



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:23 PM UTC

PDB ID : 4P57 / pdb_00004p57
Title : MHC TCR peptide complex
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Deposited on : 2014-03-14
Resolution : 2.60 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

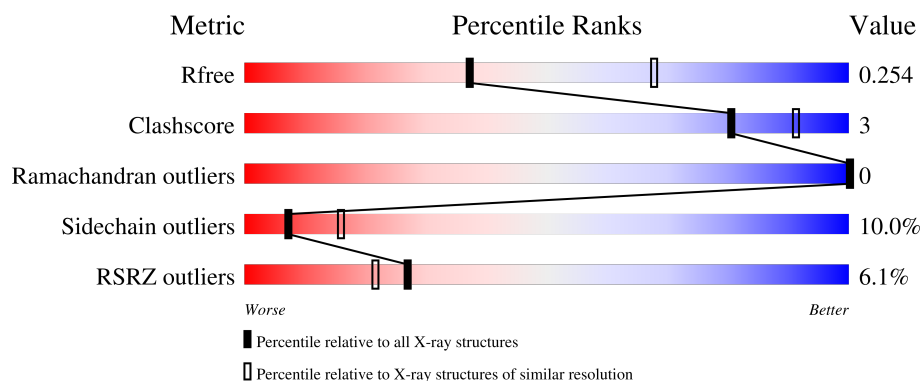
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	183	3% 79% 17% ..
1	C	183	2% 78% 19% ..
2	B	212	9% 79% 12% 7%
2	D	212	8% 77% 12% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6373 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1453	938	235	275	5			
1	C	180	Total	C	N	O	S	0	0	0
			1454	940	235	274	5			

- Molecule 2 is a protein called mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1551	983	260	300	8			
2	D	196	Total	C	N	O	S	0	0	0
			1564	989	268	299	8			

There are 32 discrepancies between the modelled and reference sequences:

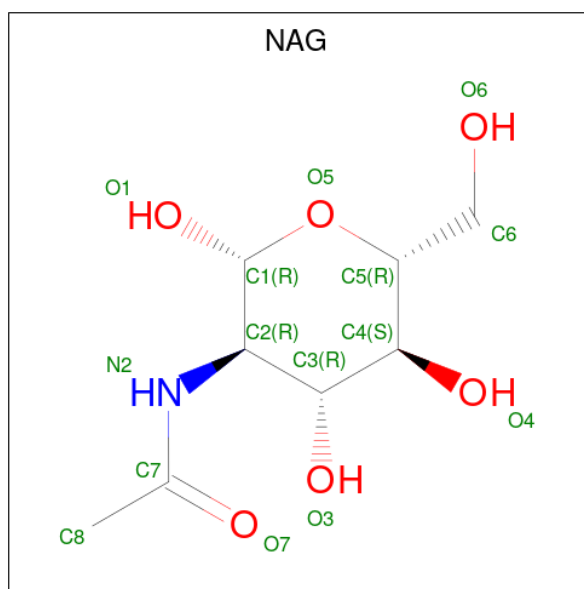
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	linker	UNP Q5EP54
B	-13	GLY	-	linker	UNP Q5EP54
B	-12	GLY	-	linker	UNP Q5EP54
B	-11	SER	-	linker	UNP Q5EP54
B	-10	LEU	-	linker	UNP Q5EP54
B	-9	VAL	-	linker	UNP Q5EP54
B	-8	PRO	-	linker	UNP Q5EP54
B	-7	ARG	-	linker	UNP Q5EP54
B	-6	GLY	-	linker	UNP Q5EP54
B	-5	SER	-	linker	UNP Q5EP54
B	-4	GLY	-	linker	UNP Q5EP54
B	-3	GLY	-	linker	UNP Q5EP54
B	-2	GLY	-	linker	UNP Q5EP54
B	-1	GLY	-	linker	UNP Q5EP54
B	3	SER	THR	variant	UNP Q5EP54
B	69	LYS	GLU	engineered mutation	UNP Q5EP54

