



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 04:40 PM EDT

PDB ID : 4P4K
Title : Structural Basis of Chronic Beryllium Disease: Bridging the Gap Between allergic hypersensitivity and auto immunity
Authors : Clayton, G.M.; Crawford, F.; Kappler, J.W.
Deposited on : 2014-03-12
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

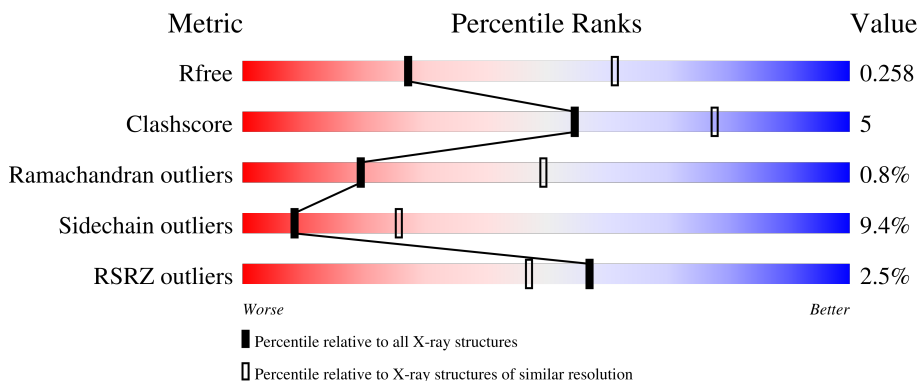
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



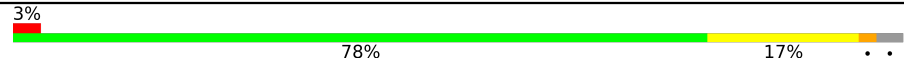

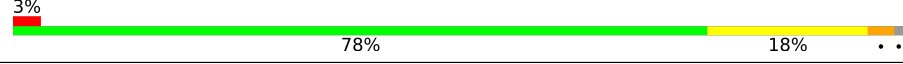
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 14% . .</p>
1	E	183	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 16% . .</p>
2	B	212	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 79% 14% 6%</p>
2	F	212	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 77% 16% . 6%</p>
3	C	209	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 75% 22% .</p>

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Mol	Chain	Length	Quality of chain
3	G	209	 <p>3% 78% 17% ..</p>
4	D	242	 <p>2% 84% 13% .</p>
4	H	242	 <p>3% 78% 18% ..</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13276 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
			Total	C	N	O	S			
1	A	178	1449	936	234	274	5	0	0	0
1	E	181	1470	951	238	276	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	199	1596	1006	275	307	8	0	0	0
2	F	199	1622	1022	283	309	8	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	linker	UNP P04440
B	-13	GLY	-	linker	UNP P04440
B	-12	GLY	-	linker	UNP P04440
B	-11	SER	-	linker	UNP P04440
B	-10	LEU	-	linker	UNP P04440
B	-9	VAL	-	linker	UNP P04440
B	-8	PRO	-	linker	UNP P04440
B	-7	ARG	-	linker	UNP P04440
B	-6	GLY	-	linker	UNP P04440
B	-5	SER	-	linker	UNP P04440
B	-4	GLY	-	linker	UNP P04440
B	-3	GLY	-	linker	UNP P04440
B	-2	GLY	-	linker	UNP P04440
B	-1	GLY	-	linker	UNP P04440
B	3	SER	THR	variant	UNP P04440
B	36	VAL	ALA	variant	UNP P04440

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	ASP	ALA	variant	UNP P04440
B	56	GLU	ALA	variant	UNP P04440
B	69	GLU	LYS	variant	UNP P04440
F	-14	GLY	-	linker	UNP P04440
F	-13	GLY	-	linker	UNP P04440
F	-12	GLY	-	linker	UNP P04440
F	-11	SER	-	linker	UNP P04440
F	-10	LEU	-	linker	UNP P04440
F	-9	VAL	-	linker	UNP P04440
F	-8	PRO	-	linker	UNP P04440
F	-7	ARG	-	linker	UNP P04440
F	-6	GLY	-	linker	UNP P04440
F	-5	SER	-	linker	UNP P04440
F	-4	GLY	-	linker	UNP P04440
F	-3	GLY	-	linker	UNP P04440
F	-2	GLY	-	linker	UNP P04440
F	-1	GLY	-	linker	UNP P04440
F	3	SER	THR	variant	UNP P04440
F	36	VAL	ALA	variant	UNP P04440
F	55	ASP	ALA	variant	UNP P04440
F	56	GLU	ALA	variant	UNP P04440
F	69	GLU	LYS	variant	UNP P04440

