



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 PM UTC

PDB ID : 3VH8 / pdb_00003vh8
Title : KIR3DL1 in complex with HLA-B*5701
Authors : Vivian, J.P.; Rossjohn, J.
Deposited on : 2011-08-24
Resolution : 1.80 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 : 4-5-2 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

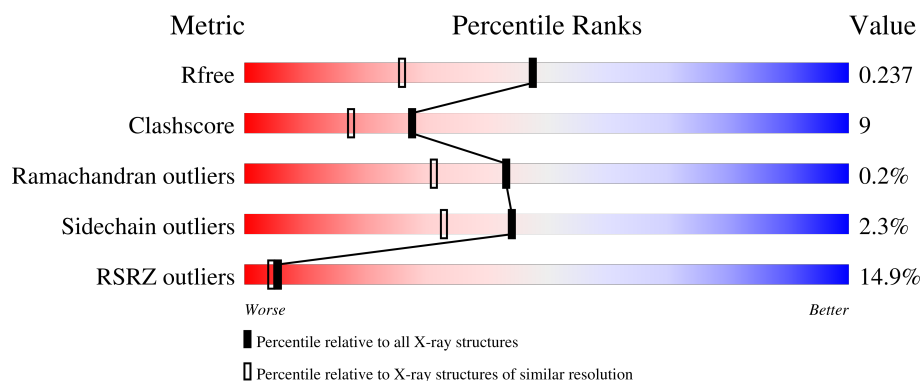
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	275	8% 91% 9%
1	D	275	8% 86% 13%
2	B	99	25% 76% 21% .
2	E	99	21% 76% 21% .
3	C	9	89% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	89% 11%
4	G	316	16% 72% 16% • 11%
4	H	316	18% 68% 13% • 16%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12223 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 I histocompatibility antigen, B-57 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2230	1391	405	425	9			
1	D	275	Total	C	N	O	S	0	0	0
			2230	1391	405	425	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	E	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called peptide of Ig kappa chain C region.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			68	44	10	14			
3	F	9	Total	C	N	O	0	0	0
			68	44	10	14			

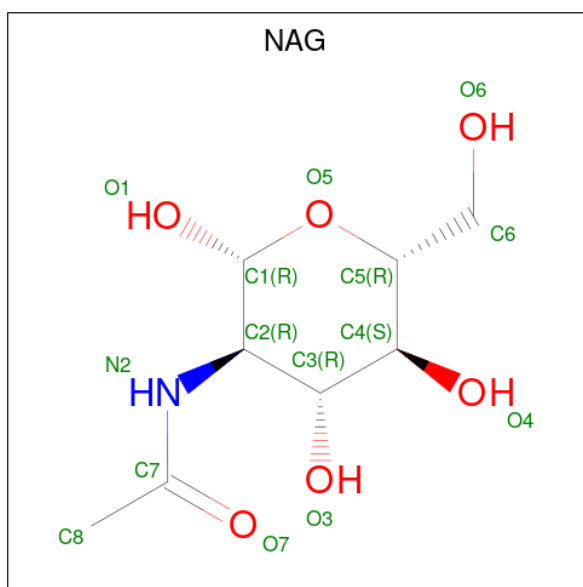
- Molecule 4 is a protein called Killer cell immunoglobulin-like receptor 3DL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	281	Total	C	N	O	S	0	0	0
			2207	1402	401	391	13			
4	H	264	Total	C	N	O	S	0	0	0
			2092	1332	379	368	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	HIS	-	expression tag	UNP P43629
G	-15	HIS	-	expression tag	UNP P43629
G	-14	HIS	-	expression tag	UNP P43629
G	-13	HIS	-	expression tag	UNP P43629
G	-12	HIS	-	expression tag	UNP P43629
G	-11	HIS	-	expression tag	UNP P43629
G	-10	GLY	-	expression tag	UNP P43629
G	-9	SER	-	expression tag	UNP P43629
G	-8	GLY	-	expression tag	UNP P43629
G	-7	SER	-	expression tag	UNP P43629
G	-6	ASP	-	expression tag	UNP P43629
G	-5	ASP	-	expression tag	UNP P43629
G	-4	ASP	-	expression tag	UNP P43629
G	-3	ASP	-	expression tag	UNP P43629
G	-2	LYS	-	expression tag	UNP P43629
G	-1	GLY	-	expression tag	UNP P43629
G	0	SER	-	expression tag	UNP P43629
H	-16	HIS	-	expression tag	UNP P43629
H	-15	HIS	-	expression tag	UNP P43629
H	-14	HIS	-	expression tag	UNP P43629
H	-13	HIS	-	expression tag	UNP P43629
H	-12	HIS	-	expression tag	UNP P43629
H	-11	HIS	-	expression tag	UNP P43629
H	-10	GLY	-	expression tag	UNP P43629
H	-9	SER	-	expression tag	UNP P43629
H	-8	GLY	-	expression tag	UNP P43629
H	-7	SER	-	expression tag	UNP P43629
H	-6	ASP	-	expression tag	UNP P43629
H	-5	ASP	-	expression tag	UNP P43629
H	-4	ASP	-	expression tag	UNP P43629
H	-3	ASP	-	expression tag	UNP P43629
H	-2	LYS	-	expression tag	UNP P43629
H	-1	GLY	-	expression tag	UNP P43629
H	0	SER	-	expression tag	UNP P43629

