



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:13 PM UTC

PDB ID : 6J31 / pdb_00006j31
Title : Crystal Structure Analysis of the Glycotransferase of kitacinnamycin
Authors : Shi, J.; Liu, C.L.; Zhang, B.; Guo, W.J.; Zhu, J.P.; Xu, X.; Xu, Q.; Jiao, R.H.;
Tan, R.X.; Ge, H.M.
Deposited on : 2019-01-03
Resolution : 2.24 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:

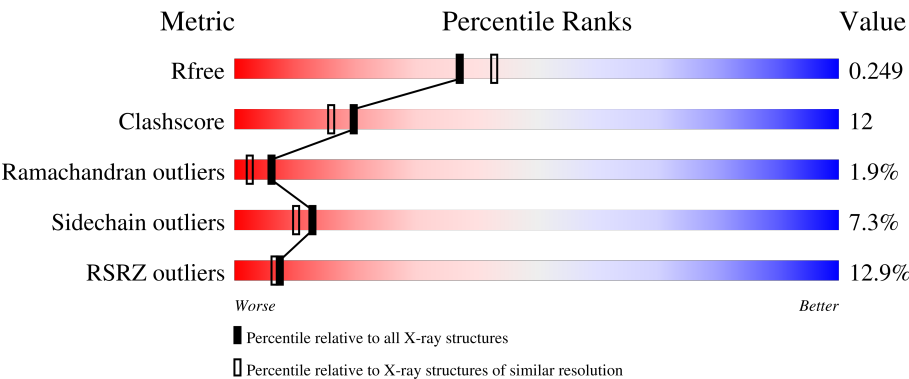
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	396	13% 71%21%5% . .
1	B	396	15% 72%20%5% . .
1	C	396	10% 77%16%5% .
1	D	396	11% 77%16%5% .
2	E	9	33% 44%33%22%

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Mol	Chain	Length	Quality of chain
2	F	9	 44% 33% 22%
2	G	9	 67% 11% 22%
2	H	9	 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12788 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.

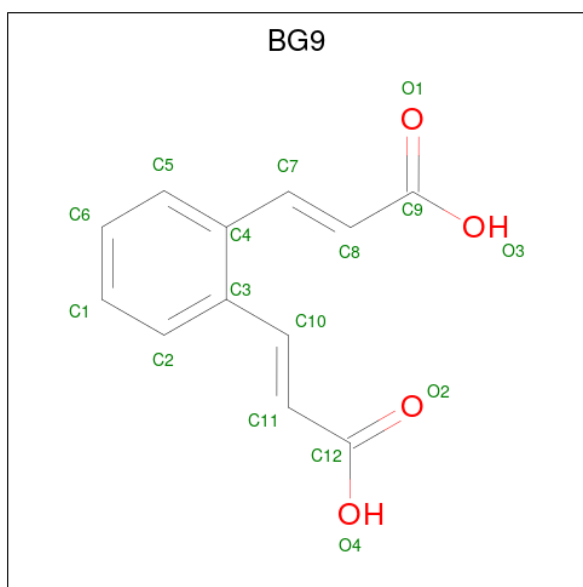
- Molecule 1 is a protein called kcn28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2970	1878	534	547	11			
1	B	387	Total	C	N	O	S	0	0	0
			2985	1888	536	549	12			
1	C	387	Total	C	N	O	S	0	0	0
			2972	1878	535	548	11			
1	D	387	Total	C	N	O	S	0	0	0
			2983	1886	536	550	11			

- Molecule 2 is a protein called DBB-DSG-VAL-MEA-VAL-GLY-GLY-DVA-DLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			64	43	10	11			
2	F	9	Total	C	N	O	0	0	0
			64	43	10	11			
2	G	9	Total	C	N	O	0	0	0
			64	43	10	11			
2	H	9	Total	C	N	O	0	0	0
			64	43	10	11			

- Molecule 3 is (2E,2'E)-3,3'-(1,2-phenylene)di(prop-2-enoic acid) (CCD ID: BG9) (formula: C₁₂H₁₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			14	12	2		
3	F	1	Total	C	O	0	0
			14	12	2		
3	G	1	Total	C	O	0	0
			14	12	2		
3	H	1	Total	C	O	0	0
			14	12	2		