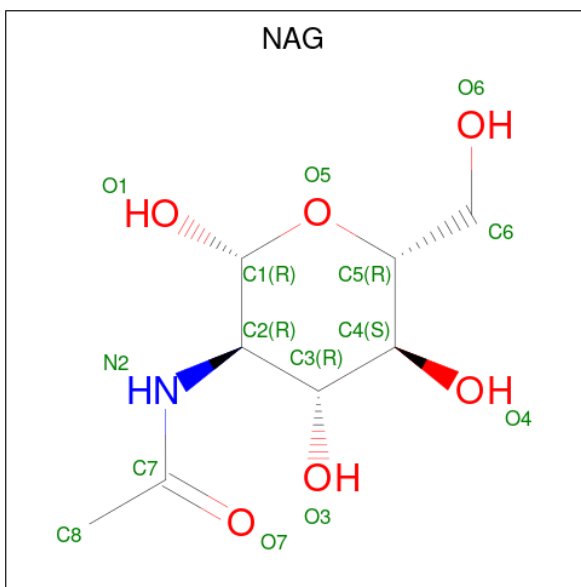
- Molecule 3 is a protein called hTCRav22 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	204	Total	C	N	O	S	0	0	0
			1522	967	236	311	8			
3	G	203	Total	C	N	O	S	0	0	0
			1496	947	233	308	8			

- Molecule 4 is a protein called hTCRav22 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1871	1178	330	357	6			
4	H	239	Total	C	N	O	S	0	0	0
			1846	1166	319	355	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	F	1	Total	Na	0	0
			1	1		

- Molecule 7 is BERYLLIUM (three-letter code: 0BE) (formula: Be).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Be	0	0
			1	1		
7	F	1	Total	Be	0	0
			1	1		

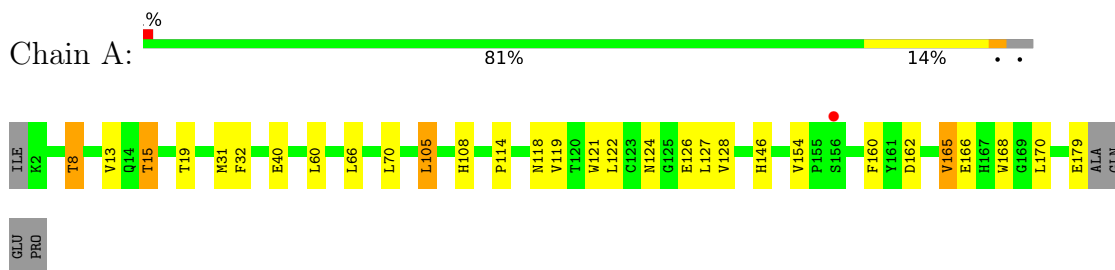
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	33	Total O 33 33	0	0
8	B	44	Total O 44 44	0	0
8	C	22	Total O 22 22	0	0
8	D	41	Total O 41 41	0	0
8	E	55	Total O 55 55	0	0
8	F	55	Total O 55 55	0	0
8	G	19	Total O 19 19	0	0
8	H	61	Total O 61 61	0	0

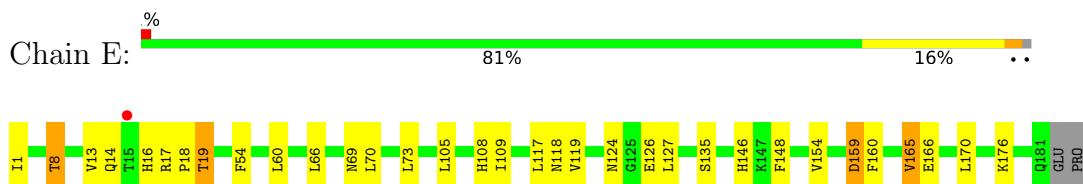
3 Residue-property plots [i](#)

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

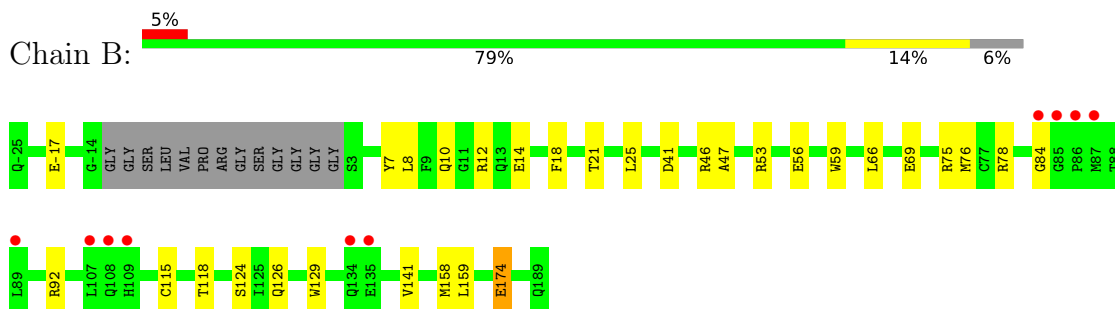
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