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	356	Total	O	0	0
			356	356		
6	B	117	Total	O	0	0
			117	117		
6	C	12	Total	O	0	0
			12	12		
6	G	311	Total	O	0	0
			311	311		
6	D	377	Total	O	0	0
			377	377		
6	E	116	Total	O	0	0
			116	116		

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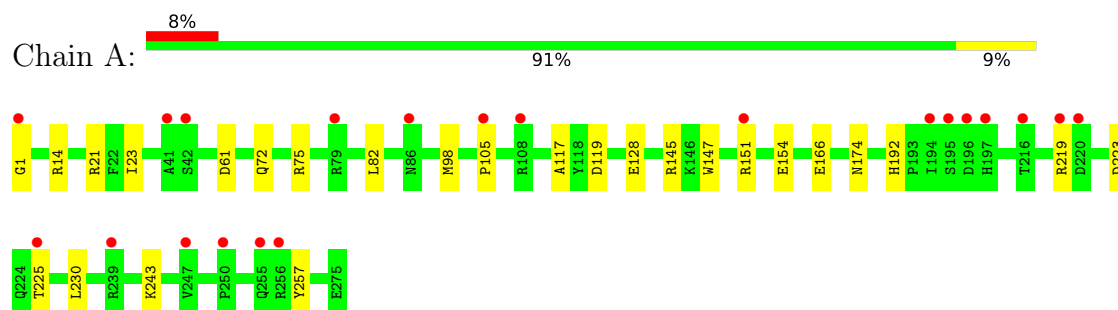
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	17	Total 17	O 17	0	0
6	H	280	Total 280	O 280	0	0

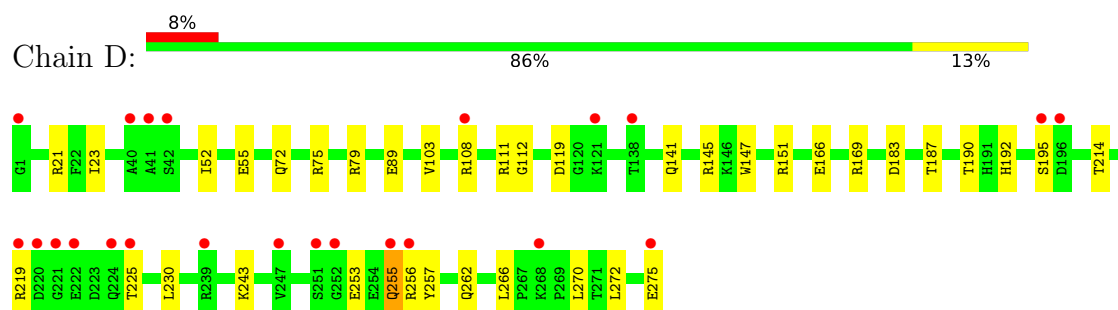
3 Residue-property plots [i](#)

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.

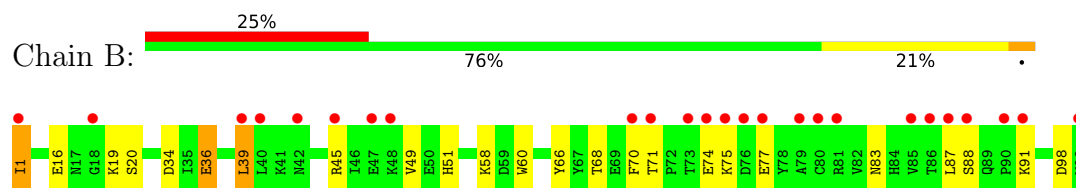
- Molecule 1: HLA class I histocompatibility antigen, B-57 alpha chain



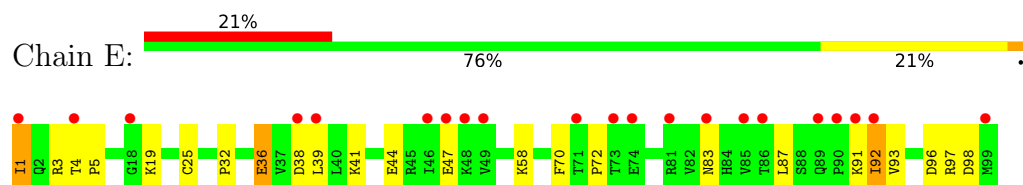
- Molecule 1: HLA class I histocompatibility antigen, B-57 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: peptide of Ig kappa chain C region

Chain C:  89% 11%



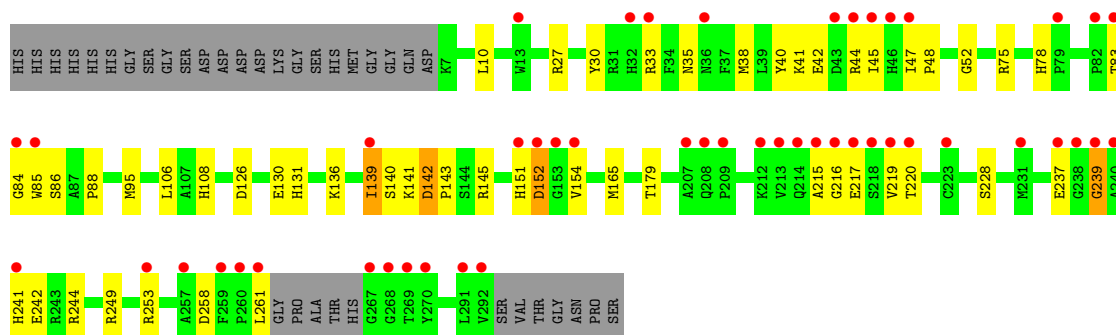
- Molecule 3: peptide of Ig kappa chain C region