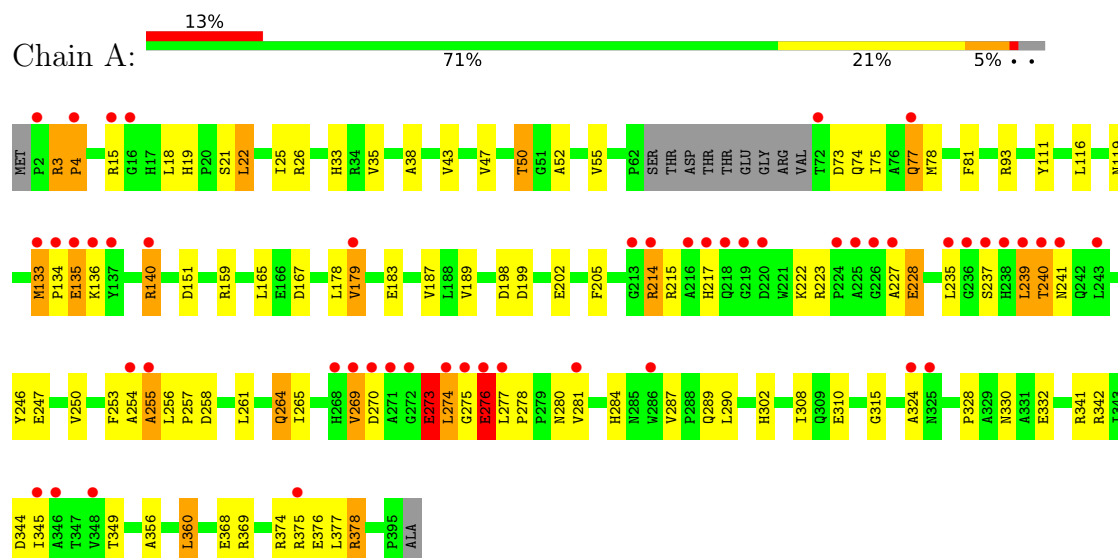
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	140	Total	O	0	0
			140	140		
4	C	135	Total	O	0	0
			135	135		
4	D	160	Total	O	0	0
			160	160		
4	E	3	Total	O	0	0
			3	3		
4	G	3	Total	O	0	0
			3	3		
4	H	7	Total	O	0	0
			7	7		

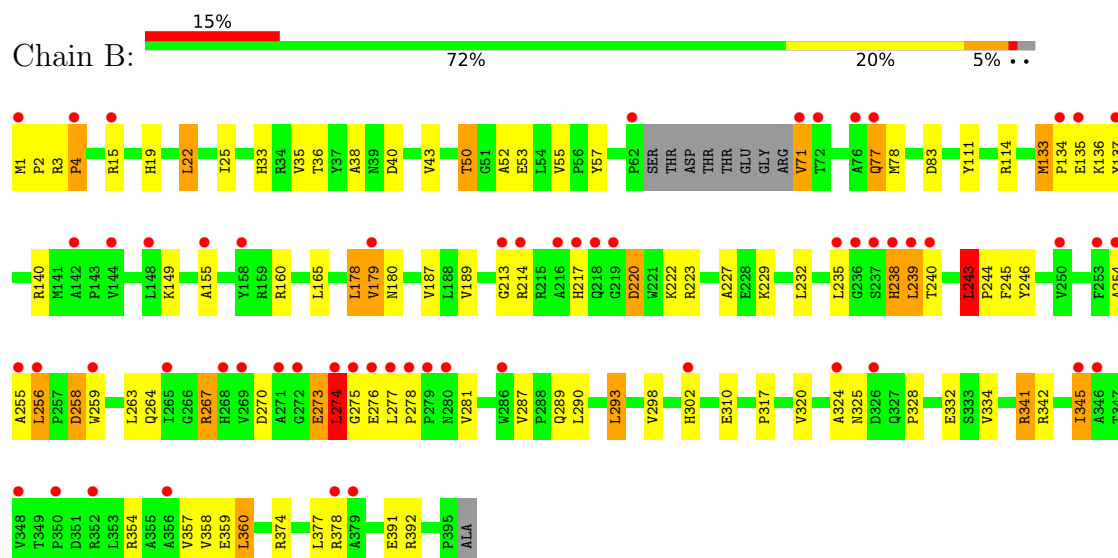
3 Residue-property plots [i](#)

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.