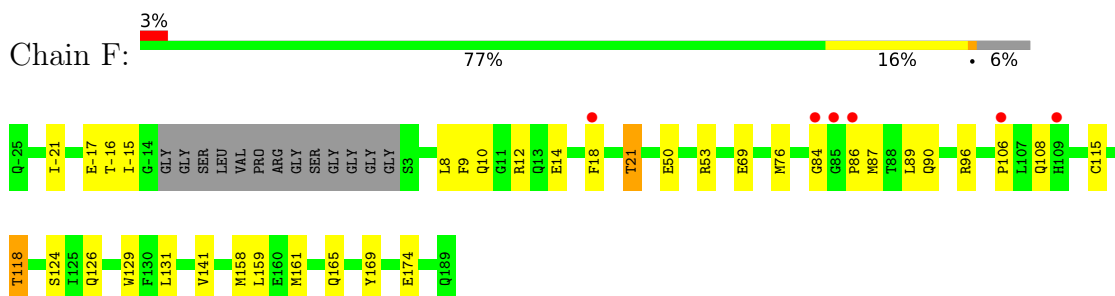
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain



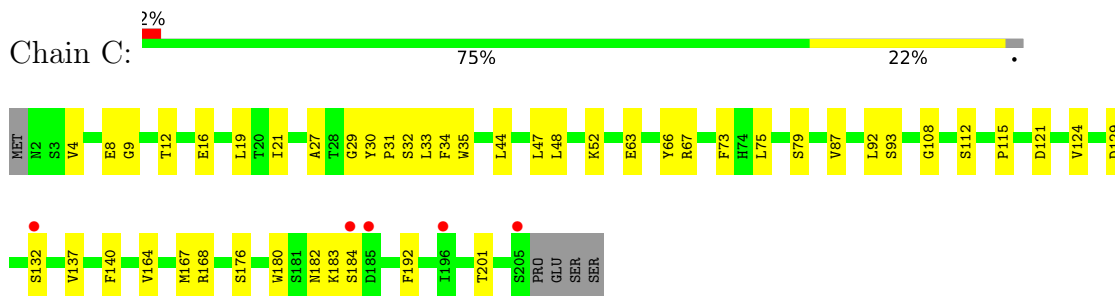
- Molecule 2: mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain



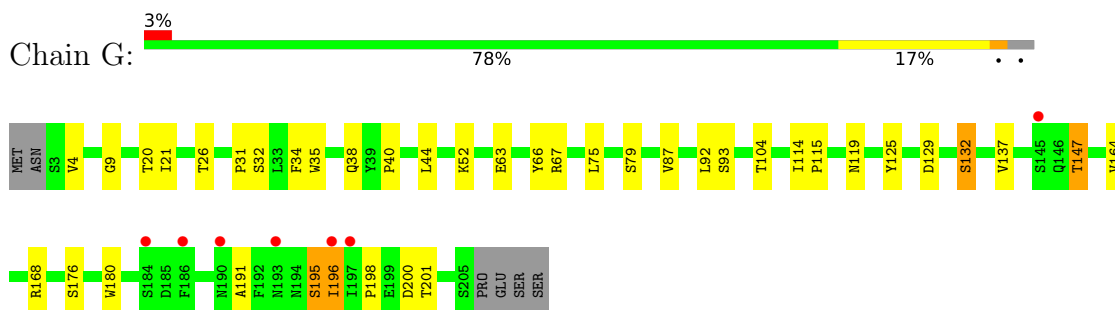
- Molecule 2: mim2 peptide,HLA class II histocompatibility antigen, DP beta 1 chain



