



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:32 AM UTC

PDB ID : 5KS9 / pdb_00005ks9
Title : Bel502-DQ8-glia-alpha1 complex
Authors : Petersen, J.; Rossjohn, J.; Reid, H.H.
Deposited on : 2016-07-08
Resolution : 2.55 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

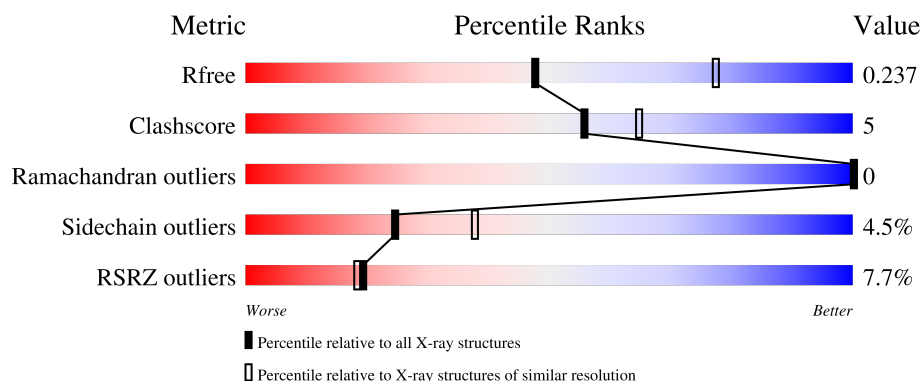
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	192	3% 81% 12% • 5%
1	C	192	• 80% 14% • 5%
2	B	230	4% 63% 14% • 21%
2	D	230	10% 58% 15% • 25%
3	E	207	14% 73% 17% •• 7%

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Mol	Chain	Length	Quality of chain
3	G	207	14% 76% 15% 7%
4	F	242	5% 86% 12%
4	H	242	5% 88% 9%
5	I	16	12% 88% 12%
5	J	16	19% 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13515 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, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1464	944	240	278	2			
1	C	182	Total	C	N	O	S	0	0	0
			1464	944	240	278	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP Q30063
A	183	SER	-	expression tag	UNP Q30063
A	184	GLY	-	expression tag	UNP Q30063
A	185	ASP	-	expression tag	UNP Q30063
A	186	ASP	-	expression tag	UNP Q30063
A	187	ASP	-	expression tag	UNP Q30063
A	188	ASP	-	expression tag	UNP Q30063
A	189	LYS	-	expression tag	UNP Q30063
C	182	THR	-	expression tag	UNP Q30063
C	183	SER	-	expression tag	UNP Q30063
C	184	GLY	-	expression tag	UNP Q30063
C	185	ASP	-	expression tag	UNP Q30063
C	186	ASP	-	expression tag	UNP Q30063
C	187	ASP	-	expression tag	UNP Q30063
C	188	ASP	-	expression tag	UNP Q30063
C	189	LYS	-	expression tag	UNP Q30063

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	1	0
			1493	946	263	277	7			
2	D	173	Total	C	N	O	S	0	0	0
			1395	890	244	254	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	linker	PDB ?
B	-12	GLY	-	linker	PDB ?
B	-11	GLY	-	linker	PDB ?
B	-10	SER	-	linker	PDB ?
B	-9	ILE	-	linker	PDB ?
B	-8	GLU	-	linker	PDB ?
B	-7	GLY	-	linker	PDB ?
B	-6	ARG	-	linker	PDB ?
B	-5	GLY	-	linker	PDB ?
B	-4	GLY	-	linker	PDB ?
B	-3	SER	-	linker	PDB ?
B	-2	GLY	-	linker	PDB ?
B	-1	ALA	-	linker	PDB ?
B	0	SER	-	linker	PDB ?
B	193	THR	-	expression tag	UNP U3PYM0
B	194	GLY	-	expression tag	UNP U3PYM0
B	195	GLY	-	expression tag	UNP U3PYM0
B	196	ASP	-	expression tag	UNP U3PYM0
B	197	ASP	-	expression tag	UNP U3PYM0
B	198	ASP	-	expression tag	UNP U3PYM0
B	199	ASP	-	expression tag	UNP U3PYM0
B	200	LYS	-	expression tag	UNP U3PYM0
D	-13	SER	-	linker	PDB ?
D	-12	GLY	-	linker	PDB ?
D	-11	GLY	-	linker	PDB ?
D	-10	SER	-	linker	PDB ?
D	-9	ILE	-	linker	PDB ?
D	-8	GLU	-	linker	PDB ?
D	-7	GLY	-	linker	PDB ?
D	-6	ARG	-	linker	PDB ?
D	-5	GLY	-	linker	PDB ?
D	-4	GLY	-	linker	PDB ?
D	-3	SER	-	linker	PDB ?
D	-2	GLY	-	linker	PDB ?
D	-1	ALA	-	linker	PDB ?
D	0	SER	-	linker	PDB ?
D	193	THR	-	expression tag	UNP U3PYM0
D	194	GLY	-	expression tag	UNP U3PYM0
D	195	GLY	-	expression tag	UNP U3PYM0
D	196	ASP	-	expression tag	UNP U3PYM0
D	197	ASP	-	expression tag	UNP U3PYM0
D	198	ASP	-	expression tag	UNP U3PYM0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	199	ASP	-	expression tag	UNP U3PYM0
D	200	LYS	-	expression tag	UNP U3PYM0