Chain F:  89% 11%



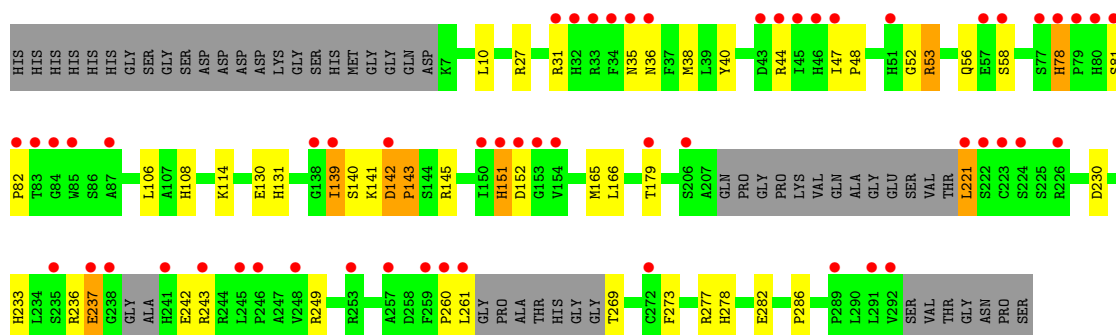
- Molecule 4: Killer cell immunoglobulin-like receptor 3DL1

Chain G:  16% 72% 16% 11%



- Molecule 4: Killer cell immunoglobulin-like receptor 3DL1

Chain H:  18% 68% 13% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.25Å 66.37Å 93.36Å 100.56° 92.83° 101.56°	Depositor
Resolution (Å)	35.85 – 1.80 35.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.85-1.80) 96.8 (35.85-1.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.211 , 0.237 0.211 , 0.237	Depositor DCC
R_{free} test set	6931 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12223	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 88.79 % 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 4.3208e-08. 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: 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	0.49	0/2291	0.77	0/3113
1	D	0.48	0/2291	0.81	1/3113 (0.0%)
2	B	0.42	0/852	0.71	0/1152
2	E	0.42	0/852	0.74	0/1152
3	C	0.48	0/69	0.85	0/91
3	F	0.51	0/69	0.79	0/91
4	G	0.47	0/2281	0.88	6/3100 (0.2%)
4	H	0.45	0/2161	0.85	5/2934 (0.2%)
All	All	0.47	0/10866	0.81	12/14746 (0.1%)

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
4	G	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	239	GLY	N-CA-C	14.86	139.14	114.48
4	H	36	ASN	N-CA-C	13.94	133.88	113.40
4	G	241	HIS	N-CA-C	7.89	121.83	110.24
4	H	237	GLU	CB-CA-C	7.54	120.19	109.71
4	H	237	GLU	N-CA-C	-7.50	99.48	110.42
4	G	239	GLY	CA-C-N	6.90	132.24	122.72
4	G	239	GLY	C-N-CA	6.90	132.24	122.72
4	G	241	HIS	CB-CA-C	-6.42	100.22	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	78	HIS	CA-C-N	5.39	124.58	118.97
4	H	78	HIS	C-N-CA	5.39	124.58	118.97
1	D	195	SER	N-CA-C	-5.35	101.71	108.45
4	G	42	GLU	N-CA-C	5.20	117.62	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	239	GLY	Peptide

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	2230	0	2100	27	0
1	D	2230	0	2100	34	0
2	B	829	0	794	27	0
2	E	829	0	794	20	0
3	C	68	0	73	1	0
3	F	68	0	73	1	0
4	G	2207	0	2131	43	0
4	H	2092	0	2011	44	0
5	G	42	0	39	0	0
5	H	42	0	39	0	0
6	A	356	0	0	9	2
6	B	117	0	0	8	0
6	C	12	0	0	0	0
6	D	377	0	0	10	2
6	E	116	0	0	9	0
6	F	17	0	0	0	0
6	G	311	0	0	12	1
6	H	280	0	0	14	3
All	All	12223	0	10154	186	4