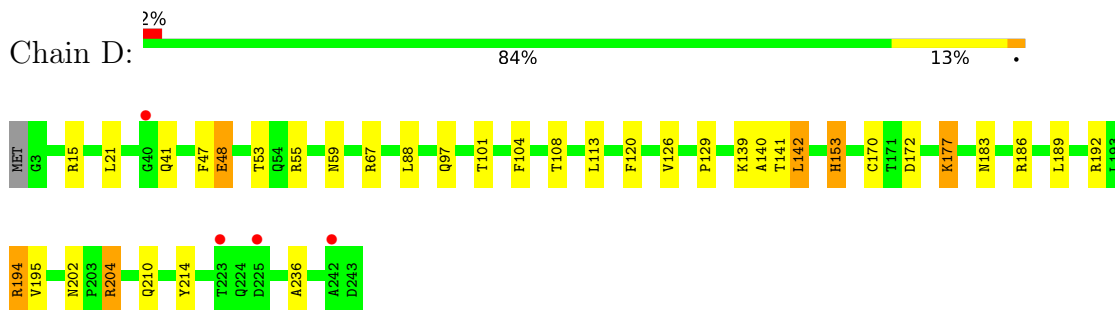
- Molecule 3: hTCRav22 alpha chain



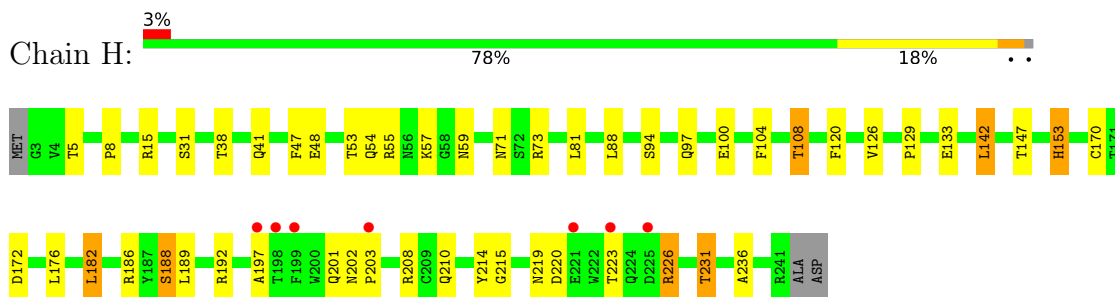
- Molecule 3: hTCRav22 alpha chain



- Molecule 4: hTCRav22 beta chain



- Molecule 4: hTCRav22 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.40Å 137.24Å 213.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.80 39.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.70-2.80) 100.0 (39.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.81Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.204 , 0.252 0.211 , 0.258	Depositor DCC
R_{free} test set	2949 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13276	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6495e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NA, OBE

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	0.51	0/1497	0.85	0/2045
1	E	0.51	0/1518	0.84	0/2074
2	B	0.53	0/1637	0.83	0/2230
2	F	0.52	0/1664	0.83	0/2263
3	C	0.54	0/1557	0.93	0/2122
3	G	0.52	0/1530	0.91	1/2090 (0.0%)
4	D	0.54	0/1922	0.83	0/2619
4	H	0.52	0/1897	0.85	0/2589
All	All	0.52	0/13222	0.86	1/18032 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	195	SER	C-N-CA	5.49	135.41	121.70

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	1449	0	1330	18	0
1	E	1470	0	1362	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1596	0	1450	12	0
2	F	1622	0	1499	16	0
3	C	1522	0	1400	23	0
3	G	1496	0	1352	18	0
4	D	1871	0	1740	17	0
4	H	1846	0	1712	21	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
5	E	28	0	26	0	0
6	B	1	0	0	0	0
6	F	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
8	A	33	0	0	0	0
8	B	44	0	0	6	0
8	C	22	0	0	0	0
8	D	41	0	0	0	0
8	E	55	0	0	2	0
8	F	55	0	0	0	0
8	G	19	0	0	0	0
8	H	61	0	0	2	0
All	All	13276	0	11910	130	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 5.