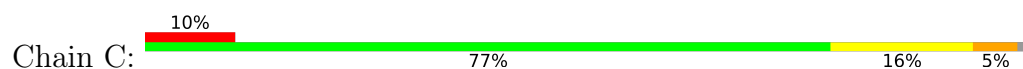
• Molecule 1: kcn28

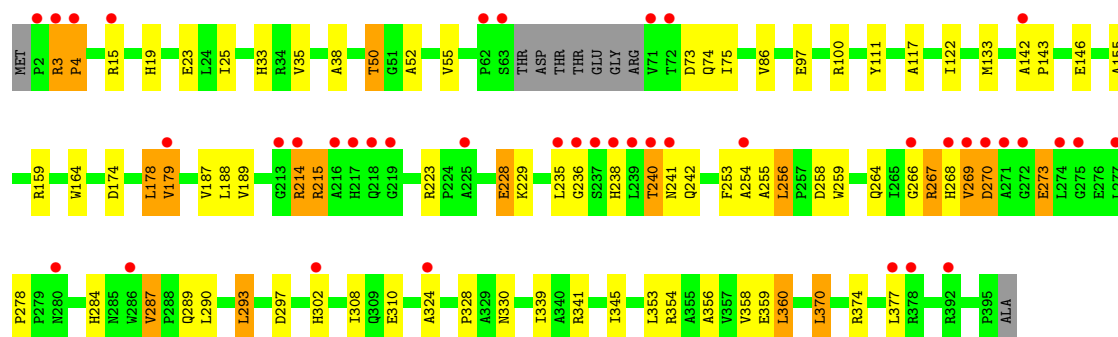


• Molecule 1: kcn28

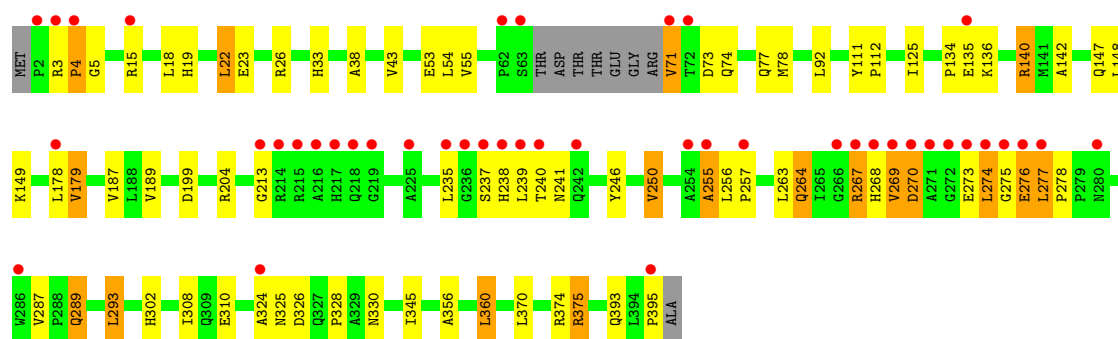
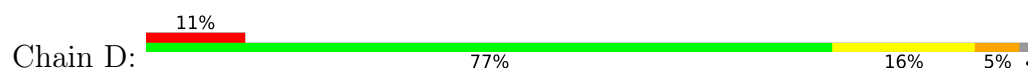


• Molecule 1: kcn28

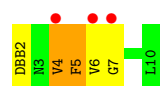
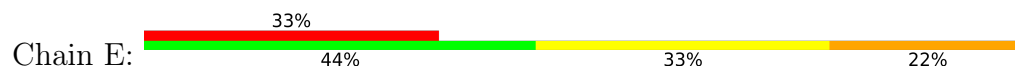




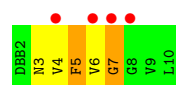
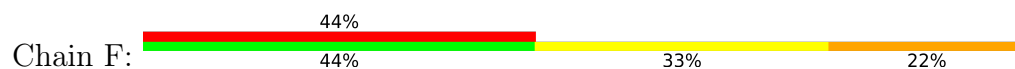
• Molecule 1: kcn28



• Molecule 2: DBB-DSG-VAL-MEA-VAL-GLY-GLY-DVA-DLE



• Molecule 2: DBB-DSG-VAL-MEA-VAL-GLY-GLY-DVA-DLE

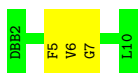


• Molecule 2: DBB-DSG-VAL-MEA-VAL-GLY-GLY-DVA-DLE



• Molecule 2: DBB-DSG-VAL-MEA-VAL-GLY-GLY-DVA-DLE





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	243.16Å 243.16Å 243.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.45 – 2.24 39.45 – 2.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.45-2.24) 99.9 (39.45-2.24)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.226 , 0.248 0.226 , 0.249	Depositor DCC
R_{free} test set	5492 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12788	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DLE, DVA, DBB, DSG, MEA, BG9