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 9.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:106:LEU:HD11	4:H:108:HIS:CE1	1.95	1.01
4:H:221:LEU:HD11	4:H:261:LEU:HD11	1.42	0.98
4:G:38:MET:HE3	4:G:48:PRO:HB3	1.47	0.94
1:D:21:ARG:CZ	1:D:23:ILE:HD11	2.02	0.90
4:H:130:GLU:OE1	4:H:179:THR:HA	1.74	0.88
4:H:78:HIS:ND1	6:H:1438:HOH:O	2.05	0.87
2:B:36:GLU:HG3	2:B:83:ASN:HB3	1.60	0.83
4:G:38:MET:HE3	4:G:48:PRO:CB	2.08	0.83
1:D:214:THR:HB	1:D:262:GLN:HG2	1.58	0.83
2:E:38:ASP:OD1	6:E:1345:HOH:O	1.95	0.83
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.08	0.83
4:H:106:LEU:HD11	4:H:108:HIS:NE2	1.97	0.79
2:E:44:GLU:O	6:E:1479:HOH:O	1.99	0.79
1:A:1:GLY:HA3	1:A:105:PRO:HA	1.65	0.78
1:D:183:ASP:OD1	6:D:1263:HOH:O	2.04	0.74
4:G:217:GLU:O	6:G:1150:HOH:O	2.06	0.74
2:B:16:GLU:HB2	2:B:19:LYS:HD3	1.71	0.73
4:G:249:ARG:NH2	4:G:253:ARG:HG2	2.03	0.73
1:A:192:HIS:HE1	2:B:98:ASP:HB3	1.55	0.72
1:D:166:GLU:HG2	6:D:1288:HOH:O	1.90	0.71
2:E:47:GLU:HB2	6:E:1365:HOH:O	1.90	0.70
4:H:221:LEU:CD1	4:H:261:LEU:HD21	2.22	0.70
2:B:49:VAL:HA	2:B:68:THR:HG22	1.73	0.70
4:H:277:ARG:HG3	4:H:278:HIS:CD2	2.27	0.70
4:H:221:LEU:HD11	4:H:261:LEU:CD1	2.20	0.69
2:E:87:LEU:O	6:E:100:HOH:O	2.09	0.69
1:D:275:GLU:O	6:D:769:HOH:O	2.12	0.67
4:G:130:GLU:OE1	4:G:179:THR:HA	1.93	0.67
4:H:236:ARG:O	4:H:237:GLU:C	2.37	0.66
1:A:128:GLU:OE2	6:A:580:HOH:O	2.14	0.66
4:H:58:SER:N	6:H:1544:HOH:O	2.28	0.66
2:B:1:ILE:O	2:B:1:ILE:HD13	1.96	0.66
1:D:253:GLU:O	1:D:256:ARG:HG2	1.97	0.65
4:G:78:HIS:ND1	6:G:559:HOH:O	2.29	0.64
2:B:88:SER:OG	6:B:1237:HOH:O	2.15	0.64
2:B:51:HIS:CE1	6:B:1503:HOH:O	2.50	0.64
4:G:139:ILE:HD11	6:G:502:HOH:O	1.97	0.64
4:G:151:HIS:CD2	4:G:152:ASP:HB2	2.33	0.64
1:D:21:ARG:NH1	1:D:23:ILE:HD11	2.11	0.64
4:H:243:ARG:HH12	4:H:260:PRO:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:38:MET:HE2	4:G:40:TYR:OH	1.99	0.63
4:G:253:ARG:NH2	6:G:497:HOH:O	2.23	0.63
2:E:1:ILE:HD11	2:E:3:ARG:HH21	1.63	0.62
4:G:44:ARG:HB3	4:G:47:ILE:HB	1.81	0.62
2:B:87:LEU:HD13	2:B:91:LYS:HG3	1.80	0.62
2:B:1:ILE:HG22	6:B:1200:HOH:O	1.98	0.62
4:H:139:ILE:HG23	4:H:141:LYS:N	2.15	0.61
1:D:225:THR:HG22	1:D:225:THR:O	2.01	0.61
4:G:244:ARG:HG3	6:G:1434:HOH:O	2.01	0.61
1:D:72:GLN:HG2	1:D:75:ARG:NH2	2.16	0.61
1:A:166:GLU:HG2	6:A:1396:HOH:O	2.00	0.61
4:G:95:MET:HE2	6:G:1569:HOH:O	2.01	0.61
1:A:192:HIS:CE1	2:B:98:ASP:HB3	2.36	0.60
1:A:1:GLY:HA3	1:A:105:PRO:CA	2.31	0.60
1:D:72:GLN:HG2	1:D:75:ARG:HH21	1.66	0.60
2:B:45:ARG:NH2	6:B:1492:HOH:O	2.35	0.59
1:A:151:ARG:NH2	6:A:1320:HOH:O	2.35	0.59
4:H:221:LEU:HD11	4:H:261:LEU:HD21	1.83	0.58
1:D:55:GLU:HG2	6:D:1444:HOH:O	2.02	0.58
4:G:139:ILE:HG23	4:G:141:LYS:N	2.19	0.58
4:G:140:SER:HB3	6:G:1155:HOH:O	2.03	0.57
1:D:119:ASP:O	2:E:1:ILE:HD12	2.05	0.57
4:H:44:ARG:O	6:H:1354:HOH:O	2.18	0.56
4:H:114:LYS:NZ	6:H:1475:HOH:O	2.39	0.56
2:B:20:SER:HA	2:B:71:THR:HG22	1.88	0.55
4:G:253:ARG:NE	6:G:497:HOH:O	2.35	0.55
1:A:21:ARG:CZ	1:A:23:ILE:CD1	2.84	0.55
4:H:273:PHE:CE1	4:H:286:PRO:HB3	2.41	0.55
1:D:79:ARG:HD3	6:D:1456:HOH:O	2.07	0.54
2:E:1:ILE:O	2:E:1:ILE:HD13	2.06	0.54
4:H:10:LEU:HD12	4:H:27:ARG:O	2.08	0.54
4:G:44:ARG:HB2	6:G:1219:HOH:O	2.08	0.54
4:G:48:PRO:HB2	4:G:52:GLY:HA2	1.90	0.54
1:D:151:ARG:NH2	6:H:1394:HOH:O	2.41	0.54
2:E:32:PRO:HB2	6:E:879:HOH:O	2.07	0.54
4:H:48:PRO:HB2	4:H:52:GLY:HA2	1.90	0.53
4:H:221:LEU:N	6:H:1195:HOH:O	2.41	0.52
1:D:21:ARG:CZ	1:D:23:ILE:CD1	2.83	0.52
4:G:38:MET:CE	4:G:48:PRO:HB3	2.32	0.51
1:D:108:ARG:NH2	6:D:1312:HOH:O	2.43	0.51
1:A:72:GLN:HG2	1:A:75:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:220:THR:HG21	4:G:258:ASP:HB3	1.93	0.51
4:G:30:TYR:CZ	4:G:86:SER:HB3	2.45	0.51
1:A:61:ASP:HB3	6:A:933:HOH:O	2.11	0.50
1:A:154:GLU:HG3	6:A:350:HOH:O	2.10	0.50
1:D:147:TRP:CH2	3:F:7:LYS:HE2	2.47	0.50
2:B:36:GLU:CG	2:B:83:ASN:HB3	2.37	0.50
4:H:53:ARG:NH2	6:H:1571:HOH:O	2.35	0.50
4:G:151:HIS:O	4:G:154:VAL:HG22	2.12	0.49
4:H:249:ARG:NH1	6:H:1442:HOH:O	2.44	0.49
1:A:223:ASP:HB3	1:A:225:THR:HG23	1.94	0.49
4:G:242:GLU:H	4:G:242:GLU:CD	2.20	0.49