All (130) 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)
3:C:183:LYS:HB3	3:C:184:SER:HA	1.54	0.90
1:E:108:HIS:HE1	1:E:146:HIS:HD2	1.24	0.84
1:A:114:PRO:HG3	8:B:339:HOH:O	1.81	0.80
4:H:8:PRO:O	4:H:108:THR:HB	1.84	0.78
1:A:108:HIS:HE1	1:A:146:HIS:CD2	2.03	0.75
1:A:114:PRO:HB3	8:B:339:HOH:O	1.87	0.74
1:A:108:HIS:HE1	1:A:146:HIS:HD2	1.31	0.74
1:E:108:HIS:HE1	1:E:146:HIS:CD2	2.04	0.74
4:D:21:LEU:HD22	4:D:108:THR:HG21	1.70	0.73
1:E:124:ASN:HD21	1:E:159:ASP:HB3	1.54	0.72
2:B:78:ARG:HD2	3:C:30:TYR:HE1	1.56	0.71
3:C:34:PHE:HE2	3:C:93:SER:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:115:PRO:HG3	3:G:164:VAL:HG21	1.74	0.69
3:G:34:PHE:HE2	3:G:93:SER:HB2	1.57	0.69
1:A:114:PRO:CB	8:B:339:HOH:O	2.39	0.69
4:D:120:PHE:CD1	4:D:186:ARG:HD3	2.28	0.68
4:D:139:LYS:HB3	4:D:194:ARG:HD3	1.77	0.66
1:A:114:PRO:CG	8:B:339:HOH:O	2.43	0.66
1:E:108:HIS:CE1	1:E:146:HIS:HD2	2.11	0.65
4:D:177:LYS:HD3	4:D:177:LYS:H	1.62	0.65
2:F:-17:GLU:OE1	2:F:69:GLU:OE2	2.15	0.64
3:G:34:PHE:CE2	3:G:93:SER:HB2	2.33	0.63
2:F:86:PRO:HA	2:F:90:GLN:HB2	1.79	0.63
3:C:34:PHE:CE2	3:C:93:SER:HB2	2.33	0.63
1:A:15:THR:HG23	2:B:7:TYR:H	1.61	0.63
3:C:183:LYS:HB3	3:C:184:SER:CA	2.29	0.62
3:G:4:VAL:CG2	3:G:92:LEU:HG	2.30	0.62
2:B:18:PHE:O	2:B:21:THR:HG22	2.00	0.62
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.83	0.61
1:E:8:THR:HG21	8:E:351:HOH:O	2.00	0.61
2:F:18:PHE:O	2:F:21:THR:HG22	2.00	0.60
2:B:53:ARG:HD3	2:F:53:ARG:NH2	2.17	0.59
2:B:47:ALA:O	8:B:327:HOH:O	2.17	0.59
1:A:108:HIS:CE1	1:A:146:HIS:HD2	2.17	0.58
2:B:8:LEU:HD21	2:B:10:GLN:HG3	1.85	0.58
4:D:202:ASN:HD21	4:D:204:ARG:HB2	1.68	0.58
1:E:118:ASN:HB2	1:E:166:GLU:HB2	1.84	0.58
2:F:8:LEU:HD21	2:F:10:GLN:HG3	1.86	0.58
4:D:177:LYS:H	4:D:177:LYS:CD	2.17	0.57
3:G:4:VAL:HG22	3:G:92:LEU:HG	1.86	0.57
4:D:55:ARG:NH2	4:D:97:GLN:O	2.35	0.57
2:B:-17:GLU:OE1	2:B:69:GLU:OE2	2.23	0.56
4:H:197:ALA:O	4:H:201:GLN:HG2	2.06	0.55
1:E:69:ASN:HD21	2:F:-16:THR:HA	1.72	0.55
1:E:146:HIS:HE1	8:E:317:HOH:O	1.90	0.54
1:E:14:GLN:NE2	1:E:16:HIS:O	2.40	0.54
1:E:17:ARG:HA	1:E:18:PRO:C	2.28	0.54
1:E:69:ASN:ND2	2:F:-15:ILE:H	2.05	0.54
3:C:47:LEU:HG	3:C:48:LEU:HD13	1.89	0.53
2:F:126:GLN:HB2	2:F:174:GLU:HB2	1.91	0.53
3:G:147:THR:HG21	3:G:198:PRO:HG3	1.91	0.52
3:G:137:VAL:HG12	3:G:180:TRP:HB3	1.91	0.52
3:C:115:PRO:HG3	3:C:164:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ARG:HA	1:E:19:THR:N	2.25	0.51
2:F:50:GLU:HG2	2:F:53:ARG:NH2	2.25	0.51
2:F:96:ARG:HB2	2:F:118:THR:HG22	1.93	0.50
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.93	0.50
3:C:129:ASP:HB3	3:C:132:SER:O	2.12	0.50
4:D:48:GLU:OE2	4:D:55:ARG:NH1	2.44	0.50
4:H:31:SER:HB3	4:H:94:SER:HB3	1.94	0.50
8:B:327:HOH:O	2:F:50:GLU:HG3	2.12	0.49
3:G:44:LEU:O	4:H:104:PHE:HB2	2.13	0.49
3:C:33:LEU:HD23	3:C:73:PHE:HB2	1.95	0.49
3:G:38:GLN:HB3	3:G:87:VAL:HG13	1.94	0.49