- Molecule 3 is a protein called Bel502 TCR alpha TRAV20*01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	193	Total	C	N	O	S	0	0	0
			1484	929	252	294	9			
3	G	192	Total	C	N	O	S	0	0	0
			1466	918	247	292	9			

- Molecule 4 is a protein called Bel502 TCR beta TRBV9*01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	240	Total	C	N	O	S	0	0	0
			1887	1193	327	362	5			
4	H	240	Total	C	N	O	S	0	0	0
			1886	1193	330	358	5			

- Molecule 5 is a protein called DQ8-glia-alpha1 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	16	Total	C	N	O	0	0	0
			112	67	19	26			
5	J	16	Total	C	N	O	0	0	0
			112	67	19	26			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total	O	0	0
			79	79		

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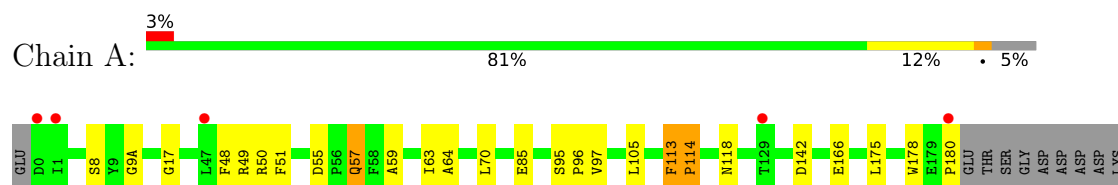
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	60	Total 60	O 60	0	0
8	C	105	Total 105	O 105	0	0
8	D	90	Total 90	O 90	0	0
8	E	75	Total 75	O 75	0	0
8	F	145	Total 145	O 145	0	0
8	G	44	Total 44	O 44	0	0
8	H	81	Total 81	O 81	0	0
8	I	9	Total 9	O 9	0	0
8	J	4	Total 4	O 4	0	0

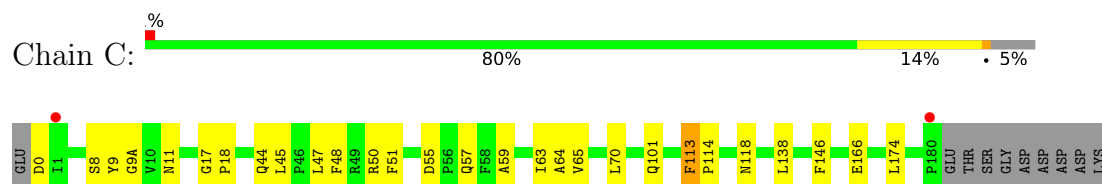
3 Residue-property plots [i](#)

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.

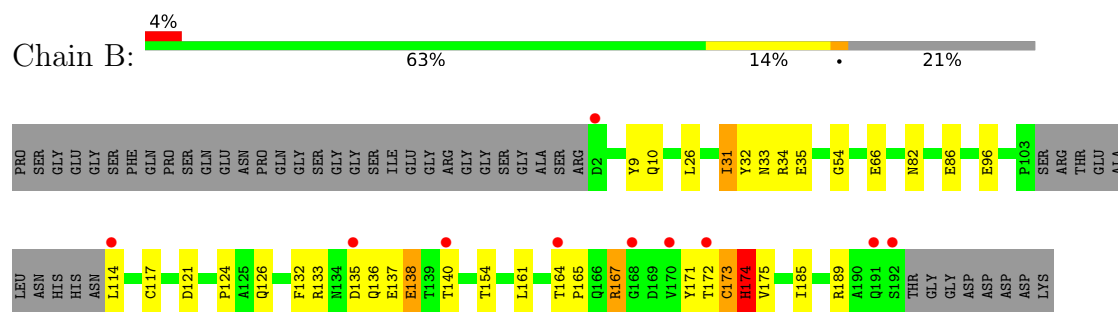
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



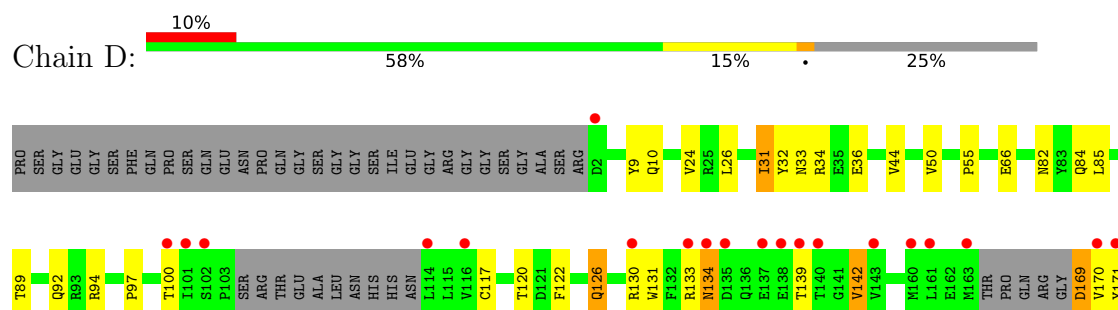
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain

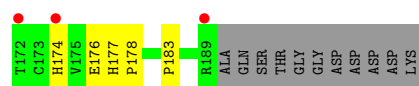


- Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain

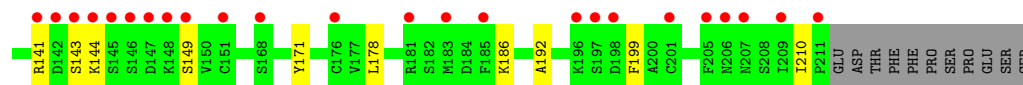
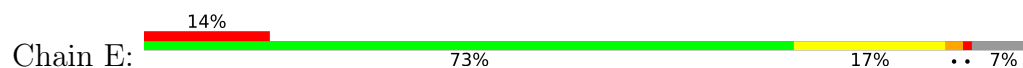


- Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain

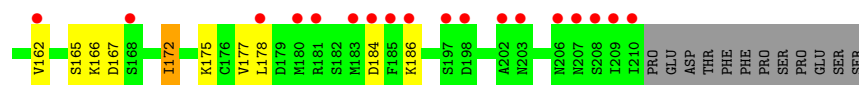
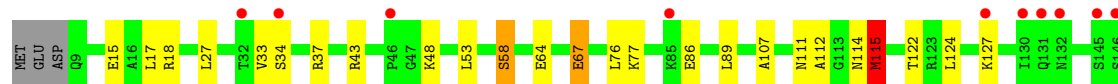
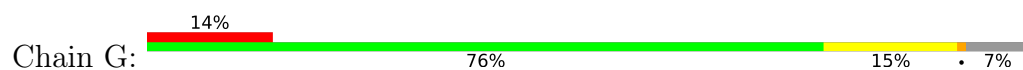




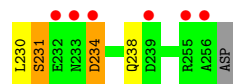
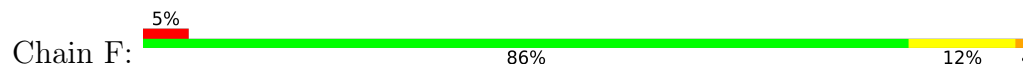
• Molecule 3: Bel502 TCR alpha TRAV20*01



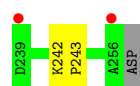
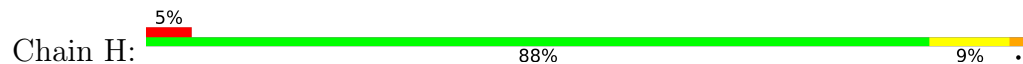
• Molecule 3: Bel502 TCR alpha TRAV20*01