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	GLY	-	linker	UNP Q5EP54
D	-13	GLY	-	linker	UNP Q5EP54
D	-12	GLY	-	linker	UNP Q5EP54
D	-11	SER	-	linker	UNP Q5EP54
D	-10	LEU	-	linker	UNP Q5EP54
D	-9	VAL	-	linker	UNP Q5EP54
D	-8	PRO	-	linker	UNP Q5EP54
D	-7	ARG	-	linker	UNP Q5EP54
D	-6	GLY	-	linker	UNP Q5EP54
D	-5	SER	-	linker	UNP Q5EP54
D	-4	GLY	-	linker	UNP Q5EP54
D	-3	GLY	-	linker	UNP Q5EP54
D	-2	GLY	-	linker	UNP Q5EP54
D	-1	GLY	-	linker	UNP Q5EP54
D	3	SER	THR	variant	UNP Q5EP54
B	69	LYS	GLU	engineered mutation	UNP Q5EP54

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



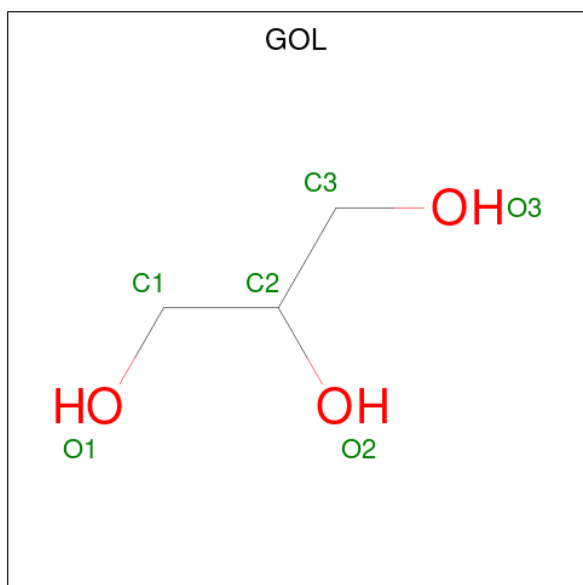
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		
6	B	57	Total	O	0	0
			57	57		

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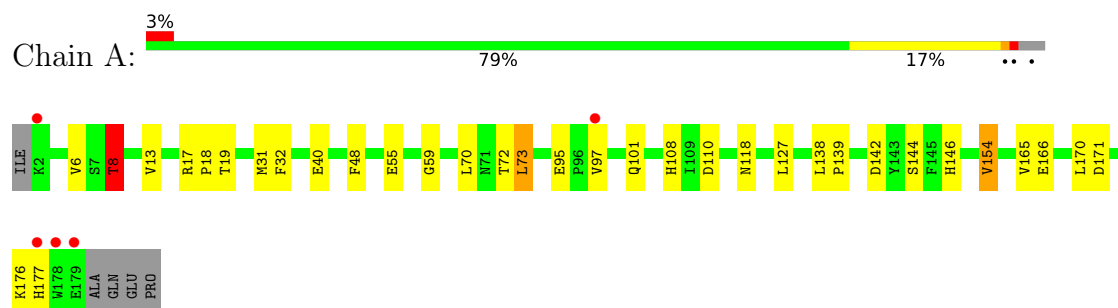
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	93	Total	O	0	0
			93	93		
6	D	50	Total	O	0	0
			50	50		

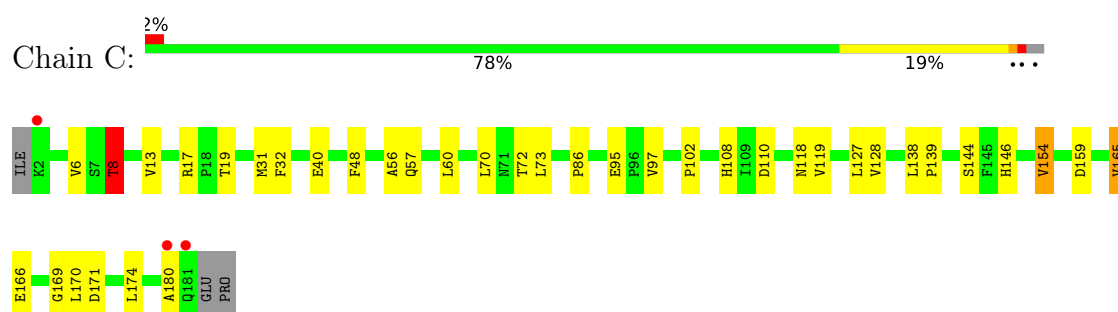
3 Residue-property plots [i](#)