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	0.21	0/3042	0.50	0/4153
1	B	0.21	0/3057	0.55	0/4174
1	C	0.18	0/3044	0.48	0/4158
1	D	0.20	0/3055	0.55	0/4171
2	E	3.65	2/20 (10.0%)	1.73	1/24 (4.2%)
2	F	3.69	2/20 (10.0%)	1.60	1/24 (4.2%)
2	G	3.64	2/20 (10.0%)	1.59	0/24
2	H	3.70	2/20 (10.0%)	1.73	0/24
All	All	0.36	8/12278 (0.1%)	0.53	2/16752 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6	VAL	C-N	10.80	1.49	1.33
2	F	6	VAL	C-N	10.77	1.49	1.33
2	G	6	VAL	C-N	10.66	1.49	1.33
2	E	6	VAL	C-N	10.58	1.49	1.33
2	F	7	GLY	C-N	10.30	1.47	1.33
2	E	7	GLY	C-N	10.29	1.47	1.33
2	G	7	GLY	C-N	10.25	1.47	1.33
2	H	7	GLY	C-N	10.24	1.47	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	VAL	N-CA-C	-5.59	95.36	111.00
2	F	4	VAL	N-CA-C	-5.49	95.64	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2939	87	0
1	B	2985	0	2961	75	0
1	C	2972	0	2931	53	0
1	D	2983	0	2953	67	0
2	E	64	0	63	5	0
2	F	64	0	62	3	0
2	G	64	0	64	1	0
2	H	64	0	62	0	0
3	E	14	0	0	0	0
3	F	14	0	0	0	0
3	G	14	0	0	0	0
3	H	14	0	0	0	0
4	A	118	0	0	16	0
4	B	140	0	0	11	0
4	C	135	0	0	5	1
4	D	160	0	0	15	0
4	E	3	0	0	0	0
4	G	3	0	0	0	0
4	H	7	0	0	0	0
All	All	12788	0	12035	280	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 12.