2:B:34:ASP:CG	6:B:966:HOH:O	2.56	0.49
1:D:190:THR:OG1	1:D:192:HIS:HE1	1.96	0.49
1:D:166:GLU:CD	6:D:771:HOH:O	2.55	0.49
2:B:87:LEU:CD2	2:B:91:LYS:HD2	2.43	0.48
1:D:214:THR:HB	1:D:262:GLN:CG	2.38	0.48
1:A:98:MET:HG3	6:A:1449:HOH:O	2.13	0.48
1:A:72:GLN:HG2	1:A:75:ARG:NH2	2.28	0.48
4:H:139:ILE:HD13	4:H:141:LYS:HB3	1.96	0.48
4:H:81:SER:HB2	4:H:82:PRO:HD2	1.96	0.47
4:H:131:HIS:CD2	4:H:145:ARG:HH11	2.32	0.47
1:D:192:HIS:NE2	2:E:98:ASP:HB3	2.30	0.47
4:G:131:HIS:CD2	4:G:145:ARG:HH11	2.32	0.47
4:G:249:ARG:NE	6:G:1332:HOH:O	2.46	0.47
4:H:27:ARG:NH2	6:H:1547:HOH:O	2.44	0.47
4:G:10:LEU:HD12	4:G:27:ARG:O	2.15	0.47
1:D:219:ARG:CG	1:D:256:ARG:HD3	2.43	0.47
2:B:39:LEU:HD23	2:B:68:THR:HG23	1.96	0.47
1:A:219:ARG:HD2	1:A:257:TYR:CZ	2.48	0.47
1:D:103:VAL:HG11	6:D:1039:HOH:O	2.14	0.47
2:E:36:GLU:HG3	2:E:83:ASN:HB3	1.97	0.46
4:G:75:ARG:NH2	4:G:88:PRO:HG3	2.30	0.46
4:G:215:ALA:HA	4:G:216:GLY:HA2	1.55	0.46
4:G:219:VAL:HG13	4:G:261:LEU:HD12	1.96	0.46
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.98	0.46
2:E:41:LYS:NZ	6:E:872:HOH:O	2.49	0.46
2:B:87:LEU:HD21	2:B:91:LYS:HD2	1.97	0.46
2:E:58:LYS:HG2	6:E:312:HOH:O	2.15	0.46
2:B:77:GLU:HB3	6:B:1372:HOH:O	2.15	0.46
1:A:147:TRP:CH2	3:C:7:LYS:HE2	2.51	0.46
4:H:139:ILE:HD11	6:H:997:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:ARG:NH2	4:H:78:HIS:CE1	2.84	0.45
2:B:39:LEU:CD2	2:B:68:THR:HG23	2.45	0.45
4:G:142:ASP:O	4:G:143:PRO:C	2.59	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.51	0.45
4:G:83:THR:HG22	4:G:84:GLY:H	1.82	0.45
2:B:1:ILE:O	2:B:1:ILE:HG23	2.15	0.45
4:H:242:GLU:HB2	6:H:1090:HOH:O	2.17	0.45
2:B:16:GLU:CB	2:B:19:LYS:HD3	2.45	0.45
4:H:31:ARG:HH21	4:H:78:HIS:CE1	2.34	0.45
1:D:255:GLN:HB2	6:D:1370:HOH:O	2.17	0.45
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.52	0.45
1:D:230:LEU:HG	1:D:243:LYS:HE3	1.99	0.45
2:E:92:ILE:HG13	2:E:93:VAL:N	2.32	0.44
4:G:237:GLU:HG3	6:G:1482:HOH:O	2.17	0.44
4:G:84:GLY:C	4:G:85:TRP:CD1	2.96	0.44
2:B:74:GLU:HG3	2:B:75:LYS:HG3	1.99	0.44
4:G:136:LYS:HB3	4:G:139:ILE:HD12	1.97	0.44
1:D:145:ARG:HH12	4:H:230:ASP:CG	2.25	0.44
1:A:145:ARG:NH2	6:A:1134:HOH:O	2.46	0.43
4:G:38:MET:HE3	4:G:48:PRO:CG	2.47	0.43
4:G:139:ILE:HD13	4:G:141:LYS:HB3	1.99	0.43
4:H:269:THR:HA	6:H:1136:HOH:O	2.18	0.43
1:A:1:GLY:CA	1:A:105:PRO:HA	2.42	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.43
2:E:58:LYS:NZ	6:E:1307:HOH:O	2.50	0.43
2:E:96:ASP:O	2:E:98:ASP:N	2.51	0.43
1:D:141:GLN:O	1:D:145:ARG:HG3	2.17	0.43
2:E:4:THR:OG1	2:E:5:PRO:HD2	2.18	0.43
4:H:106:LEU:HD12	4:H:106:LEU:C	2.44	0.43
4:H:142:ASP:O	4:H:143:PRO:C	2.60	0.43
4:H:221:LEU:HD11	4:H:261:LEU:CG	2.48	0.43
1:A:145:ARG:HD2	4:G:228:SER:HB2	2.01	0.43
1:A:219:ARG:HD2	1:A:257:TYR:OH	2.19	0.43
4:H:273:PHE:CZ	4:H:286:PRO:HB3	2.54	0.43
4:H:140:SER:HB3	6:H:1299:HOH:O	2.18	0.42
1:A:145:ARG:NE	6:A:1134:HOH:O	2.29	0.42
4:G:242:GLU:HB2	6:G:1135:HOH:O	2.19	0.42
2:B:77:GLU:C	6:B:1196:HOH:O	2.62	0.42
1:D:219:ARG:HD3	1:D:257:TYR:CZ	2.53	0.42
4:H:38:MET:HE3	4:H:40:TYR:OH	2.19	0.42
4:H:233:HIS:HA	4:H:243:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:LYS:HE2	6:E:1267:HOH:O	2.19	0.42
4:G:83:THR:HG22	4:G:84:GLY:N	2.34	0.42
1:A:174:ASN:ND2	6:A:1447:HOH:O	2.52	0.42
2:E:25:CYS:HB2	2:E:39:LEU:HD21	2.02	0.42
4:H:35:ASN:HB2	4:H:56:GLN:O	2.19	0.42
4:G:220:THR:CG2	4:G:258:ASP:HB3	2.50	0.41
1:D:111:ARG:HG3	1:D:112:GLY:N	2.35	0.41
1:D:169:ARG:HD2	6:D:771:HOH:O	2.20	0.41
1:D:187:THR:OG1	1:D:272:LEU:HD21	2.20	0.41
2:E:96:ASP:C	2:E:98:ASP:H	2.28	0.41
4:H:221:LEU:CD1	4:H:261:LEU:CD2	2.96	0.41
1:A:119:ASP:O	2:B:1:ILE:HD12	2.19	0.41
2:E:19:LYS:O	2:E:72:PRO:HD2	2.20	0.41
4:G:106:LEU:HD11	4:G:108:HIS:CE1	2.56	0.41
1:A:230:LEU:HG	1:A:243:LYS:HE3	2.03	0.41
2:B:58:LYS:HG2	6:B:1031:HOH:O	2.20	0.41
4:H:243:ARG:NH1	4:H:260:PRO:HD2	2.31	0.41
4:H:166:LEU:HD13	4:H:282:GLU:HB3	2.03	0.40
4:G:33:ARG:NH1	4:G:35:ASN:OD1	2.48	0.40
1:D:225:THR:O	1:D:225:THR:CG2	2.68	0.40
4:H:27:ARG:NE	6:H:1547:HOH:O	2.49	0.40
4:G:216:GLY:N	4:H:151:HIS:CE1	2.90	0.40
1:D:52:ILE:HG13	1:D:52:ILE:O	2.22	0.40

