



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:43 PM BST

PDB ID : 3VH8
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 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	:	2.13.1
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)	:	2.13.1

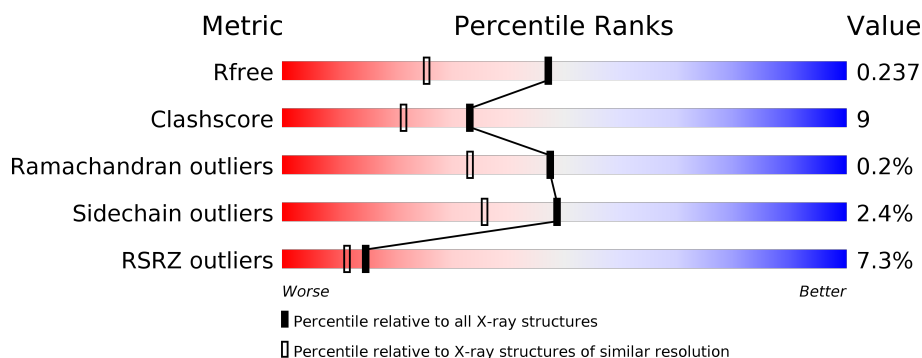
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on 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	
1	D	275	
2	B	99	
2	E	99	
3	C	9	
3	F	9	

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Mol	Chain	Length	Quality of chain
4	G	316	<div><div></div><div>12%</div><div></div><div>73%</div><div></div><div>15%</div><div></div><div>11%</div></div>
4	H	316	<div><div></div><div>8%</div><div></div><div>69%</div><div></div><div>14%</div><div></div><div>16%</div></div>

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 (three-letter code: 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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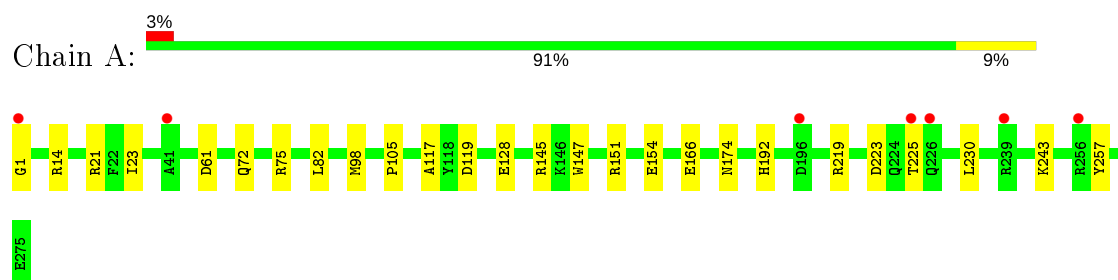
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	17	Total 17	O 17	0	0
6	H	280	Total 280	O 280	0	0

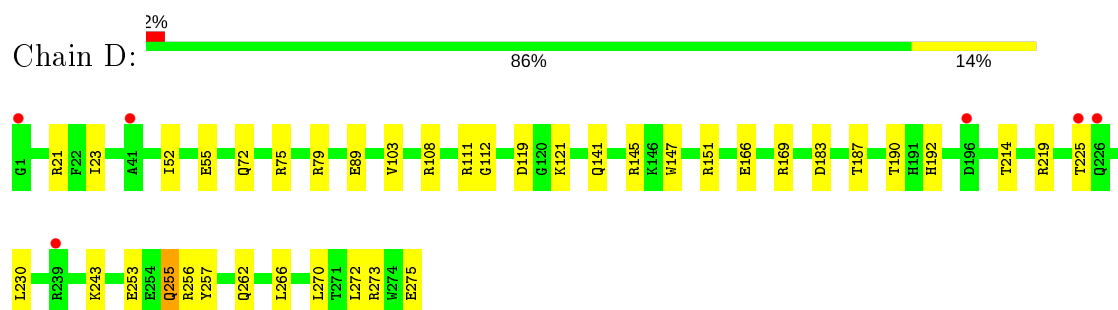
3 Residue-property plots [i](#)

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.