All (280) 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)
1:A:223:ARG:NH1	1:A:227:ALA:O	1.92	1.01
1:A:214:ARG:HA	1:A:214:ARG:HH11	1.24	0.99
1:D:264:GLN:OE1	4:D:401:HOH:O	1.83	0.97
1:B:15:ARG:O	1:B:15:ARG:NH1	1.96	0.96
1:C:242:GLN:NE2	4:C:402:HOH:O	1.98	0.96
1:D:257:PRO:O	4:D:402:HOH:O	1.85	0.94
1:C:23:GLU:OE1	4:C:401:HOH:O	1.85	0.93
1:A:15:ARG:O	1:A:15:ARG:NH1	2.04	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HE1	2:E:5:MEA:HB1	1.52	0.91
1:A:374:ARG:NH1	4:A:402:HOH:O	1.94	0.90
1:A:360:LEU:O	4:A:401:HOH:O	1.91	0.89
1:B:274:LEU:HD22	1:B:277:LEU:HG	1.54	0.87
1:C:374:ARG:NH2	4:C:403:HOH:O	2.06	0.87
1:D:147:GLN:OE1	4:D:403:HOH:O	1.95	0.84
1:D:237:SER:O	1:D:239:LEU:N	2.10	0.84
1:C:341:ARG:NH2	1:C:359:GLU:OE2	2.11	0.84
1:A:19:HIS:HA	1:A:22:LEU:HD22	1.59	0.83
1:A:198:ASP:OD2	4:A:403:HOH:O	1.97	0.83
1:B:135:GLU:OE2	4:B:401:HOH:O	1.98	0.82
1:D:3:ARG:HH12	1:D:395:PRO:HG2	1.46	0.81
1:A:375:ARG:NH2	4:A:409:HOH:O	2.13	0.81
1:A:214:ARG:HA	1:A:214:ARG:NH1	1.95	0.80
1:B:374:ARG:NH1	4:B:404:HOH:O	2.14	0.80
1:C:15:ARG:NH1	1:C:19:HIS:H	1.80	0.80
1:B:19:HIS:HA	1:B:22:LEU:HD22	1.62	0.80
1:B:223:ARG:NH1	1:B:227:ALA:O	2.16	0.79
1:A:274:LEU:HD23	1:A:278:PRO:HD3	1.65	0.79
1:A:15:ARG:HH22	1:A:19:HIS:HB2	1.47	0.78
1:B:273:GLU:O	1:B:274:LEU:HB3	1.81	0.78
1:D:53:GLU:OE1	4:D:405:HOH:O	2.03	0.76
1:D:326:ASP:OD2	4:D:404:HOH:O	2.03	0.76
1:D:19:HIS:HA	1:D:22:LEU:HD22	1.68	0.74
1:B:4:PRO:O	1:B:33:HIS:ND1	2.20	0.74
1:D:374:ARG:NH1	4:D:410:HOH:O	2.19	0.74
1:C:15:ARG:O	1:C:15:ARG:NE	2.20	0.74
1:A:368:GLU:OE1	4:A:405:HOH:O	2.06	0.74
1:A:376:GLU:OE2	4:A:404:HOH:O	2.06	0.73
1:D:289:GLN:NE2	1:D:310:GLU:OE1	2.22	0.73
1:B:71:VAL:HG11	1:B:77:GLN:HB3	1.70	0.73
1:D:15:ARG:NE	1:D:15:ARG:O	2.22	0.73
1:D:267:ARG:HG3	1:D:267:ARG:HH21	1.54	0.72
1:B:15:ARG:HH22	1:B:19:HIS:HB2	1.53	0.72
1:A:369:ARG:NH1	4:A:413:HOH:O	2.21	0.72
1:B:274:LEU:HD11	1:B:277:LEU:HA	1.70	0.72
1:A:75:ILE:HA	1:A:78:MET:HE3	1.73	0.71
1:D:15:ARG:NH1	4:D:408:HOH:O	2.16	0.71
1:A:289:GLN:NE2	1:A:310:GLU:OE1	2.24	0.71
1:D:142:ALA:O	4:D:407:HOH:O	2.09	0.70
1:C:266:GLY:O	1:C:268:HIS:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ARG:NH2	1:D:19:HIS:H	1.89	0.70
1:D:54:LEU:O	4:D:406:HOH:O	2.09	0.70
1:D:3:ARG:NH1	1:D:395:PRO:HG2	2.06	0.69
1:B:258:ASP:OD1	1:B:258:ASP:N	2.21	0.69
1:C:15:ARG:HH12	1:C:19:HIS:H	1.39	0.69
1:B:274:LEU:CD2	1:B:277:LEU:HG	2.22	0.69
1:D:274:LEU:O	1:D:276:GLU:N	2.25	0.69
1:A:21:SER:OG	4:A:406:HOH:O	2.10	0.69
1:A:344:ASP:OD1	4:A:407:HOH:O	2.10	0.69
1:C:155:ALA:HB1	1:C:159:ARG:HH12	1.59	0.68
1:A:228:GLU:HG3	1:A:258:ASP:HB3	1.75	0.67
1:B:180:ASN:ND2	2:F:7:GLY:O	2.27	0.67
1:B:256:LEU:HD21	1:B:354:ARG:HG3	1.77	0.67
1:D:15:ARG:HH22	1:D:19:HIS:H	1.43	0.67
1:A:151:ASP:OD2	4:A:408:HOH:O	2.12	0.67
1:B:238:HIS:O	1:B:240:THR:N	2.27	0.67
1:A:240:THR:O	1:A:240:THR:OG1	2.12	0.66
1:C:50:THR:HG22	1:C:52:ALA:H	1.61	0.66
1:B:274:LEU:HG	1:B:275:GLY:N	2.09	0.66
