	3.1
3	G	35	PHE	3.0
4	H	1095	VAL	3.0
1	E	75	ASN	3.0
1	E	27	PHE	3.0
2	B	52	SER	3.0
3	G	172	LEU	3.0
2	F	13	ALA	3.0
4	H	1057	ALA	3.0
1	E	30	SER	3.0
2	F	56	TYR	3.0
2	B	54	LEU	2.9
4	H	1138	GLU	2.9
4	H	1153	TRP	2.9
3	G	59	GLN	2.9
3	G	11	TYR	2.9
4	D	1163	MET	2.9
4	H	1130	ARG	2.9
3	G	89	PRO	2.9
4	H	1131	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	35	ILE	2.9
4	H	1012	LYS	2.9
2	F	52	SER	2.9
1	E	1	GLN	2.8
1	E	88	ARG	2.8
4	H	1188	TRP	2.8
2	F	82	ASP	2.8
3	G	94	PHE	2.8
4	H	1116	VAL	2.8
1	E	86	SER	2.8
2	B	130	SER	2.8
2	F	60	ALA	2.8
4	D	1032	TYR	2.8
4	D	1131	TRP	2.8
1	A	105	TYR	2.8
4	H	1171	TYR	2.8
3	C	175	PRO	2.8
4	D	1050	VAL	2.8
4	H	1140	ALA	2.8
1	A	164	LEU	2.7
3	C	176	LEU	2.7
2	B	103	VAL	2.7
3	C	74	SER	2.7
1	E	119	ALA	2.7
1	E	126	VAL	2.7
4	D	1011	PHE	2.7
2	B	124	LEU	2.7
1	E	101	ILE	2.7
4	H	1104	SER	2.7
4	H	1129	VAL	2.7
2	F	72	THR	2.7
1	E	128	PRO	2.7
4	D	0	ILE	2.6
1	A	169	HIS	2.6
3	G	103	GLN	2.6
4	D	1166	GLN	2.6
1	A	1	GLN	2.6
1	E	64	TRP	2.6
2	B	99	GLN	2.6
1	A	157	VAL	2.6
2	F	85	VAL	2.6
1	E	85	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	83	PHE	2.6
3	G	100	THR	2.5
2	B	75	ILE	2.5
2	F	94	VAL	2.5
1	E	120	SER	2.5
3	G	15	LEU	2.5
1	E	41	ALA	2.5
1	E	63	SER	2.5
3	C	167	VAL	2.5
2	B	179	THR	2.5
2	F	102	LYS	2.5
1	E	26	GLY	2.5
4	H	1067	ILE	2.4
4	H	1151	GLY	2.4
1	A	13	GLN	2.4
1	E	11	VAL	2.4
1	E	121	THR	2.4
1	E	114	VAL	2.4
1	E	29	PHE	2.4
4	H	1164	THR	2.4
2	B	119	PRO	2.4
1	E	62	ALA	2.4
2	F	50	TYR	2.4
3	C	177	LEU	2.4
4	H	1121	ASP	2.4
3	C	174	LYS	2.4
4	H	1072	ARG	2.4
2	F	11	LEU	2.3
3	G	51	LEU	2.3
4	H	1053	LEU	2.3
4	D	1067	ILE	2.3
4	H	1186	VAL	2.3
4	H	7	ALA	2.3
4	H	1026	LEU	2.3
2	F	86	TYR	2.3
3	G	19	TYR	2.3
4	H	1139	THR	2.3
1	A	159	TRP	2.3
2	F	43	PRO	2.3
3	C	62	LEU	2.3
4	D	1174	HIS	2.3
2	B	128	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	42	LYS	2.3
2	B	3	GLN	2.3
2	B	132	VAL	2.3
4	H	1184	ILE	2.3
2	B	10	SER	2.3
2	F	103	VAL	2.3
4	H	0	ILE	2.2
4	H	1013	GLY	2.2
1	E	23	ALA	2.2
3	G	179	HIS	2.2
4	H	1099	VAL	2.2
2	F	55	ALA	2.2
1	E	61	TYR	2.2
1	E	8	GLY	2.2
4	D	1114	LEU	2.2
4	D	1135	ASP	2.2
4	H	1115	LEU	2.2
2	F	58	ILE	2.2
1	E	90	GLU	2.2
1	E	54	THR	2.2
2	B	26	THR	2.2
4	H	1019	ASN	2.2
4	H	1033	ASN	2.2
2	B	178	LEU	2.2
1	E	68	ARG	2.1
4	D	1130	ARG	2.1
4	D	1056	PRO	2.1
3	G	163	TYR	2.1
1	E	87	LEU	2.1
2	F	15	VAL	2.1
1	A	130	ALA	2.1
1	E	16	ARG	2.1
3	G	39	LEU	2.1
3	G	155	LEU	2.1
4	D	1053	LEU	2.1
4	H	1158	LEU	2.1
2	B	131	VAL	2.1
4	H	1128	LYS	2.1
4	H	1150	ASN	2.1
2	B	50	TYR	2.1
3	G	8	VAL	2.1
4	D	1164	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	124	LEU	2.1
4	D	1083	TYR	2.1
3	G	93	VAL	2.1
3	C	142	LYS	2.0
1	E	124	PRO	2.0
1	A	12	VAL	2.0
4	D	1064	GLN	2.0
4	H	1161	LEU	2.0
1	A	103	ILE	2.0
3	G	108	ILE	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
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.