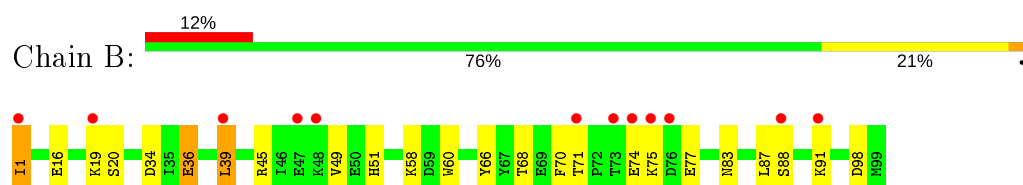
- Molecule 1: HLA class I histocompatibility antigen, B-57 alpha chain



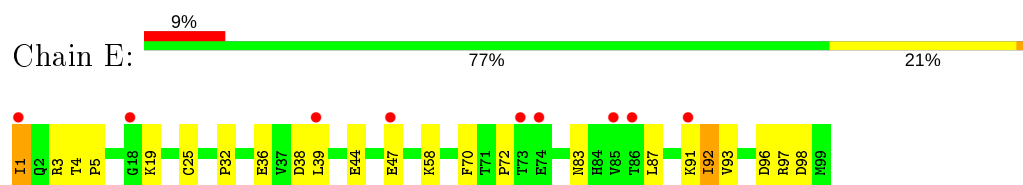
- Molecule 1: HLA class I histocompatibility antigen, B-57 alpha chain




- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: peptide of Ig kappa chain C region

Chain C:  89% 11%




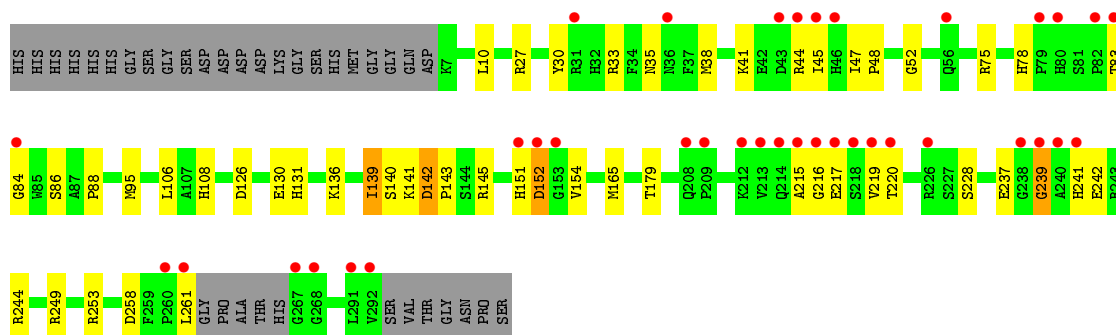
- Molecule 3: peptide of Ig kappa chain C region

Chain F:  89% 11%



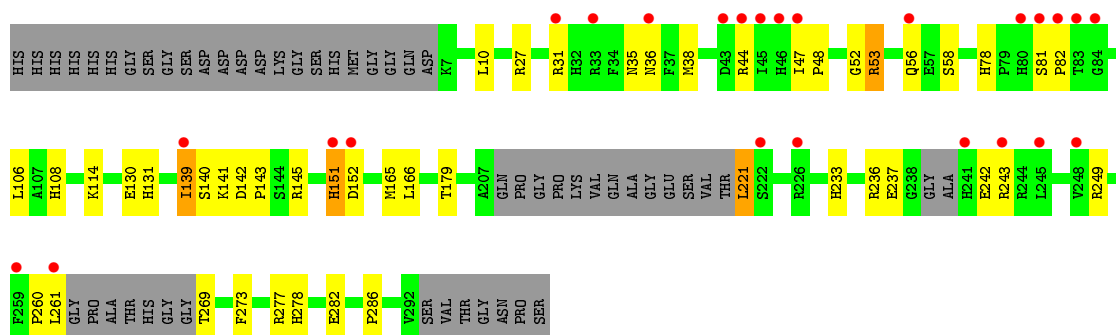
- Molecule 4: Killer cell immunoglobulin-like receptor 3DL1