1:B:50:THR:HG22	1:B:52:ALA:H	1.61	0.66
1:B:114:ARG:NH1	1:B:178:LEU:HA	2.11	0.65
1:A:4:PRO:O	1:A:33:HIS:ND1	2.26	0.65
1:B:289:GLN:NE2	1:B:310:GLU:OE1	2.28	0.65
1:C:235:LEU:HB3	1:C:302:HIS:CD2	2.32	0.64
1:B:2:PRO:HG3	1:B:391:GLU:HB3	1.80	0.64
1:D:3:ARG:HH12	1:D:395:PRO:CG	2.11	0.64
1:D:375:ARG:HG2	1:D:375:ARG:HH21	1.62	0.64
1:B:83:ASP:OD1	1:B:160:ARG:NH2	2.28	0.63
1:C:289:GLN:NE2	1:C:310:GLU:OE1	2.32	0.62
1:B:15:ARG:NH2	4:B:403:HOH:O	2.06	0.62
1:D:149:LYS:NZ	4:D:417:HOH:O	2.33	0.61
1:A:81:PHE:HE2	2:E:2:DBB:HG1	1.67	0.60
1:C:240:THR:O	1:C:242:GLN:HG2	2.01	0.60
1:A:240:THR:OG1	1:A:246:TYR:OH	2.18	0.60
1:A:315:GLY:O	4:A:410:HOH:O	2.16	0.60
1:A:26:ARG:NH1	4:A:411:HOH:O	2.17	0.59
1:A:235:LEU:HB3	1:A:302:HIS:CD2	2.36	0.59
1:C:324:ALA:O	1:C:328:PRO:HD3	2.02	0.59
1:D:15:ARG:HH22	1:D:19:HIS:N	2.00	0.59
1:D:26:ARG:NH1	4:D:412:HOH:O	2.27	0.59
1:D:273:GLU:N	1:D:273:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:H	1:A:3:ARG:HD3	1.68	0.58
1:C:236:GLY:H	1:C:302:HIS:HB2	1.69	0.58
1:B:341:ARG:NH2	1:B:359:GLU:OE1	2.36	0.58
1:B:325:ASN:HB3	2:F:3:DSG:O	2.03	0.58
1:B:15:ARG:NH2	1:B:19:HIS:HB2	2.19	0.57
1:A:264:GLN:HG3	1:A:287:VAL:HG13	1.85	0.57
1:B:277:LEU:HD22	1:B:281:VAL:HB	1.86	0.57
1:B:317:PRO:HB2	1:B:360:LEU:HG	1.86	0.57
1:A:375:ARG:O	1:A:378:ARG:HD2	2.05	0.57
1:B:111:TYR:OH	4:B:405:HOH:O	2.17	0.57
1:C:273:GLU:N	1:C:273:GLU:OE1	2.36	0.56
1:D:71:VAL:HG12	1:D:77:GLN:HG3	1.86	0.56
1:A:179:VAL:O	4:A:412:HOH:O	2.18	0.56
1:C:15:ARG:HH12	1:C:19:HIS:N	2.02	0.56
1:C:267:ARG:HG3	1:C:268:HIS:CD2	2.41	0.56
1:A:73:ASP:OD1	1:A:74:GLN:N	2.39	0.56
1:A:15:ARG:NH2	1:A:19:HIS:HB2	2.19	0.56
1:D:325:ASN:HA	4:D:439:HOH:O	2.06	0.56
1:A:183:GLU:HG2	4:A:504:HOH:O	2.06	0.56
1:C:354:ARG:NH1	4:C:407:HOH:O	2.24	0.55
1:D:255:ALA:O	4:D:409:HOH:O	2.17	0.55
1:D:264:GLN:HG3	1:D:287:VAL:HG13	1.89	0.55
1:D:267:ARG:HH21	1:D:267:ARG:CG	2.18	0.55
1:A:275:GLY:O	1:A:276:GLU:HB2	2.07	0.55
1:B:298:VAL:HG11	1:B:357:VAL:HG13	1.87	0.55
1:A:290:LEU:HD21	1:A:310:GLU:HG2	1.88	0.55
1:A:324:ALA:O	1:A:328:PRO:HD3	2.06	0.55
1:B:354:ARG:NH1	4:B:412:HOH:O	2.37	0.55
1:C:100:ARG:O	4:C:406:HOH:O	2.18	0.54
1:A:253:PHE:O	1:A:280:ASN:ND2	2.34	0.54
1:D:324:ALA:O	1:D:328:PRO:HD3	2.08	0.54
1:C:215:ARG:HB3	1:C:215:ARG:CZ	2.38	0.54
1:D:269:VAL:O	1:D:270:ASP:HB2	2.08	0.53
1:D:375:ARG:HH21	1:D:375:ARG:CG	2.22	0.53
1:C:256:LEU:HB3	1:C:259:TRP:HB2	1.90	0.53
1:A:255:ALA:C	1:A:257:PRO:HD3	2.34	0.52
1:C:155:ALA:HB1	1:C:159:ARG:NH1	2.24	0.52
1:C:228:GLU:HG3	1:C:258:ASP:HB3	1.91	0.52
1:D:136:LYS:HD2	1:D:199:ASP:OD2	2.10	0.52
1:A:273:GLU:OE1	1:A:273:GLU:N	2.43	0.52
1:B:36:THR:HG22	1:B:53:GLU:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLN:HG3	1:C:287:VAL:HG13	1.92	0.51
1:A:159:ARG:NH2	1:B:222:LYS:HD2	2.25	0.51
1:A:167:ASP:OD1	1:B:217:HIS:ND1	2.44	0.51
1:B:324:ALA:O	1:B:328:PRO:HD3	2.10	0.51
1:A:356:ALA:O	1:A:360:LEU:HB2	2.10	0.51