All (4) 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)
6:G:914:HOH:O	6:D:908:HOH:O[1_645]	1.72	0.48
6:A:1351:HOH:O	6:H:1357:HOH:O[1_554]	1.97	0.23
6:D:494:HOH:O	6:H:652:HOH:O[1_565]	2.14	0.06
6:A:1247:HOH:O	6:H:530:HOH:O[1_454]	2.17	0.03

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	273/275 (99%)	265 (97%)	8 (3%)	0	100	100
1	D	273/275 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	E	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	12	4
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	G	277/316 (88%)	267 (96%)	10 (4%)	0	100	100
4	H	256/316 (81%)	247 (96%)	8 (3%)	1 (0%)	30	19
All	All	1287/1398 (92%)	1248 (97%)	37 (3%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	97	ARG
4	H	143	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	229/229 (100%)	228 (100%)	1 (0%)	84	83
1	D	229/229 (100%)	227 (99%)	2 (1%)	70	67
2	B	94/94 (100%)	90 (96%)	4 (4%)	26	13
2	E	94/94 (100%)	90 (96%)	4 (4%)	26	13
3	C	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
4	G	243/270 (90%)	236 (97%)	7 (3%)	37	25
4	H	231/270 (86%)	223 (96%)	8 (4%)	32	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1138/1204 (94%)	1112 (98%)	26 (2%)	44 33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
2	B	1	ILE
2	B	36	GLU
2	B	39	LEU
2	B	70	PHE
4	G	41	LYS
4	G	45	ILE
4	G	126	ASP
4	G	139	ILE
4	G	142	ASP
4	G	152	ASP
4	G	165	MET
1	D	89	GLU
1	D	255	GLN
2	E	1	ILE
2	E	36	GLU
2	E	70	PHE
2	E	92	ILE
4	H	47	ILE
4	H	53	ARG
4	H	139	ILE
4	H	142	ASP
4	H	151	HIS
4	H	152	ASP
4	H	165	MET
4	H	221	LEU