Chain G:  12% 73% 15% 11%



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

Chain H:  8% 69% 14% 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 35.84 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.85-1.80) 96.8 (35.84-1.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 1.81Å)	Xtrriage
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 (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.3	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	0.96	EDS
Total number of atoms	12223	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.39	0/2291	0.56	0/3113
1	D	0.38	0/2291	0.58	0/3113
2	B	0.36	0/852	0.51	0/1152
2	E	0.36	0/852	0.51	0/1152
3	C	0.42	0/69	0.56	0/91
3	F	0.43	0/69	0.58	0/91
4	G	0.37	0/2281	0.60	2/3100 (0.1%)
4	H	0.36	0/2161	0.58	1/2934 (0.0%)
All	All	0.37	0/10866	0.57	3/14746 (0.0%)

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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	239	GLY	N-CA-C	10.42	139.14	113.10
4	H	36	ASN	N-CA-C	8.48	133.88	111.00
4	G	241	HIS	CB-CA-C	-5.09	100.22	110.40

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	33	0
2	B	829	0	794	26	0
2	E	829	0	794	17	0
3	C	68	0	73	1	0
3	F	68	0	73	1	0
4	G	2207	0	2131	42	0
4	H	2092	0	2011	41	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	7	0
6	C	12	0	0	0	0
6	D	377	0	0	10	2
6	E	116	0	0	7	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	178	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 (178) 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
1:D:21:ARG:CZ	1:D:23:ILE:HD11	2.02	0.90
4:H:78:HIS:ND1	6:H:1438:HOH:O	2.05	0.89
4:H:130:GLU:OE1	4:H:179:THR:HA	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLU:HG3	2:B:83:ASN:HB3	1.60	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
4:G:38:MET:HE3	4:G:48:PRO:HG3	1.73	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
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
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
4:G:38:MET:HE2	4:G:48:PRO:HB3	1.81	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
4:H:236:ARG:O	4:H:237:GLU:C	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:HG22	1:D:225:THR:O	2.01	0.61
1:D:72:GLN:HG2	1:D:75:ARG:NH2	2.16	0.61
4:G:244:ARG:HG3	6:G:1434:HOH:O	2.01	0.61
1:A:166:GLU:HG2	6:A:1396:HOH:O	2.00	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
4:G:38:MET:CE	4:G:48:PRO:HB3	2.32	0.60
2:B:45:ARG:NH2	6:B:1492:HOH:O	2.35	0.59
4:G:95:MET:HE2	6:G:1569:HOH:O	2.03	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
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
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:154:GLU:HG3	6:A:350:HOH:O	2.10	0.50
1:A:61:ASP:HB3	6:A:933:HOH:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:151:HIS:O	4:G:154:VAL:HG22	2.12	0.49
4:G:38:MET:HE3	4:G:48:PRO:CG	2.41	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
1:D:190:THR:OG1	1:D:192:HIS:HE1	1.96	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
1:D:219:ARG:CG	1:D:256:ARG:HD3	2.43	0.47
4:G:10:LEU:HD12	4:G:27:ARG:O	2.15	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: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
4:G:75:ARG:NH2	4:G:88:PRO:HG3	2.30	0.46
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.98	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:GLU:H	4:G:242:GLU:CD	2.20	0.44
4:G:237:GLU:HG3	6:G:1482:HOH:O	2.17	0.44
2:B:34:ASP:CG	6:B:966:HOH:O	2.56	0.44
1:D:166:GLU:CD	6:D:771:HOH:O	2.55	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:A:145:ARG:NH2	6:A:1134:HOH:O	2.46	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:HA	1:A:82:LEU:HD23	1.88	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: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
1:D:219:ARG:HD3	1:D:257:TYR:CZ	2.53	0.42
4:H:233:HIS:HA	4:H:243:ARG:O	2.19	0.42
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
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
4:G:220:THR:CG2	4:G:258:ASP:HB3	2.50	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
4:H:38:MET:HE2	4:H:38:MET:HB2	1.90	0.41
2:E:19:LYS:O	2:E:72:PRO:HD2	2.20	0.41
4:G:38:MET:HE3	4:G:48:PRO:CB	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:142:ASP:O	4:G:143:PRO:C	2.59	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:O	1:D:52:ILE:HG13	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 ⓘ