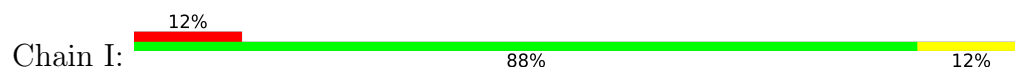
• Molecule 4: Bel502 TCR beta TRBV9*01



• Molecule 4: Bel502 TCR beta TRBV9*01



• Molecule 5: DQ8-glia-alpha1 peptide





- Molecule 5: DQ8-glia-alpha1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.56Å 56.87Å 232.05Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	46.90 – 2.55 46.90 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.90-2.55) 98.8 (46.90-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.199 , 0.224 0.215 , 0.237	Depositor DCC
R_{free} test set	1263 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13515	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.45 % 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 2.7305e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.96	4/1508 (0.3%)	1.14	3/2061 (0.1%)
1	C	1.15	6/1508 (0.4%)	1.22	3/2061 (0.1%)
2	B	1.17	11/1534 (0.7%)	1.25	13/2092 (0.6%)
2	D	1.12	8/1430 (0.6%)	1.18	8/1951 (0.4%)
3	E	1.17	11/1514 (0.7%)	1.13	4/2050 (0.2%)
3	G	0.95	3/1495 (0.2%)	1.07	0/2026
4	F	0.90	11/1938 (0.6%)	1.10	3/2644 (0.1%)
4	H	0.83	1/1937 (0.1%)	1.06	2/2642 (0.1%)
5	I	0.70	0/115	1.09	0/156
5	J	0.63	0/115	1.11	0/156
All	All	1.02	55/13094 (0.4%)	1.14	36/17839 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	115	MET	SD-CE	-12.61	1.48	1.79
3	G	115	MET	SD-CE	-11.45	1.50	1.79
2	B	174[A]	HIS	CA-C	9.84	1.64	1.52
2	B	174[B]	HIS	CA-C	9.84	1.64	1.52
2	B	33	ASN	C-O	-6.71	1.18	1.24
3	E	76	LEU	C-O	-6.44	1.16	1.24
3	E	125	MET	C-O	-6.43	1.16	1.24
3	E	124	LEU	C-O	-6.38	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	33	ASN	C-O	-6.21	1.18	1.24
3	E	124	LEU	N-CA	-6.17	1.38	1.46
4	F	64	GLU	C-O	-6.13	1.16	1.23
2	B	31	ILE	C-O	-6.08	1.17	1.24
1	C	64	ALA	C-O	-6.01	1.17	1.24
2	D	32	TYR	C-O	-5.95	1.17	1.24
4	F	55	GLN	C-O	-5.91	1.16	1.24
2	D	36	GLU	C-O	-5.91	1.17	1.24
2	B	164	THR	C-N	5.81	1.40	1.33
2	B	173	CYS	C-O	-5.76	1.17	1.24
2	B	175	VAL	C-O	-5.73	1.18	1.24
4	F	18	ARG	C-O	-5.73	1.16	1.24
4	H	64	GLU	C-O	-5.72	1.16	1.23
1	C	65	VAL	C-O	-5.64	1.17	1.24
3	G	107	ALA	C-O	-5.60	1.17	1.24
2	B	32	TYR	C-O	-5.54	1.17	1.24
2	B	35	GLU	C-O	-5.52	1.17	1.24
2	D	82	ASN	C-O	-5.52	1.17	1.24
1	A	114	PRO	N-CD	5.49	1.55	1.47
3	E	14	PRO	N-CD	5.48	1.55	1.47
3	E	126	VAL	C-O	-5.47	1.18	1.24
3	E	107	ALA	C-O	-5.44	1.17	1.24
2	D	84	GLN	C-O	-5.43	1.17	1.24
3	E	109	ASN	C-O	-5.39	1.17	1.24
1	A	57	GLN	C-O	-5.35	1.17	1.24
1	C	47	LEU	C-O	-5.34	1.17	1.24
4	F	63	GLY	C-O	-5.32	1.16	1.24
3	G	76	LEU	C-O	-5.32	1.17	1.24
1	C	44	GLN	C-O	-5.31	1.17	1.24
2	D	126	GLN	C-O	-5.26	1.17	1.23
4	F	19	VAL	C-O	-5.25	1.18	1.24
4	F	65	GLU	C-O	-5.21	1.17	1.23
2	B	165	PRO	N-CD	5.19	1.55	1.47
3	E	77	LYS	C-O	-5.14	1.18	1.23
2	D	31	ILE	C-O	-5.13	1.18	1.24
1	A	64	ALA	C-O	-5.12	1.18	1.24
4	F	54	ILE	C-O	-5.11	1.17	1.23
1	A	48	PHE	C-O	-5.11	1.18	1.24
4	F	21	LEU	C-O	-5.11	1.17	1.24
2	B	96	GLU	C-N	5.07	1.40	1.33
4	F	67	ALA	C-O	-5.06	1.17	1.23
4	F	20	THR	C-O	-5.05	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	34	ARG	C-O	-5.05	1.17	1.24
3	E	67	GLU	C-O	-5.04	1.18	1.24
4	F	57	TYR	C-O	-5.03	1.18	1.24
1	C	57	GLN	C-O	-5.02	1.17	1.24
1	C	18	PRO	N-CD	5.01	1.54	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	ARG	N-CA-C	9.05	121.23	111.36
1	C	17	GLY	C-N-CD	8.17	138.57	120.60
1	C	113	PHE	C-N-CD	8.04	138.28	120.60
2	B	140	THR	N-CA-C	7.81	119.58	111.14
1	A	113	PHE	C-N-CD	7.69	137.52	120.60
3	E	13	SER	C-N-CD	7.66	137.45	120.60
1	A	17	GLY	C-N-CD	7.36	136.79	120.60
2	D	31	ILE	N-CA-C	7.27	118.28	108.11
2	B	174[A]	HIS	N-CA-C	7.18	120.22	108.52
2	B	174[B]	HIS	N-CA-C	7.18	120.22	108.52
4	F	76	PHE	CA-CB-CG	6.93	120.73	113.80
2	B	31	ILE	N-CA-C	6.78	117.60	108.11
2	B	164	THR	CA-C-N	-6.33	112.97	120.13
2	B	164	THR	C-N-CA	-6.33	112.97	120.13
4	H	76	PHE	CA-CB-CG	6.32	120.11	113.80
2	B	96	GLU	CA-C-N	-6.29	113.50	119.85
2	B	96	GLU	C-N-CA	-6.29	113.50	119.85
2	D	142	VAL	N-CA-C	6.08	116.62	107.80
2	B	173	CYS	CA-CB-SG	5.92	128.02	114.40
2	D	120	THR	CA-C-N	5.75	130.98	122.82
2	D	120	THR	C-N-CA	5.75	130.98	122.82
3	E	143	SER	CA-C-N	5.72	128.52	120.28
3	E	143	SER	C-N-CA	5.72	128.52	120.28
4	F	84	ASP	CA-CB-CG	5.72	118.32	112.60
4	H	84	ASP	CA-CB-CG	5.60	118.20	112.60
2	D	55	PRO	N-CA-C	5.59	117.52	110.70
2	D	44	VAL	N-CA-C	-5.52	106.32	111.45
2	B	124	PRO	CA-C-N	5.47	127.61	120.28
2	B	124	PRO	C-N-CA	5.47	127.61	120.28
2	D	50	VAL	N-CA-C	-5.30	107.66	112.96
3	E	119	GLY	N-CA-C	-5.17	104.72	112.89
1	C	146	PHE	CA-CB-CG	5.14	118.94	113.80
2	D	134	ASN	CB-CA-C	-5.11	110.71	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	65	GLU	N-CA-C	5.11	117.62	109.96
2	B	54	GLY	N-CA-C	5.07	122.69	112.34
1	A	142	ASP	CA-CB-CG	5.05	117.66	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	174[B]	HIS	Mainchain