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	144	GLN
1	A	174	ASN
2	B	51	HIS
4	G	149	GLN
4	G	151	HIS
4	G	214	GLN

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Mol	Chain	Res	Type
4	G	256	GLN
1	D	141	GLN
1	D	144	GLN
1	D	192	HIS
1	D	255	GLN
4	H	46	HIS
4	H	78	HIS
4	H	278	HIS

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](#)

6 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	H	301	4	14,14,15	0.69	0	17,19,21	1.75	3 (17%)
5	NAG	G	300	4	14,14,15	0.71	0	17,19,21	1.21	2 (11%)
5	NAG	H	300	4	14,14,15	0.63	0	17,19,21	0.83	1 (5%)
5	NAG	H	302	4	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
5	NAG	G	301	4	14,14,15	0.56	0	17,19,21	1.66	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	302	4	14,14,15	0.72	0	17,19,21	1.51	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	H	301	4	-	1/6/23/26	0/1/1/1
5	NAG	G	300	4	-	0/6/23/26	0/1/1/1
5	NAG	H	300	4	-	0/6/23/26	0/1/1/1
5	NAG	H	302	4	-	2/6/23/26	0/1/1/1
5	NAG	G	301	4	-	1/6/23/26	0/1/1/1
5	NAG	G	302	4	-	0/6/23/26	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(°)
5	G	302	NAG	C2-N2-C7	-5.19	115.94	122.90
5	H	301	NAG	C2-N2-C7	-4.82	116.44	122.90
5	G	301	NAG	C4-C3-C2	-3.90	105.30	111.02
5	H	301	NAG	C1-O5-C5	3.72	117.17	112.19
5	G	301	NAG	O5-C1-C2	-2.91	106.80	111.29
5	H	302	NAG	C1-O5-C5	2.90	116.07	112.19
5	G	301	NAG	C1-O5-C5	2.85	116.01	112.19
5	G	301	NAG	C6-C5-C4	-2.74	106.29	113.02
5	G	300	NAG	C2-N2-C7	-2.62	119.39	122.90
5	H	301	NAG	C6-C5-C4	-2.22	107.56	113.02
5	H	300	NAG	C2-N2-C7	-2.13	120.05	122.90
5	G	300	NAG	C1-O5-C5	2.13	115.04	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	301	NAG	C3-C2-N2-C7
5	H	302	NAG	C4-C5-C6-O6
5	H	302	NAG	O5-C5-C6-O6
5	H	301	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	275/275 (100%)	0.44	21 (7%) 20 18	10, 22, 44, 51	23 (8%)
1	D	275/275 (100%)	0.38	23 (8%) 17 15	8, 22, 45, 60	24 (8%)
2	B	99/99 (100%)	1.45	25 (25%) 1 1	13, 28, 50, 59	9 (9%)
2	E	99/99 (100%)	1.24	21 (21%) 2 2	14, 28, 42, 51	10 (10%)
3	C	9/9 (100%)	-0.45	0 100 100	14, 17, 18, 19	0
3	F	9/9 (100%)	-0.43	0 100 100	13, 17, 18, 18	0
4	G	281/316 (88%)	1.01	49 (17%) 4 3	13, 28, 51, 67	0
4	H	264/316 (83%)	1.03	56 (21%) 2 2	13, 28, 55, 67	0
All	All	1311/1398 (93%)	0.79	195 (14%) 5 4	8, 25, 48, 67	66 (5%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	SER	8.3
4	G	267	GLY	7.3
1	A	1	GLY	6.8
4	G	216	GLY	6.8
4	G	215	ALA	6.8
4	H	82	PRO	6.7
4	G	84	GLY	5.7
4	H	45	ILE	5.6
4	G	239	GLY	5.3
4	G	240	ALA	5.3
1	D	1	GLY	5.2
2	E	1	ILE	5.2
4	H	84	GLY	5.2
4	G	45	ILE	5.0
4	H	259	PHE	5.0
4	G	219	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	91	LYS	5.0
4	H	43	ASP	4.9
4	H	36	ASN	4.7
4	G	218	SER	4.6
4	G	238	GLY	4.5
4	G	268	GLY	4.4
2	B	1	ILE	4.4
4	G	214	GLN	4.3
4	H	139	ILE	4.3
4	H	238	GLY	4.3
4	H	83	THR	4.2
2	B	85	VAL	4.1
2	E	91	LYS	4.1
4	G	83	THR	4.1
2	B	86	THR	4.0
4	G	241	HIS	4.0
1	D	239	ARG	3.9
4	H	222	SER	3.9
1	A	225	THR	3.9
1	D	225	THR	3.9
2	B	39	LEU	3.8
4	G	43	ASP	3.8
1	A	256	ARG	3.7
4	G	291	LEU	3.7