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	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%)	15	5
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	H	256/316 (81%)	247 (96%)	8 (3%)	1 (0%)	34 21
All	All	1287/1398 (92%)	1248 (97%)	37 (3%)	2 (0%)	47 33

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%)	91 89
1	D	229/229 (100%)	225 (98%)	4 (2%)	60 51
2	B	94/94 (100%)	90 (96%)	4 (4%)	29 14
2	E	94/94 (100%)	91 (97%)	3 (3%)	39 25
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%)	42 29
4	H	231/270 (86%)	223 (96%)	8 (4%)	36 21
All	All	1138/1204 (94%)	1111 (98%)	27 (2%)	49 36

All (27) 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

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Mol	Chain	Res	Type
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	121	LYS
1	D	255	GLN
1	D	273	ARG
2	E	1	ILE
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
2	B	51	HIS
4	G	151	HIS
4	G	256	GLN
1	D	192	HIS
1	D	224	GLN
1	D	255	GLN
4	H	46	HIS
4	H	78	HIS

5.3.3 RNA ⓘ

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](#)

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	0.70	0	17,19,21	1.70	3 (17%)
5	NAG	G	300	4	14,14,15	0.72	0	17,19,21	1.24	2 (11%)
5	NAG	G	301	4	14,14,15	0.58	0	17,19,21	1.68	4 (23%)
5	NAG	H	300	4	14,14,15	0.64	0	17,19,21	0.84	1 (5%)
5	NAG	G	302	4	14,14,15	0.73	0	17,19,21	1.48	1 (5%)
5	NAG	H	302	4	14,14,15	0.58	0	17,19,21	1.12	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	-	0/6/23/26	0/1/1/1
5	NAG	G	300	4	-	0/6/23/26	0/1/1/1
5	NAG	G	301	4	-	1/6/23/26	0/1/1/1
5	NAG	H	300	4	-	0/6/23/26	0/1/1/1
5	NAG	G	302	4	-	0/6/23/26	0/1/1/1
5	NAG	H	302	4	-	2/6/23/26	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	-4.89	115.94	122.90
5	H	301	NAG	C2-N2-C7	-4.54	116.44	122.90
5	G	301	NAG	C4-C3-C2	-3.90	105.30	111.02
5	H	301	NAG	C1-O5-C5	3.67	117.17	112.19
5	G	301	NAG	C6-C5-C4	-2.86	106.29	113.00
5	H	302	NAG	C1-O5-C5	2.86	116.07	112.19
5	G	301	NAG	O5-C1-C2	-2.84	106.80	111.29
5	G	301	NAG	C1-O5-C5	2.82	116.01	112.19
5	G	300	NAG	C2-N2-C7	-2.47	119.39	122.90
5	H	301	NAG	C6-C5-C4	-2.32	107.56	113.00
5	G	300	NAG	C1-O5-C5	2.10	115.04	112.19
5	H	300	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