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

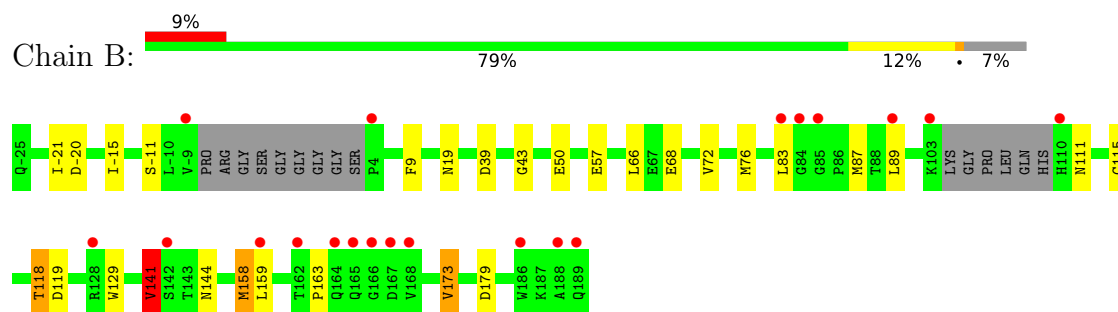
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



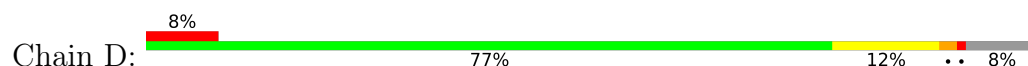
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

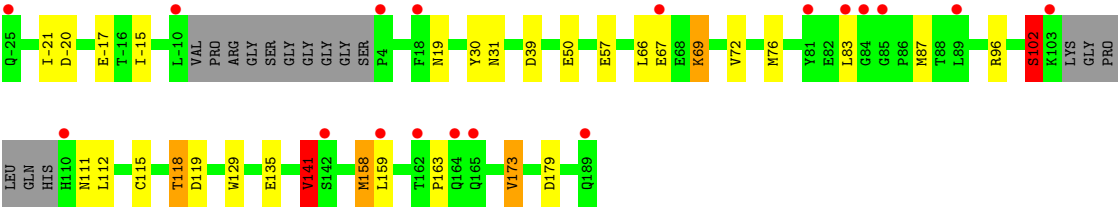


- Molecule 2: mim2 peptide, HLA class II histocompatibility antigen, DP beta 1 chain



- Molecule 2: mim2 peptide, HLA class II histocompatibility antigen, DP beta 1 chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.39Å 102.39Å 234.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.10 – 2.60 77.10 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (77.10-2.60) 95.8 (77.10-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.208 , 0.245 0.216 , 0.254	Depositor DCC
R_{free} test set	1895 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.95% 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, CA, GOL