3:G:129:ASP:HB3	3:G:132:SER:O	2.13	0.49
4:H:226:ARG:HH11	4:H:226:ARG:HB3	1.78	0.49
4:D:129:PRO:HD3	4:D:142:LEU:HG	1.95	0.49
1:E:109:ILE:HG21	1:E:117:LEU:HD21	1.93	0.49
4:H:71:ASN:OD1	4:H:73:ARG:HB2	2.13	0.49
3:C:12:THR:HG23	3:C:112:SER:HB2	1.94	0.48
4:D:172:ASP:HB2	4:D:189:LEU:HD12	1.95	0.48
4:D:126:VAL:HG23	4:D:236:ALA:HB3	1.94	0.48
4:H:126:VAL:HG23	4:H:236:ALA:HB3	1.95	0.48
2:B:46:ARG:HA	2:B:56:GLU:HG3	1.95	0.47
4:D:202:ASN:ND2	4:D:204:ARG:HB2	2.28	0.47
1:E:135:SER:HB2	1:E:148:PHE:H	1.79	0.47
4:H:129:PRO:HD3	4:H:142:LEU:HG	1.96	0.47
4:H:55:ARG:NH2	4:H:97:GLN:O	2.41	0.47
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.50	0.46
4:H:172:ASP:HB2	4:H:189:LEU:HD12	1.97	0.46
4:D:141:THR:OG1	4:D:194:ARG:HG3	2.15	0.46
1:E:124:ASN:HA	1:E:160:PHE:CE2	2.51	0.46
3:G:21:ILE:HD12	3:G:75:LEU:HD23	1.98	0.45
2:F:115:CYS:HB2	2:F:129:TRP:CZ2	2.51	0.45
3:G:34:PHE:HE2	3:G:93:SER:CB	2.28	0.45
1:A:121:TRP:CB	1:A:128:VAL:HG22	2.46	0.45
3:C:137:VAL:HG12	3:C:180:TRP:HB3	1.98	0.45
2:B:115:CYS:HB2	2:B:129:TRP:CZ2	2.52	0.44
3:C:183:LYS:CB	3:C:184:SER:HA	2.34	0.44
4:D:129:PRO:HG3	4:D:140:ALA:HB1	2.00	0.44
4:H:120:PHE:CD2	4:H:186:ARG:HD3	2.53	0.44
2:F:131:LEU:HD13	2:F:169:TYR:CE1	2.52	0.44
2:B:126:GLN:HB2	2:B:174:GLU:HB2	2.00	0.44
4:H:54:GLN:NE2	4:H:57:LYS:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:PHE:HE2	3:C:93:SER:CB	2.28	0.43
3:G:93:SER:OG	4:H:100:GLU:HG2	2.18	0.43
1:E:54:PHE:HE1	2:F:-21:ILE:HG23	1.83	0.43
3:C:44:LEU:O	4:D:104:PHE:HB2	2.18	0.43
3:G:32:SER:HB2	3:G:93:SER:HB3	2.00	0.43
3:C:4:VAL:HG22	3:C:92:LEU:HG	2.00	0.43
3:G:35:TRP:CE2	3:G:75:LEU:HB2	2.54	0.43
3:G:92:LEU:HB2	3:G:104:THR:HB	2.01	0.43
3:C:32:SER:HB2	3:C:93:SER:HB3	2.00	0.43
4:H:5:THR:HA	8:H:351:HOH:O	2.18	0.43
3:C:35:TRP:CE2	3:C:75:LEU:HB2	2.54	0.42
1:A:121:TRP:HB2	1:A:128:VAL:HG22	2.01	0.42
1:A:8:THR:HB	2:B:14:GLU:HA	2.01	0.42
3:C:21:ILE:HD12	3:C:75:LEU:HD23	2.02	0.42
3:C:140:PHE:HB2	3:C:192:PHE:CE1	2.55	0.42
4:H:54:GLN:HE22	4:H:57:LYS:HD3	1.85	0.41
4:H:202:ASN:HA	4:H:203:PRO:HD3	1.89	0.41
3:C:4:VAL:CG2	3:C:92:LEU:HG	2.50	0.41
3:G:31:PRO:HB2	3:G:92:LEU:HD22	2.01	0.41
4:D:153:HIS:HB3	4:D:214:TYR:HB2	2.02	0.41
4:H:208:ARG:NH2	8:H:301:HOH:O	2.45	0.41
4:H:215:GLY:H	4:H:231:THR:HG22	1.85	0.41
4:H:147:THR:HG22	4:H:188:SER:HB3	2.03	0.41
3:C:31:PRO:HB2	3:C:92:LEU:HD22	2.03	0.41
4:H:153:HIS:HB3	4:H:214:TYR:HB2	2.02	0.41
2:B:-17:GLU:HB2	2:B:59:TRP:CZ2	2.56	0.41
3:C:167:MET:SD	4:D:194:ARG:HD2	2.61	0.41
1:E:73:LEU:HD13	2:F:9:PHE:HE2	1.86	0.41
3:G:125:TYR:CE1	4:H:133:GLU:HG3	2.56	0.41
1:A:119:VAL:HG22	1:A:165:VAL:HB	2.03	0.40
1:A:31:MET:HG2	1:A:32:PHE:HD2	1.86	0.40
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.96	0.40
1:E:8:THR:HB	2:F:14:GLU:HA	2.03	0.40
3:C:27:ALA:HB3	3:C:31:PRO:HG3	2.02	0.40
1:E:119:VAL:HG22	1:E:165:VAL:HB	2.04	0.40
1:A:168:TRP:CD1	5:A:202:NAG:H82	2.57	0.40