2	B	74	GLU	3.7
2	B	73	THR	3.7
4	G	209	PRO	3.7
4	H	44	ARG	3.7
4	H	46	HIS	3.6
2	E	85	VAL	3.6
4	H	260	PRO	3.6
1	A	255	GLN	3.6
4	G	208	GLN	3.6
4	H	81	SER	3.6
4	H	261	LEU	3.6
1	A	239	ARG	3.6
2	B	76	ASP	3.6
2	B	48	LYS	3.6
4	G	217	GLU	3.5
1	A	196	ASP	3.5
4	H	248	VAL	3.5
4	H	47	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
4	G	213	VAL	3.5
2	B	71	THR	3.4
4	H	223	CYS	3.4
4	H	138	GLY	3.4
4	H	87	ALA	3.4
1	A	42	SER	3.4
4	G	85	TRP	3.4
4	H	151	HIS	3.3
4	G	292	VAL	3.3
2	E	39	LEU	3.3
4	H	241	HIS	3.3
1	D	196	ASP	3.3
4	G	139	ILE	3.3
4	G	207	ALA	3.3
1	D	256	ARG	3.3
4	H	257	ALA	3.2
4	G	220	THR	3.2
2	E	90	PRO	3.2
4	G	260	PRO	3.2
4	G	153	GLY	3.2
1	D	42	SER	3.2
1	D	251	SER	3.2
4	G	44	ARG	3.2
1	D	255	GLN	3.2
2	B	18	GLY	3.2
4	H	245	LEU	3.1
2	E	86	THR	3.1
4	H	79	PRO	3.1
4	H	221	LEU	3.1
2	B	77	GLU	3.1
2	E	18	GLY	3.1
4	H	237	GLU	3.0
4	G	152	ASP	3.0
2	E	4	THR	2.9
1	D	138	THR	2.9
2	E	73	THR	2.9
2	B	70	PHE	2.9
4	G	212	LYS	2.9
1	A	195	SER	2.9
4	H	291	LEU	2.9
2	B	47	GLU	2.8
4	H	152	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	H	243	ARG	2.8
4	H	292	VAL	2.8
1	A	41	ALA	2.8
4	H	32	HIS	2.8
4	H	289	PRO	2.8
4	H	154	VAL	2.8
2	B	79	ALA	2.8
4	H	31	ARG	2.8
4	G	151	HIS	2.8
4	H	58	SER	2.7
4	H	253	ARG	2.7
4	G	259	PHE	2.7
4	G	269	THR	2.7
4	H	224	SER	2.7
4	G	261	LEU	2.7
4	G	13	TRP	2.7
4	G	270	TYR	2.7
2	B	80	CYS	2.7
2	E	92	ILE	2.7
1	D	221	GLY	2.6
2	E	81	ARG	2.6
2	E	47	GLU	2.6
2	E	83	ASN	2.6
4	H	80	HIS	2.6
1	A	197	HIS	2.5
1	D	222	GLU	2.5
4	H	206	SER	2.5
1	D	275	GLU	2.5
4	G	82	PRO	2.5
4	H	57	GLU	2.5
4	H	150	ILE	2.5
1	A	108	ARG	2.5
4	G	223	CYS	2.5
2	B	81	ARG	2.5
1	A	194	ILE	2.5
2	B	90	PRO	2.5
4	H	153	GLY	2.4
4	H	34	PHE	2.4
4	G	47	ILE	2.4
4	G	253	ARG	2.4
2	B	40	LEU	2.4
2	E	38	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	179	THR	2.4
4	H	51	HIS	2.4
2	B	87	LEU	2.4
1	A	220	ASP	2.4
2	E	89	GLN	2.4
4	H	85	TRP	2.4
2	E	48	LYS	2.4
1	D	108	ARG	2.3
4	H	33	ARG	2.3
4	H	246	PRO	2.3
4	H	235	SER	2.3
1	A	216	THR	2.3
1	A	86	ASN	2.3
1	A	250	PRO	2.3
4	G	237	GLU	2.3
4	G	36	ASN	2.3
4	G	46	HIS	2.3
2	E	99	MET	2.3
1	D	252	GLY	2.3
4	H	226	ARG	2.3
2	E	74	GLU	2.3
2	B	99	MET	2.3
2	E	49	VAL	2.2
4	H	35	ASN	2.2
2	E	71	THR	2.2
4	H	77	SER	2.2
2	B	42	ASN	2.2
2	B	75	LYS	2.2
4	G	33	ARG	2.2
1	D	247	VAL	2.2
1	D	220	ASP	2.2
4	H	142	ASP	2.2
4	G	79	PRO	2.2
4	G	32	HIS	2.2
1	D	41	ALA	2.2
1	A	219	ARG	2.2
1	A	79	ARG	2.1
1	D	268	LYS	2.1
2	B	45	ARG	2.1
4	G	231	MET	2.1
1	D	40	ALA	2.1
1	D	195	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	121	LYS	2.1
1	A	151	ARG	2.1
1	A	105	PRO	2.1
4	H	272	CYS	2.1
4	G	257	ALA	2.1
1	D	219	ARG	2.1
1	D	224	GLN	2.0
4	G	154	VAL	2.0
2	E	46	ILE	2.0
4	H	78	HIS	2.0
1	A	247	VAL	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(Å ²)	Q<0.9
5	NAG	H	301	14/15	0.68	0.15	36,39,42,42	0
5	NAG	H	302	14/15	0.71	0.14	46,48,49,49	0
5	NAG	G	301	14/15	0.77	0.13	36,40,40,41	0
5	NAG	H	300	14/15	0.81	0.12	33,35,37,37	0
5	NAG	G	302	14/15	0.85	0.11	38,41,42,42	0
5	NAG	G	300	14/15	0.87	0.10	32,35,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.