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	0.83	0/1501	1.46	16/2050 (0.8%)
1	C	0.85	0/1502	1.47	16/2054 (0.8%)
2	B	0.88	0/1589	1.41	11/2164 (0.5%)
2	D	0.84	0/1602	1.41	11/2178 (0.5%)
All	All	0.85	0/6194	1.44	54/8446 (0.6%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	ASN	CA-CB-CG	9.95	122.55	112.60
2	D	19	ASN	CA-CB-CG	8.29	120.89	112.60
1	C	48	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	48	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	154	VAL	N-CA-CB	6.87	120.83	111.21
1	C	56	ALA	CA-C-N	6.70	129.55	120.38
1	C	56	ALA	C-N-CA	6.70	129.55	120.38
2	D	72	VAL	N-CA-CB	6.65	115.64	110.45
1	C	128	VAL	N-CA-CB	6.58	119.75	111.46
1	C	97	VAL	N-CA-CB	6.45	118.25	110.31
1	A	55	GLU	CA-C-N	6.35	129.08	120.38
1	A	55	GLU	C-N-CA	6.35	129.08	120.38
2	B	72	VAL	N-CA-CB	6.23	115.31	110.45
2	B	163	PRO	N-CA-C	6.18	120.63	110.55
1	A	154	VAL	CB-CA-C	6.17	118.28	111.18
2	B	141	VAL	N-CA-CB	6.02	119.46	111.64
1	A	97	VAL	N-CA-CB	6.00	117.69	110.31
2	D	50	GLU	CB-CG-CD	5.92	122.66	112.60
2	B	19	ASN	OD1-CG-ND2	5.80	128.41	122.60
2	B	119	ASP	CA-CB-CG	5.76	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	110	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	177	HIS	CA-C-N	5.69	132.41	121.54
1	A	177	HIS	C-N-CA	5.69	132.41	121.54
2	B	118	THR	N-CA-CB	-5.66	101.71	111.55
2	D	119	ASP	CA-CB-CG	5.65	118.25	112.60
2	D	141	VAL	N-CA-CB	5.61	118.94	111.64
2	B	39	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	59	GLY	CA-C-N	5.58	128.03	120.38
1	A	59	GLY	C-N-CA	5.58	128.03	120.38
1	C	86	PRO	O-C-N	5.56	123.76	121.15
2	D	173	VAL	N-CA-CB	5.56	118.47	111.46
2	D	163	PRO	N-CA-C	5.52	120.76	111.32
2	D	39	ASP	CA-CB-CG	5.51	118.11	112.60
2	B	173	VAL	N-CA-CB	5.47	118.35	111.46
1	A	18	PRO	CA-C-N	5.42	128.09	120.28
1	A	18	PRO	C-N-CA	5.42	128.09	120.28
1	C	169	GLY	CA-C-N	5.41	129.60	122.30
1	C	169	GLY	C-N-CA	5.41	129.60	122.30
1	A	8	THR	N-CA-C	5.39	117.87	108.76
1	C	8	THR	N-CA-C	5.36	117.82	108.76
2	B	76	MET	N-CA-C	5.35	117.19	111.36
2	D	102	SER	N-CA-C	5.34	117.77	110.24
1	C	57	GLN	CA-C-N	5.32	125.88	119.98
1	C	57	GLN	C-N-CA	5.32	125.88	119.98
2	D	76	MET	N-CA-CB	5.29	118.09	110.20
1	A	177	HIS	N-CA-C	5.28	117.01	109.14
1	C	159	ASP	CA-CB-CG	5.24	117.84	112.60
2	D	67	GLU	N-CA-C	5.22	117.05	111.36
1	A	97	VAL	N-CA-C	5.20	115.80	109.30
1	C	97	VAL	N-CA-C	5.18	115.78	109.30
1	A	142	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	180	ALA	N-CA-C	-5.11	102.08	109.59
2	B	-20	ASP	N-CA-C	-5.05	100.80	109.24

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	1453	0	1336	9	0
1	C	1454	0	1331	10	0
2	B	1551	0	1402	6	0
2	D	1564	0	1434	9	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
3	C	28	0	26	0	0
4	A	6	0	8	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	73	0	0	0	0
6	B	57	0	0	1	0
6	C	93	0	0	0	0
6	D	50	0	0	1	0
All	All	6373	0	5576	30	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (30) 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)
2:D:96:ARG:HB3	2:D:118:THR:HG22	1.55	0.87
1:C:108:HIS:HE1	1:C:146:HIS:CD2	2.15	0.65
1:A:108:HIS:HE1	1:A:146:HIS:CD2	2.16	0.63
1:A:108:HIS:HE1	1:A:146:HIS:HD2	1.52	0.57
1:C:108:HIS:HE1	1:C:146:HIS:HD2	1.52	0.57
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.88	0.56
2:D:141:VAL:HG12	6:D:306:HOH:O	2.06	0.55
1:C:119:VAL:HG22	1:C:165:VAL:HB	1.90	0.54
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.92	0.52
1:A:72:THR:HG21	2:B:15:ILE:HG22	1.90	0.52
2:B:141:VAL:HG13	2:B:158:MET:HG2	1.94	0.50
2:D:141:VAL:HG13	2:D:158:MET:HG2	1.94	0.49
1:C:72:THR:HG21	2:D:-15:ILE:HG22	1.94	0.48
1:A:31:MET:HG2	1:A:32:PHE:HD1	1.80	0.47
1:C:31:MET:HG2	1:C:32:PHE:HD1	1.80	0.47
2:D:-20:ASP:OD2	2:D:69:LYS:NZ	2.49	0.45
2:D:-17:GLU:HG2	2:D:69:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:GLY:HA3	1:C:102:PRO:HD2	1.99	0.45
2:B:115:CYS:HB2	2:B:129:TRP:CZ2	2.52	0.45
1:C:138:LEU:HA	1:C:139:PRO:HD3	1.89	0.45
2:D:102:SER:HB2	2:D:112:LEU:HB3	1.99	0.45
1:A:108:HIS:CE1	1:A:146:HIS:HD2	2.35	0.44
2:D:30:TYR:O	2:D:31:ASN:HB2	2.17	0.44
2:B:141:VAL:HG12	6:B:306:HOH:O	2.16	0.44
2:D:115:CYS:HB2	2:D:129:TRP:CZ2	2.52	0.44
1:A:6:VAL:HG12	1:A:8:THR:HG22	2.02	0.42
1:A:138:LEU:HA	1:A:139:PRO:HD3	1.88	0.42
1:C:6:VAL:HG12	1:C:8:THR:HG22	2.02	0.42
1:C:108:HIS:CE1	1:C:146:HIS:HD2	2.34	0.41
1:A:73:LEU:HD13	2:B:9:PHE:HE2	1.86	0.41