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	176/183 (96%)	173 (98%)	3 (2%)	0	100	100
1	E	179/183 (98%)	174 (97%)	5 (3%)	0	100	100
2	B	195/212 (92%)	183 (94%)	11 (6%)	1 (0%)	29	61
2	F	195/212 (92%)	184 (94%)	9 (5%)	2 (1%)	15	44
3	C	202/209 (97%)	178 (88%)	20 (10%)	4 (2%)	7	24
3	G	201/209 (96%)	182 (90%)	14 (7%)	5 (2%)	5	19
4	D	239/242 (99%)	231 (97%)	8 (3%)	0	100	100
4	H	237/242 (98%)	225 (95%)	11 (5%)	1 (0%)	34	66
All	All	1624/1692 (96%)	1530 (94%)	81 (5%)	13 (1%)	19	49

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	29	GLY
3	C	168	ARG
2	F	84	GLY
3	G	40	PRO
3	G	168	ARG
3	C	9	GLY
2	F	106	PRO
2	B	84	GLY
4	H	182	LEU
3	G	191	ALA
3	G	196	ILE
3	C	108	GLY
3	G	9	GLY

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	157/164 (96%)	142 (90%)	15 (10%)	8	24
1	E	159/164 (97%)	144 (91%)	15 (9%)	8	26
2	B	168/186 (90%)	155 (92%)	13 (8%)	13	35
2	F	174/186 (94%)	161 (92%)	13 (8%)	13	37
3	C	164/184 (89%)	150 (92%)	14 (8%)	10	31
3	G	159/184 (86%)	143 (90%)	16 (10%)	7	22
4	D	198/211 (94%)	178 (90%)	20 (10%)	7	22
4	H	197/211 (93%)	174 (88%)	23 (12%)	5	16
All	All	1376/1490 (92%)	1247 (91%)	129 (9%)	8	26

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	13	VAL
1	A	15	THR
1	A	19	THR
1	A	40	GLU
1	A	60	LEU
1	A	66	LEU
1	A	70	LEU
1	A	105	LEU
1	A	126	GLU
1	A	127	LEU
1	A	154	VAL
1	A	165	VAL
1	A	170	LEU
1	A	179	GLU
2	B	12	ARG
2	B	25	LEU
2	B	41	ASP
2	B	66	LEU

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Mol	Chain	Res	Type
2	B	75	ARG
2	B	76	MET
2	B	92	ARG
2	B	118	THR
2	B	124	SER
2	B	141	VAL
2	B	158	MET
2	B	159	LEU
2	B	174	GLU
3	C	8	GLU
3	C	16	GLU
3	C	19	LEU
3	C	52	LYS
3	C	63	GLU
3	C	66	TYR
3	C	67	ARG
3	C	79	SER
3	C	87	VAL
3	C	121	ASP
3	C	124	VAL
3	C	176	SER
3	C	182	ASN
3	C	201	THR
4	D	15	ARG
4	D	41	GLN
4	D	47	PHE
4	D	48	GLU
4	D	53	THR
4	D	59	ASN
4	D	67	ARG
4	D	88	LEU
4	D	101	THR
4	D	113	LEU
4	D	142	LEU
4	D	153	HIS
4	D	170	CYS
4	D	177	LYS
4	D	183	ASN
4	D	192	ARG
4	D	194	ARG
4	D	195	VAL
4	D	204	ARG

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Mol	Chain	Res	Type
4	D	210	GLN
1	E	1	ILE
1	E	8	THR
1	E	13	VAL
1	E	19	THR
1	E	60	LEU
1	E	66	LEU
1	E	70	LEU
1	E	105	LEU
1	E	126	GLU
1	E	127	LEU
1	E	154	VAL
1	E	159	ASP
1	E	165	VAL
1	E	170	LEU
1	E	176	LYS
2	F	12	ARG
2	F	21	THR
2	F	76	MET
2	F	87	MET
2	F	89	LEU
2	F	108	GLN
2	F	118	THR
2	F	124	SER
2	F	141	VAL
2	F	158	MET
2	F	159	LEU
2	F	161	MET
2	F	165	GLN
3	G	20	THR
3	G	26	THR
3	G	52	LYS
3	G	63	GLU
3	G	66	TYR
3	G	67	ARG
3	G	79	SER
3	G	114	ILE
3	G	119	ASN
3	G	132	SER
3	G	147	THR
3	G	176	SER
3	G	195	SER

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Mol	Chain	Res	Type
3	G	196	ILE
3	G	200	ASP
3	G	201	THR
4	H	15	ARG
4	H	38	THR
4	H	41	GLN
4	H	47	PHE
4	H	48	GLU
4	H	53	THR
4	H	59	ASN
4	H	81	LEU
4	H	88	LEU
4	H	108	THR
4	H	142	LEU
4	H	153	HIS
4	H	170	CYS
4	H	176	LEU
4	H	182	LEU
4	H	188	SER
4	H	192	ARG
4	H	210	GLN
4	H	219	ASN
4	H	220	ASP
4	H	223	THR
4	H	226	ARG
4	H	231	THR

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	68	ASN
1	A	108	HIS
1	A	146	HIS
4	D	77	ASN
4	D	202	ASN
1	E	68	ASN
1	E	69	ASN
1	E	108	HIS
1	E	146	HIS
3	G	81	GLN
4	H	54	GLN
4	H	102	GLN