1:B:274:LEU:HD21	1:B:277:LEU:N	2.26	0.51
1:B:245:PHE:N	4:B:407:HOH:O	2.44	0.50
1:B:274:LEU:HD11	1:B:277:LEU:CA	2.41	0.50
1:D:111:TYR:CG	1:D:179:VAL:HG22	2.46	0.50
1:B:290:LEU:HD21	1:B:310:GLU:HG2	1.94	0.50
1:D:3:ARG:NH1	1:D:395:PRO:C	2.69	0.50
1:C:214:ARG:NE	1:C:214:ARG:HA	2.27	0.50
1:D:73:ASP:OD1	1:D:74:GLN:N	2.45	0.49
1:A:3:ARG:H	1:A:3:ARG:CD	2.25	0.49
1:B:246:TYR:N	4:B:407:HOH:O	2.30	0.49
1:B:320:VAL:HG21	1:B:334:VAL:HG21	1.95	0.49
1:A:136:LYS:HE3	1:A:199:ASP:HB3	1.95	0.49
1:C:75:ILE:HD12	1:C:75:ILE:H	1.78	0.48
1:D:235:LEU:HB3	1:D:302:HIS:CD2	2.48	0.48
1:D:178:LEU:O	1:D:179:VAL:HB	2.13	0.48
1:B:217:HIS:HB2	4:B:448:HOH:O	2.12	0.48
1:A:15:ARG:HD2	1:A:15:ARG:HA	1.50	0.48
1:D:136:LYS:O	1:D:140:ARG:HG3	2.13	0.48
1:A:250:VAL:HG12	1:A:281:VAL:HG11	1.96	0.48
1:B:77:GLN:HG3	1:B:78:MET:N	2.29	0.48
1:C:356:ALA:O	1:C:360:LEU:HB2	2.14	0.48
1:A:111:TYR:CG	1:A:179:VAL:HG22	2.49	0.47
1:A:178:LEU:O	1:A:179:VAL:HB	2.14	0.47
1:C:25:ILE:HG23	1:C:35:VAL:HG11	1.95	0.47
1:B:240:THR:OG1	1:B:267:ARG:NH1	2.47	0.47
1:D:276:GLU:O	1:D:277:LEU:HB2	2.14	0.47
1:B:235:LEU:HB3	1:B:302:HIS:CE1	2.49	0.47
1:D:3:ARG:HH12	1:D:395:PRO:C	2.22	0.47
1:D:274:LEU:HD21	1:D:278:PRO:HD3	1.95	0.47
1:B:254:ALA:HB2	1:B:278:PRO:HG2	1.96	0.47
1:D:274:LEU:HG	1:D:277:LEU:HA	1.96	0.47
1:C:38:ALA:HA	1:C:55:VAL:O	2.15	0.47
1:B:378:ARG:NH1	4:B:417:HOH:O	2.47	0.47
1:A:77:GLN:HG3	1:A:78:MET:N	2.30	0.46
1:A:368:GLU:HB3	4:A:405:HOH:O	2.14	0.46
1:C:269:VAL:O	1:C:270:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LEU:HD21	1:C:310:GLU:HG2	1.97	0.46
1:D:246:TYR:CD1	1:D:263:LEU:HD11	2.49	0.46
1:A:261:LEU:HD23	1:A:281:VAL:HG22	1.97	0.46
1:A:332:GLU:OE2	1:A:342:ARG:NH1	2.48	0.46
1:B:136:LYS:NZ	1:B:140:ARG:HD3	2.31	0.46
1:A:140:ARG:H	1:A:140:ARG:HG2	1.51	0.46
1:C:178:LEU:O	1:C:179:VAL:HB	2.16	0.46
1:D:74:GLN:O	1:D:78:MET:HG3	2.16	0.45
1:D:125:ILE:HD11	1:D:393:GLN:HG3	1.97	0.45
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.81	0.45
1:A:15:ARG:HH12	1:A:19:HIS:H	1.63	0.45
1:B:133:MET:SD	2:F:5:MEA:HB1	2.56	0.45
1:B:243:LEU:H	1:B:244:PRO:CD	2.29	0.45
1:B:341:ARG:HH11	1:B:341:ARG:HG2	1.81	0.45
1:B:345:ILE:HD12	1:B:345:ILE:HA	1.71	0.45
1:A:265:ILE:HG12	1:A:284:HIS:O	2.17	0.45
1:B:33:HIS:NE2	1:B:391:GLU:OE2	2.50	0.45
1:B:232:LEU:HD23	1:B:293:LEU:HD13	1.98	0.45
1:D:23:GLU:HG3	1:D:213:GLY:N	2.32	0.45
1:D:38:ALA:HA	1:D:55:VAL:O	2.17	0.45
1:D:256:LEU:HD12	1:D:256:LEU:HA	1.79	0.45
1:A:93:ARG:HH22	1:A:119:ASN:ND2	2.14	0.45
1:B:245:PHE:HB3	4:B:407:HOH:O	2.16	0.45
1:D:267:ARG:HG3	1:D:267:ARG:NH2	2.24	0.45
1:A:75:ILE:HD12	1:A:75:ILE:H	1.80	0.45
1:B:332:GLU:OE2	1:B:342:ARG:NH1	2.50	0.45
1:C:133:MET:SD	2:G:5:MEA:HB1	2.57	0.45
1:A:187:VAL:HG12	1:A:189:VAL:HG22	1.99	0.45
1:B:178:LEU:O	1:B:179:VAL:HB	2.17	0.45
1:C:4:PRO:O	1:C:33:HIS:ND1	2.40	0.45
1:A:47:VAL:O	1:A:50:THR:HG22	2.17	0.45
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.83	0.45