All (3) 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

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	275/275 (100%)	0.01	7 (2%) 57 52	13, 23, 45, 52	23 (8%)
1	D	275/275 (100%)	-0.01	6 (2%) 62 57	12, 22, 45, 60	24 (8%)
2	B	99/99 (100%)	0.61	12 (12%) 4 3	17, 29, 50, 59	9 (9%)
2	E	99/99 (100%)	0.47	9 (9%) 9 7	17, 28, 42, 51	10 (10%)
3	C	9/9 (100%)	-0.53	0 100 100	14, 17, 18, 19	0
3	F	9/9 (100%)	-0.38	0 100 100	13, 17, 18, 18	0
4	G	281/316 (88%)	0.56	37 (13%) 3 2	13, 28, 51, 67	0
4	H	264/316 (83%)	0.40	25 (9%) 8 6	13, 28, 55, 67	0
All	All	1311/1398 (93%)	0.28	96 (7%) 15 11	12, 25, 48, 67	66 (5%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	215	ALA	10.8
4	G	239	GLY	10.3
4	G	241	HIS	9.9
4	G	216	GLY	7.3
4	G	267	GLY	6.8
2	E	1	ILE	6.6
4	H	261	LEU	6.2
4	G	218	SER	6.1
4	G	45	ILE	6.1
2	B	1	ILE	6.0
4	G	240	ALA	5.7
2	B	48	LYS	5.4
4	H	82	PRO	5.3
4	G	209	PRO	5.0
4	H	43	ASP	5.0
1	D	239	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
4	H	45	ILE	4.7
4	H	44	ARG	4.7
4	G	217	GLU	4.7
4	H	259	PHE	4.7
4	G	214	GLN	4.7
4	H	36	ASN	4.4
4	G	260	PRO	4.2
4	G	212	LYS	4.2
2	B	75	LYS	4.1
1	A	239	ARG	4.1
1	A	1	GLY	4.1
4	G	238	GLY	4.1
4	G	151	HIS	4.1
4	G	208	GLN	4.0
1	A	41	ALA	4.0
1	A	226	GLN	3.9
4	G	84	GLY	3.7
1	A	225	THR	3.6
4	G	292	VAL	3.6
4	H	151	HIS	3.6
2	B	47	GLU	3.6
4	G	268	GLY	3.5
2	B	71	THR	3.5
4	H	243	ARG	3.5
1	D	225	THR	3.5
4	H	83	THR	3.4
2	B	76	ASP	3.3
2	B	74	GLU	3.3
4	G	82	PRO	3.3
2	E	74	GLU	3.2
4	H	152	ASP	3.2
4	G	213	VAL	3.2
4	H	80	HIS	3.1
1	D	226	GLN	3.1
4	H	46	HIS	3.1
4	G	43	ASP	3.0
2	E	47	GLU	3.0
4	G	220	THR	3.0
4	H	56	GLN	3.0
1	D	196	ASP	3.0
2	B	19	LYS	3.0
4	G	261	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	H	47	ILE	2.9
2	B	73	THR	2.9
4	G	44	ARG	2.8
4	G	36	ASN	2.8
4	H	241	HIS	2.8
2	B	91	LYS	2.8
1	A	196	ASP	2.8
2	E	18	GLY	2.7
2	E	86	THR	2.7
4	G	79	PRO	2.6
4	G	83	THR	2.6
4	H	81	SER	2.6
1	D	41	ALA	2.5
4	G	56	GLN	2.4
2	E	39	LEU	2.4
1	D	1	GLY	2.3
4	H	248	VAL	2.3
4	G	153	GLY	2.3
4	H	84	GLY	2.3
2	E	73	THR	2.3
4	G	219	VAL	2.3
2	B	39	LEU	2.3
2	E	91	LYS	2.3
2	E	85	VAL	2.2
4	H	139	ILE	2.2
4	G	291	LEU	2.2
4	H	226	ARG	2.2
4	H	222	SER	2.2
4	G	152	ASP	2.2
2	B	88	SER	2.2
4	G	46	HIS	2.2
4	G	80	HIS	2.1
4	H	33	ARG	2.1
4	G	31	ARG	2.1
4	H	245	LEU	2.1
1	A	256	ARG	2.0
4	H	31	ARG	2.0
4	G	226	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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	H	301	14/15	0.74	0.26	36,39,42,42	0
5	NAG	G	301	14/15	0.80	0.25	36,40,40,41	0
5	NAG	H	300	14/15	0.84	0.17	33,35,37,37	0
5	NAG	H	302	14/15	0.84	0.28	46,48,49,49	0
5	NAG	G	302	14/15	0.86	0.22	38,41,42,42	0
5	NAG	G	300	14/15	0.88	0.14	32,35,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.