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Mol	Chain	Res	Type
4	H	161	ASN
4	H	205	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
5	NAG	E	201	1	14,14,15	0.32	0	17,19,21	1.29	1 (5%)
5	NAG	A	201	1	14,14,15	0.35	0	17,19,21	1.03	3 (17%)
5	NAG	E	202	1	14,14,15	0.38	0	17,19,21	1.21	3 (17%)
5	NAG	A	202	1	14,14,15	0.38	0	17,19,21	2.65	3 (17%)
5	NAG	B	201	2	14,14,15	0.34	0	17,19,21	0.70	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	E	201	1	-	2/6/23/26	0/1/1/1
5	NAG	A	201	1	-	0/6/23/26	0/1/1/1
5	NAG	E	202	1	-	0/6/23/26	0/1/1/1
5	NAG	A	202	1	-	4/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	202	NAG	C1-C2-N2	9.37	126.49	110.49
5	A	202	NAG	C1-O5-C5	4.77	118.66	112.19
5	E	201	NAG	C1-C2-N2	-4.65	102.54	110.49
5	E	202	NAG	C1-O5-C5	3.19	116.51	112.19
5	E	202	NAG	C1-C2-N2	2.52	114.79	110.49
5	A	201	NAG	C1-O5-C5	2.48	115.55	112.19
5	E	202	NAG	O5-C1-C2	-2.48	107.38	111.29
5	A	202	NAG	C2-N2-C7	2.47	126.42	122.90
5	B	201	NAG	C1-O5-C5	2.36	115.39	112.19
5	A	201	NAG	C1-C2-N2	2.28	114.38	110.49
5	A	201	NAG	O5-C1-C2	-2.21	107.80	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	202	NAG	C8-C7-N2-C2
5	A	202	NAG	O7-C7-N2-C2
5	E	201	NAG	O5-C5-C6-O6
5	A	202	NAG	C1-C2-N2-C7
5	A	202	NAG	C3-C2-N2-C7
5	E	201	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	A	202	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

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%)	0.01	1 (0%) 89 86	38, 53, 72, 86	0
1	E	181/183 (98%)	-0.10	1 (0%) 89 86	37, 51, 70, 95	0
2	B	199/212 (93%)	0.19	10 (5%) 28 19	40, 57, 93, 107	0
2	F	199/212 (93%)	0.03	6 (3%) 50 40	35, 50, 89, 106	0
3	C	204/209 (97%)	0.21	5 (2%) 57 47	43, 67, 101, 113	0
3	G	203/209 (97%)	0.21	7 (3%) 45 35	43, 70, 94, 113	0
4	D	241/242 (99%)	0.05	4 (1%) 70 63	39, 56, 86, 110	0
4	H	239/242 (98%)	-0.03	7 (2%) 51 41	34, 52, 89, 103	0
All	All	1644/1692 (97%)	0.07	41 (2%) 57 47	34, 57, 92, 113	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	84	GLY	4.6
2	F	85	GLY	4.3
2	B	107	LEU	3.9
2	F	84	GLY	3.7
3	G	190	ASN	3.6
2	B	108	GLN	3.4
2	F	106	PRO	3.4
3	C	196	ILE	3.1
2	B	109	HIS	3.1
2	F	109	HIS	3.0
3	C	132	SER	2.9
2	B	85	GLY	2.9
4	D	242	ALA	2.9
3	G	193	ASN	2.9
2	B	89	LEU	2.9
3	C	184	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	87	MET	2.8
4	H	225	ASP	2.7
2	F	86	PRO	2.6
4	D	223	THR	2.6
2	B	86	PRO	2.5
1	E	15	THR	2.5
3	C	185	ASP	2.5
4	H	221	GLU	2.4
3	G	145	SER	2.4
2	F	18	PHE	2.4
3	G	197	ILE	2.3
4	H	203	PRO	2.3
4	H	223	THR	2.3
4	D	40	GLY	2.2
4	H	199	PHE	2.1
1	A	156	SER	2.1
4	H	197	ALA	2.1
4	H	198	THR	2.1
3	C	205	SER	2.1
3	G	186	PHE	2.1
2	B	134	GLN	2.0
3	G	184	SER	2.0
2	B	135	GLU	2.0
3	G	196	ILE	2.0
4	D	225	ASP	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 monosaccharides 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(\AA^2)	Q<0.9
5	NAG	E	202	14/15	0.71	0.33	102,103,107,108	0
5	NAG	A	201	14/15	0.76	0.32	117,120,121,121	0
5	NAG	B	201	14/15	0.77	0.27	108,113,114,115	0
5	NAG	E	201	14/15	0.81	0.27	72,84,93,96	0
7	0BE	F	202	1/1	0.86	0.38	18,18,18,18	0
5	NAG	A	202	14/15	0.89	0.28	72,74,78,80	0
6	NA	B	202	1/1	0.90	0.30	63,63,63,63	0
6	NA	F	201	1/1	0.93	0.23	52,52,52,52	0
7	0BE	B	203	1/1	0.95	0.26	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.