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	176/183 (96%)	175 (99%)	1 (1%)	0	100	100
1	C	178/183 (97%)	178 (100%)	0	0	100	100
2	B	191/212 (90%)	186 (97%)	5 (3%)	0	100	100
2	D	190/212 (90%)	186 (98%)	4 (2%)	0	100	100
All	All	735/790 (93%)	725 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	158/164 (96%)	142 (90%)	16 (10%)	7	15
1	C	156/164 (95%)	140 (90%)	16 (10%)	7	15
2	B	161/186 (87%)	144 (89%)	17 (11%)	6	14
2	D	164/186 (88%)	149 (91%)	15 (9%)	9	19
All	All	639/700 (91%)	575 (90%)	64 (10%)	7	16

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	13	VAL
1	A	17	ARG
1	A	19	THR
1	A	40	GLU
1	A	70	LEU
1	A	73	LEU
1	A	95	GLU
1	A	101	GLN
1	A	127	LEU
1	A	144	SER
1	A	154	VAL
1	A	165	VAL
1	A	170	LEU
1	A	171	ASP
1	A	176	LYS
2	B	-21	ILE
2	B	-11	SER
2	B	50	GLU
2	B	57	GLU
2	B	66	LEU
2	B	68	GLU
2	B	83	LEU
2	B	87	MET

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Mol	Chain	Res	Type
2	B	89	LEU
2	B	111	ASN
2	B	118	THR
2	B	141	VAL
2	B	144	ASN
2	B	158	MET
2	B	159	LEU
2	B	173	VAL
2	B	179	ASP
1	C	8	THR
1	C	13	VAL
1	C	17	ARG
1	C	19	THR
1	C	40	GLU
1	C	60	LEU
1	C	70	LEU
1	C	73	LEU
1	C	95	GLU
1	C	127	LEU
1	C	144	SER
1	C	154	VAL
1	C	165	VAL
1	C	170	LEU
1	C	171	ASP
1	C	174	LEU
2	D	-21	ILE
2	D	57	GLU
2	D	66	LEU
2	D	69	LYS
2	D	83	LEU
2	D	87	MET
2	D	102	SER
2	D	111	ASN
2	D	118	THR
2	D	135	GLU
2	D	141	VAL
2	D	158	MET
2	D	159	LEU
2	D	173	VAL
2	D	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	84	ASN
1	A	101	GLN
1	A	108	HIS
1	A	124	ASN
1	A	146	HIS
2	B	98	ASN
1	C	16	HIS
1	C	57	GLN
1	C	67	ASN
1	C	84	ASN
1	C	108	HIS
1	C	146	HIS
2	D	98	ASN