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	1464	0	1395	16	0
1	C	1464	0	1395	13	0
2	B	1493	0	1426	20	1
2	D	1395	0	1309	19	0
3	E	1484	0	1420	18	0
3	G	1466	0	1388	19	0
4	F	1887	0	1784	11	1
4	H	1886	0	1789	14	0
5	I	112	0	94	2	0
5	J	112	0	94	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	A	79	0	0	0	0
8	B	60	0	0	0	0
8	C	105	0	0	0	0
8	D	90	0	0	0	0
8	E	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	145	0	0	0	0
8	G	44	0	0	0	0
8	H	81	0	0	0	0
8	I	9	0	0	0	0
8	J	4	0	0	0	0
All	All	13515	0	12146	117	1

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 (117) 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:B:132:PHE:CD1	2:B:174[B]:HIS:CD2	2.17	1.33
2:B:117:CYS:SG	2:B:173:CYS:SG	1.36	1.22
3:E:15:GLU:OE1	3:E:123:ARG:NH2	1.86	1.07
4:H:234:ASP:O	4:H:242:LYS:NZ	1.88	1.07
2:B:132:PHE:CE1	2:B:174[B]:HIS:CD2	2.48	1.02
2:B:132:PHE:CD1	2:B:174[B]:HIS:HD2	1.68	0.97
2:B:132:PHE:CD1	2:B:174[B]:HIS:NE2	2.35	0.95
2:B:132:PHE:HD1	2:B:174[B]:HIS:CD2	1.70	0.95
2:B:117:CYS:CB	2:B:173:CYS:SG	2.54	0.94
3:G:111:ASN:HB3	3:G:115:MET:HE3	1.50	0.94
4:H:231:SER:HB2	4:H:233:ASN:OD1	1.76	0.85
3:E:111:ASN:HB3	3:E:115:MET:CE	2.11	0.81
2:B:132:PHE:HD1	2:B:174[B]:HIS:HD2	1.11	0.79
2:B:172:THR:HG21	2:B:174[B]:HIS:CE1	2.20	0.76
3:G:178:LEU:HB3	4:H:184:CYS:HB3	1.66	0.76
2:D:139:THR:O	2:D:142:VAL:HG12	1.86	0.74
3:E:111:ASN:HB3	3:E:115:MET:HE2	1.70	0.73
3:E:67:GLU:HG3	3:E:77:LYS:HG3	1.71	0.73
3:G:33:VAL:HG12	3:G:34:SER:N	2.03	0.73
3:G:33:VAL:HG12	3:G:34:SER:H	1.54	0.72
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.70	0.71
2:B:172:THR:CG2	2:B:174[B]:HIS:CE1	2.73	0.71
3:G:111:ASN:HB3	3:G:115:MET:CE	2.20	0.69
3:G:58:SER:O	3:G:64:GLU:HB2	1.93	0.69
4:H:21:LEU:HD22	4:H:122:THR:HG21	1.74	0.68
3:G:67:GLU:HG3	3:G:77:LYS:HG3	1.79	0.64
1:A:50:ARG:HG2	1:A:51:PHE:CE1	2.33	0.64
3:G:67:GLU:HG3	3:G:77:LYS:CG	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:178:LEU:HB3	4:F:184:CYS:HB3	1.80	0.61
2:B:132:PHE:CE1	2:B:174[B]:HIS:HD2	2.05	0.60
1:C:50:ARG:HD2	1:C:51:PHE:CZ	2.36	0.60
1:A:50:ARG:HG2	1:A:51:PHE:CD1	2.36	0.60
1:C:48:PHE:CE1	2:D:89:THR:HB	2.37	0.60
3:E:58:SER:O	3:E:64:GLU:HB2	2.02	0.59
2:D:130:ARG:HB2	2:D:174:HIS:HB3	1.85	0.59
2:D:169:ASP:N	2:D:169:ASP:OD1	2.34	0.58
4:H:22:ARG:HG2	4:H:88:GLU:HG2	1.85	0.58
1:A:57:GLN:OE1	4:H:66:ARG:NH2	2.36	0.58
3:E:67:GLU:HG3	3:E:77:LYS:CG	2.34	0.58
2:D:85:LEU:HD21	5:I:-2:SER:HB3	1.86	0.57
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.85	0.57
3:G:18:ARG:HH21	3:G:127:LYS:HE2	1.71	0.56
2:D:142:VAL:O	2:D:142:VAL:HG13	2.04	0.56
3:E:33:VAL:HG12	3:E:34:SER:N	2.20	0.55
2:B:133:ARG:HD3	2:B:171:TYR:CE2	2.41	0.55
3:G:165:SER:HB2	3:G:172:ILE:HG12	1.88	0.55
3:G:27:LEU:HD22	3:G:122:THR:HG21	1.88	0.54
3:E:27:LEU:HD22	3:E:122:THR:HG21	1.90	0.54
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.90	0.54
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.88	0.53