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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	NAG	B	201	2	14,14,15	0.51	0	17,19,21	1.46	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	201	1	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
3	NAG	C	201	1	14,14,15	0.38	0	17,19,21	0.92	1 (5%)
4	GOL	A	203	-	5,5,5	0.18	0	5,5,5	0.39	0
3	NAG	C	202	1	14,14,15	0.33	0	17,19,21	2.68	4 (23%)
3	NAG	A	202	1	14,14,15	0.29	0	17,19,21	2.62	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
3	NAG	B	201	2	-	1/6/23/26	0/1/1/1
3	NAG	A	201	1	-	0/6/23/26	0/1/1/1
3	NAG	C	201	1	-	0/6/23/26	0/1/1/1
4	GOL	A	203	-	-	2/4/4/4	-
3	NAG	C	202	1	-	1/6/23/26	0/1/1/1
3	NAG	A	202	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	NAG	C1-C2-N2	9.14	124.83	110.43
3	A	202	NAG	C1-C2-N2	8.33	123.56	110.43
3	A	202	NAG	O5-C1-C2	-5.40	102.93	111.29
3	B	201	NAG	C1-C2-N2	4.48	117.49	110.43
3	C	202	NAG	O5-C1-C2	-4.42	104.45	111.29
3	A	202	NAG	C2-N2-C7	3.08	127.03	122.90
3	C	202	NAG	C1-O5-C5	2.71	115.82	112.19
3	B	201	NAG	C1-O5-C5	2.65	115.74	112.19
3	A	201	NAG	C1-O5-C5	2.62	115.69	112.19
3	C	201	NAG	C1-O5-C5	2.55	115.61	112.19
3	C	202	NAG	C2-N2-C7	2.44	126.17	122.90
3	B	201	NAG	C2-N2-C7	2.37	126.08	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	NAG	C1-C2-N2-C7
3	C	202	NAG	C1-C2-N2-C7
4	A	203	GOL	C1-C2-C3-O3
4	A	203	GOL	O2-C2-C3-O3
3	B	201	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	178/183 (97%)	-0.05	5 (2%) 55 49	26, 37, 62, 97	0
1	C	180/183 (98%)	-0.13	3 (1%) 69 64	26, 36, 56, 67	0
2	B	197/212 (92%)	0.71	20 (10%) 12 9	23, 44, 77, 106	0
2	D	196/212 (92%)	0.66	18 (9%) 14 11	28, 47, 70, 100	0
All	All	751/790 (95%)	0.31	46 (6%) 27 22	23, 42, 70, 106	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	189	GLN	9.2
2	B	189	GLN	8.2
2	B	-9	VAL	7.3
2	D	110	HIS	5.7
2	B	84	GLY	5.6
1	A	179	GLU	4.7
2	B	110	HIS	4.5
2	B	164	GLN	4.3
2	D	162	THR	4.1
2	B	165	GLN	4.0
2	B	103	LYS	3.8
2	B	166	GLY	3.8
2	B	188	ALA	3.4
2	D	85	GLY	3.4
2	D	-25	GLN	3.3
2	D	89	LEU	3.2
2	B	162	THR	3.0
1	A	178	TRP	3.0
2	D	84	GLY	2.9
2	B	168	VAL	2.8
2	B	186	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	83	LEU	2.8
2	B	85	GLY	2.7
2	D	103	LYS	2.7
1	C	2	LYS	2.6
1	C	180	ALA	2.6
2	D	159	LEU	2.6
2	B	89	LEU	2.5
1	C	181	GLN	2.5
2	B	83	LEU	2.5
2	B	4	PRO	2.5
2	D	-10	LEU	2.5
1	A	2	LYS	2.4
2	B	167	ASP	2.4
2	D	4	PRO	2.4
2	B	142	SER	2.3
2	D	18	PHE	2.3
2	D	164	GLN	2.3
1	A	177	HIS	2.2
2	B	128	ARG	2.2
2	D	67	GLU	2.1
2	D	142	SER	2.1
2	D	165	GLN	2.1
2	D	81	TYR	2.1
1	A	97	VAL	2.1
2	B	159	LEU	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	NAG	B	201	14/15	0.41	0.22	107,109,112,112	0
3	NAG	C	201	14/15	0.65	0.20	95,97,98,98	0
4	GOL	A	203	6/6	0.70	0.19	58,59,61,61	0
3	NAG	A	201	14/15	0.72	0.16	80,83,84,85	0
3	NAG	A	202	14/15	0.82	0.16	45,57,62,63	0
3	NAG	C	202	14/15	0.87	0.13	56,61,68,69	0
5	CA	B	202	1/1	0.91	0.10	49,49,49,49	0
5	CA	D	201	1/1	0.96	0.05	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.