2:D:176:GLU:HG3	2:D:183:PRO:HB3	1.89	0.53
2:D:117:CYS:HB2	2:D:131:TRP:CZ2	2.43	0.53
4:H:44:GLN:HB2	4:H:50:LEU:HD13	1.91	0.53
1:C:50:ARG:HD2	1:C:51:PHE:CE2	2.44	0.53
2:B:172:THR:HG22	2:B:174[B]:HIS:CE1	2.46	0.51
1:A:50:ARG:NE	1:A:51:PHE:CE1	2.79	0.51
3:G:37:ARG:HH21	3:G:114:ASN:HD21	1.58	0.50
1:A:97:VAL:HG11	1:A:180:PRO:HB3	1.93	0.50
4:H:234:ASP:OD1	4:H:234:ASP:N	2.27	0.50
1:C:45:LEU:HB2	1:C:48:PHE:CD2	2.47	0.50
1:C:8:SER:C	1:C:9(A):GLY:HA2	2.36	0.50
1:C:48:PHE:CD1	2:D:89:THR:HB	2.47	0.49
2:D:85:LEU:HD13	5:I:1:GLU:OE2	2.13	0.49
4:F:231:SER:N	4:F:234:ASP:OD1	2.46	0.49
1:C:70:LEU:HD13	2:D:9:TYR:HB2	1.96	0.48
1:C:59:ALA:O	1:C:63:ILE:HG12	2.15	0.47
3:E:141:ARG:HB2	4:F:142:GLU:HB2	1.95	0.47
4:H:167:HIS:HB3	4:H:228:TYR:HB2	1.97	0.47
1:A:85:GLU:HG3	2:B:34:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:233:ASN:CG	4:H:234:ASP:N	2.73	0.47
2:D:97:PRO:HB3	2:D:122:PHE:HB3	1.96	0.47
1:C:48:PHE:HE1	2:D:89:THR:HB	1.80	0.47
4:F:5:THR:OG1	4:F:24:SER:HB2	2.15	0.47
1:A:59:ALA:O	1:A:63:ILE:HG12	2.16	0.46
2:B:121:ASP:HA	2:B:154:THR:HB	1.97	0.46
1:A:55:ASP:CG	3:G:112:ALA:HA	2.40	0.46
2:B:138:GLU:HG3	2:B:161:LEU:HD11	1.96	0.46
4:F:167:HIS:HB3	4:F:228:TYR:HB2	1.97	0.46
2:D:133:ARG:O	2:D:134:ASN:HB2	2.16	0.46
4:H:39:VAL:HG21	4:H:87:SER:HB2	1.98	0.46
1:A:105:LEU:HD21	1:A:178:TRP:CD2	2.50	0.46
2:D:10:GLN:HB2	2:D:31:ILE:HB	1.98	0.45
4:F:166:ASP:HB2	4:F:189:PRO:HG2	1.98	0.45
4:F:8:PRO:HG3	4:F:11:LEU:HD13	1.99	0.45
3:G:33:VAL:CG1	3:G:34:SER:N	2.73	0.45
1:A:70:LEU:HD13	2:B:9:TYR:HB2	1.98	0.45
2:D:133:ARG:HG3	2:D:171:TYR:HE1	1.80	0.45
3:E:33:VAL:CG1	3:E:34:SER:N	2.79	0.45
1:A:8:SER:C	1:A:9(A):GLY:HA2	2.42	0.44
3:E:149:SER:HB2	3:E:199:PHE:HD2	1.81	0.44
1:A:50:ARG:HD3	1:A:51:PHE:CZ	2.53	0.44
3:G:43:ARG:HB3	3:G:53:LEU:HD11	1.99	0.44
3:G:17:LEU:HB3	3:G:124:LEU:HD12	2.00	0.44
3:E:171:TYR:O	3:E:192:ALA:HA	2.17	0.44
1:A:95:SER:HB2	1:A:96:PRO:CD	2.46	0.44
1:C:113:PHE:CG	1:C:114:PRO:HA	2.52	0.44
3:E:49:GLY:HA2	4:F:103:PHE:CE1	2.53	0.44
3:E:96:PRO:HG2	3:E:186:LYS:HE2	2.00	0.43
4:H:133:VAL:O	4:H:243:PRO:HG3	2.18	0.43
3:G:33:VAL:CG1	3:G:34:SER:H	2.26	0.42
4:H:19:VAL:HG22	4:H:94:LEU:HD11	2.01	0.42
3:G:27:LEU:HD12	3:G:89:LEU:HD23	2.00	0.42
2:D:177:HIS:CD2	2:D:178:PRO:HD2	2.54	0.42
4:F:21:LEU:HD22	4:F:122:THR:HG21	2.02	0.42
4:F:234:ASP:OD1	4:F:234:ASP:N	2.53	0.42
2:D:26:LEU:C	2:D:26:LEU:HD12	2.45	0.42
2:B:82:ASN:O	2:B:86:GLU:HG2	2.20	0.41
3:E:102:TYR:CE1	3:E:124:LEU:HD23	2.55	0.41
1:C:9:TYR:N	1:C:9(A):GLY:HA2	2.34	0.41
2:B:172:THR:HG23	2:B:185:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ASP:CG	3:E:112:ALA:HA	2.46	0.41
2:D:133:ARG:HG3	2:D:171:TYR:CE1	2.55	0.41
4:F:9:LYS:HB3	4:F:10:HIS:CD2	2.55	0.41
4:H:233:ASN:OD1	4:H:233:ASN:N	2.52	0.41
1:A:113:PHE:CG	1:A:114:PRO:HA	2.56	0.40
3:E:43:ARG:HG2	3:E:53:LEU:HD21	2.03	0.40
3:G:112:ALA:C	3:G:115:MET:HE1	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:NH2	4:F:238:GLN:O[1_546]	1.05	1.15

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	180/192 (94%)	178 (99%)	2 (1%)	0	100	100
1	C	180/192 (94%)	175 (97%)	5 (3%)	0	100	100
2	B	178/230 (77%)	170 (96%)	8 (4%)	0	100	100
2	D	167/230 (73%)	160 (96%)	7 (4%)	0	100	100
3	E	191/207 (92%)	185 (97%)	6 (3%)	0	100	100
3	G	190/207 (92%)	185 (97%)	5 (3%)	0	100	100
4	F	238/242 (98%)	230 (97%)	8 (3%)	0	100	100
4	H	238/242 (98%)	229 (96%)	9 (4%)	0	100	100
5	I	14/16 (88%)	14 (100%)	0	0	100	100
5	J	14/16 (88%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1590/1774 (90%)	1540 (97%)	50 (3%)	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	165/176 (94%)	163 (99%)	2 (1%)	63	78
1	C	165/176 (94%)	160 (97%)	5 (3%)	36	53
2	B	163/203 (80%)	154 (94%)	9 (6%)	19	29
2	D	147/203 (72%)	139 (95%)	8 (5%)	20	30
3	E	163/183 (89%)	152 (93%)	11 (7%)	15	21
3	G	159/183 (87%)	145 (91%)	14 (9%)	9	12
4	F	204/210 (97%)	198 (97%)	6 (3%)	37	55
4	H	203/210 (97%)	196 (97%)	7 (3%)	32	48
5	I	12/13 (92%)	12 (100%)	0	100	100
5	J	12/13 (92%)	12 (100%)	0	100	100
All	All	1393/1570 (89%)	1331 (96%)	62 (4%)	24	38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	175	LEU
2	B	26	LEU
2	B	66	GLU
2	B	114	LEU
2	B	126	GLN
2	B	135	ASP
2	B	136	GLN
2	B	137	GLU

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Mol	Chain	Res	Type
2	B	138	GLU
2	B	189	ARG
1	C	0	ASP
1	C	11	ASN
1	C	101	GLN
1	C	138	LEU
1	C	174	LEU
2	D	24	VAL
2	D	66	GLU
2	D	92	GLN
2	D	94	ARG
2	D	100	THR
2	D	126	GLN
2	D	169	ASP
2	D	170	VAL
3	E	10	VAL
3	E	15	GLU
3	E	48	LYS
3	E	58	SER
3	E	66	LYS
3	E	68	LYS
3	E	77	LYS
3	E	82	LYS
3	E	115	MET
3	E	144	LYS
3	E	210	ILE
4	F	46	LEU
4	F	128	GLU
4	F	184	CYS
4	F	230	LEU
4	F	231	SER
4	F	234	ASP
3	G	15	GLU
3	G	48	LYS
3	G	58	SER
3	G	67	GLU
3	G	86	GLU
3	G	115	MET
3	G	162	VAL
3	G	166	LYS
3	G	167	ASP
3	G	172	ILE

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Mol	Chain	Res	Type
3	G	175	LYS
3	G	177	VAL
3	G	184	ASP
3	G	186	LYS
4	H	64	GLU
4	H	66	ARG
4	H	86	HIS
4	H	128	GLU
4	H	184	CYS
4	H	206	ARG
4	H	234	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	84	ASN
1	A	101	GLN
1	A	111	ASN
2	B	64	GLN
2	B	134	ASN
2	B	156	GLN
2	B	166	GLN
1	C	14	GLN
1	C	62	ASN
2	D	64	GLN
2	D	84	GLN
2	D	174	HIS
3	E	28	ASN
3	E	110	ASN
3	E	139	GLN
3	E	203	ASN
4	F	79	GLN
4	F	132	ASN
3	G	28	ASN
3	G	114	ASN
3	G	132	ASN
3	G	139	GLN
3	G	203	ASN
4	H	70	ASN
4	H	180	HIS
4	H	216	ASN

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Mol	Chain	Res	Type
4	H	238	GLN
5	I	10	ASN

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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
6	NAG	A	301	1	14,14,15	0.32	0	17,19,21	0.54	0
6	NAG	C	301	1	14,14,15	0.30	0	17,19,21	0.56	0
6	NAG	D	1000	2	14,14,15	0.33	0	17,19,21	0.53	0
6	NAG	B	1000	2	14,14,15	0.30	0	17,19,21	0.79	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
6	NAG	A	301	1	-	0/6/23/26	0/1/1/1
6	NAG	C	301	1	-	0/6/23/26	0/1/1/1
6	NAG	D	1000	2	-	0/6/23/26	0/1/1/1
6	NAG	B	1000	2	-	0/6/23/26	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($^{\circ}$)	Ideal($^{\circ}$)
6	B	1000	NAG	O5-C1-C2	-2.20	107.89	111.29

There are no chirality outliers.

There are no torsion outliers.

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	182/192 (94%)	0.13	5 (2%) 56 57	14, 30, 60, 70	0
1	C	182/192 (94%)	0.21	2 (1%) 78 79	8, 29, 70, 94	0
2	B	181/230 (78%)	0.33	10 (5%) 30 30	13, 30, 75, 109	1 (0%)
2	D	173/230 (75%)	0.50	23 (13%) 7 6	7, 26, 98, 128	0
3	E	193/207 (93%)	0.75	29 (15%) 5 5	10, 37, 72, 87	0
3	G	192/207 (92%)	0.76	28 (14%) 6 5	16, 42, 74, 96	0
4	F	240/242 (99%)	0.40	11 (4%) 37 38	8, 26, 53, 82	0
4	H	240/242 (99%)	0.41	12 (5%) 34 33	12, 35, 76, 102	0
5	I	16/16 (100%)	0.38	2 (12%) 8 7	10, 18, 58, 65	0
5	J	16/16 (100%)	0.51	3 (18%) 3 2	16, 24, 64, 73	0
All	All	1615/1774 (91%)	0.44	125 (7%) 19 18	7, 32, 74, 128	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	256	ALA	6.7
4	F	256	ALA	5.5
2	D	140	THR	4.9
5	J	-4	ALA	4.6
2	D	189	ARG	4.4
3	E	168	SER	4.4
2	D	163	MET	4.4
3	E	146	SER	4.2
2	D	137	GLU	4.1
3	G	210	ILE	4.0
3	G	146	SER	4.0
2	D	114	LEU	3.9
2	B	140	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	192	SER	3.6
3	G	183	MET	3.6
3	E	148	LYS	3.6
4	F	234	ASP	3.4
3	G	185	PHE	3.4
3	G	32	THR	3.4
3	E	144	LYS	3.3
3	E	211	PRO	3.3
3	G	145	SER	3.2
3	E	147	ASP	3.2
2	D	135	ASP	3.2
2	D	143	VAL	3.2
1	A	47	LEU	3.1
2	B	114	LEU	3.1
2	D	130	ARG	3.1
3	G	181	ARG	3.1
3	G	209	ILE	3.1
4	H	174	VAL	3.1
3	G	202	ALA	3.0
2	D	2	ASP	3.0
3	G	184	ASP	3.0
3	E	206	ASN	3.0
5	I	12	GLN	3.0
3	E	207	ASN	2.9
2	D	138	GLU	2.9
3	E	136	ALA	2.9
3	G	46	PRO	2.9
3	G	131	GLN	2.9
4	H	177	LYS	2.9
2	B	164	THR	2.9
1	A	0	ASP	2.9
2	B	135	ASP	2.9
3	E	198	ASP	2.8
1	C	180	PRO	2.8
2	D	101	ILE	2.8
4	H	231	SER	2.8
3	E	131	GLN	2.8
2	D	134	ASN	2.7
4	F	129	ASP	2.7
5	I	-4	ALA	2.7
5	J	12	GLN	2.6
4	H	237	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	102	SER	2.6
2	D	133	ARG	2.5
2	B	168	GLY	2.5
3	G	162	VAL	2.5
3	E	201	CYS	2.5
3	G	186	LYS	2.5
3	E	151	CYS	2.5
5	J	-3	PRO	2.5
4	F	239	ASP	2.5
2	D	160	MET	2.5
3	G	203	ASN	2.5
3	G	206	ASN	2.5
4	F	216	ASN	2.5
2	D	100	THR	2.5
3	E	205	PHE	2.4
2	D	139	THR	2.4
2	B	170	VAL	2.4
1	A	180	PRO	2.4
4	H	181	SER	2.4
3	E	183	MET	2.4
4	F	149	SER	2.4
3	E	209	ILE	2.4
4	H	232	GLU	2.4
2	D	116	VAL	2.3
2	D	172	THR	2.3
4	H	149	SER	2.3
2	B	191	GLN	2.3
3	E	142	ASP	2.3
3	E	185	PHE	2.3
3	E	196	LYS	2.3
3	G	127	LYS	2.3
4	F	219	ASN	2.3
2	D	161	LEU	2.3
4	H	239	ASP	2.3
4	F	233	ASN	2.3
3	G	178	LEU	2.3
3	E	33	VAL	2.3
3	G	168	SER	2.2
4	H	183	VAL	2.2
3	E	176	CYS	2.2
3	E	143	SER	2.2
3	G	130	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	181	ARG	2.2
2	D	171	TYR	2.2
3	E	197	SER	2.2
2	D	170	VAL	2.1
2	D	174	HIS	2.1
4	F	211	ALA	2.1
1	A	1	ILE	2.1
3	G	34	SER	2.1
3	G	85	LYS	2.1
4	H	46	LEU	2.1
3	E	34	SER	2.1
3	E	145	SER	2.1
3	E	149	SER	2.1
3	G	207	ASN	2.1
3	E	141	ARG	2.1
4	F	255	ARG	2.1
1	A	129	THR	2.1
1	C	1	ILE	2.1
3	G	198	ASP	2.1
3	G	208	SER	2.1
3	G	132	ASN	2.0
4	F	232	GLU	2.0
3	E	32	THR	2.0
3	G	197	SER	2.0
2	B	172	THR	2.0
2	B	2	ASP	2.0
3	G	180	MET	2.0
4	H	234	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 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
6	NAG	A	301	14/15	0.62	0.19	81,87,92,94	0
6	NAG	B	1000	14/15	0.67	0.19	82,85,88,88	0
7	CA	G	301	1/1	0.67	0.17	118,118,118,118	0
6	NAG	D	1000	14/15	0.69	0.16	70,73,75,77	0
6	NAG	C	301	14/15	0.76	0.15	66,76,82,82	0
7	CA	E	301	1/1	0.85	0.09	66,66,66,66	0
7	CA	C	302	1/1	0.86	0.16	65,65,65,65	0
7	CA	A	302	1/1	0.95	0.10	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.