1:C:97:GLU:OE1	1:C:100:ARG:NH2	2.41	0.45
1:A:135:GLU:CD	1:A:135:GLU:H	2.24	0.44
1:A:270:ASP:OD1	1:A:273:GLU:OE2	2.35	0.44
1:C:111:TYR:CG	1:C:179:VAL:HG22	2.52	0.44
1:B:38:ALA:HA	1:B:55:VAL:O	2.18	0.44
1:B:274:LEU:CD1	1:B:277:LEU:HA	2.43	0.44
1:B:15:ARG:HD2	1:B:15:ARG:HA	1.48	0.44
1:D:308:ILE:HD12	1:D:330:ASN:HB3	2.00	0.44
1:A:215:ARG:NH2	1:A:217:HIS:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HG23	1:B:35:VAL:HG11	1.98	0.44
1:A:81:PHE:CE2	2:E:2:DBB:HG1	2.49	0.43
1:A:159:ARG:HD3	1:B:220:ASP:O	2.18	0.43
1:C:3:ARG:HG2	1:C:3:ARG:HH21	1.82	0.43
1:D:22:LEU:HD12	1:D:22:LEU:HA	1.89	0.43
1:B:134:PRO:HD2	1:B:137:TYR:HB2	2.01	0.43
1:C:229:LYS:HA	1:C:297:ASP:OD2	2.19	0.43
1:A:202:GLU:HA	1:A:205:PHE:O	2.19	0.43
1:A:276:GLU:O	1:A:277:LEU:HB2	2.18	0.43
1:D:147:GLN:HB3	4:D:436:HOH:O	2.18	0.43
1:D:308:ILE:CD1	1:D:330:ASN:HB3	2.48	0.43
1:A:133:MET:H	1:A:133:MET:HG2	1.67	0.43
1:A:222:LYS:HD2	1:A:222:LYS:HA	1.85	0.43
1:A:273:GLU:HB2	1:A:274:LEU:H	1.56	0.43
1:C:73:ASP:OD1	1:C:74:GLN:N	2.51	0.43
1:C:253:PHE:HA	1:C:256:LEU:HB2	2.01	0.43
1:C:254:ALA:HB2	1:C:278:PRO:HG2	2.00	0.43
1:D:4:PRO:O	1:D:33:HIS:ND1	2.38	0.43
1:D:204:ARG:NH2	4:D:434:HOH:O	2.51	0.43
1:A:18:LEU:HD21	1:A:43:VAL:HB	2.01	0.42
1:D:4:PRO:HB2	1:D:5:GLY:H	1.61	0.42
1:B:111:TYR:CG	1:B:179:VAL:HG22	2.55	0.42
1:B:235:LEU:HB3	1:B:302:HIS:NE2	2.34	0.42
1:B:246:TYR:CD1	1:B:263:LEU:HD11	2.54	0.42
1:C:284:HIS:HB2	1:C:287:VAL:HG12	2.01	0.42
1:D:134:PRO:C	1:D:136:LYS:H	2.26	0.42
1:B:213:GLY:O	1:B:214:ARG:HB3	2.18	0.42
1:B:264:GLN:HG3	1:B:287:VAL:HG13	2.02	0.42
1:D:187:VAL:HG12	1:D:189:VAL:HG22	2.02	0.42
1:A:38:ALA:HA	1:A:55:VAL:O	2.19	0.42
1:B:187:VAL:HG12	1:B:189:VAL:HG22	2.01	0.42
1:A:239:LEU:HD13	1:A:239:LEU:HA	1.78	0.42
1:A:254:ALA:HB2	1:A:278:PRO:HG2	2.02	0.42
1:C:15:ARG:NH1	1:C:19:HIS:HB2	2.34	0.41
1:C:142:ALA:N	1:C:143:PRO:HD2	2.35	0.41
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.93	0.41
4:A:515:HOH:O	2:E:4:VAL:HB	2.20	0.41
1:C:308:ILE:CD1	1:C:330:ASN:HB3	2.50	0.41
1:D:111:TYR:CD1	1:D:112:PRO:HD3	2.55	0.41
1:D:136:LYS:NZ	1:D:140:ARG:HD3	2.35	0.41
1:D:250:VAL:HG21	1:D:274:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HB3	1:A:277:LEU:HA	2.02	0.41
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.36	0.41
1:A:74:GLN:HG2	1:A:78:MET:HE2	2.01	0.41
1:A:50:THR:CG2	1:A:52:ALA:H	2.34	0.41
1:B:274:LEU:HD21	1:B:277:LEU:H	1.84	0.41
1:A:25:ILE:HG23	1:A:35:VAL:HG11	2.03	0.41
1:A:50:THR:HG22	1:A:52:ALA:H	1.86	0.41
1:A:237:SER:O	1:A:239:LEU:N	2.51	0.41
1:C:339:ILE:HG21	1:C:370:LEU:HD13	2.02	0.41
1:A:133:MET:HE1	2:E:5:MEA:CB	2.36	0.41
1:B:40:ASP:HA	1:B:57:TYR:O	2.21	0.41
1:B:229:LYS:O	1:B:259:TRP:HA	2.21	0.41
1:C:187:VAL:HG12	1:C:189:VAL:HG22	2.02	0.41
1:C:293:LEU:HD12	1:C:293:LEU:HA	1.89	0.41
1:D:18:LEU:HD21	1:D:43:VAL:HB	2.02	0.41
1:A:250:VAL:HG12	1:A:281:VAL:HG21	2.02	0.41
1:C:117:ALA:HB1	1:C:122:ILE:O	2.21	0.41
1:A:308:ILE:CD1	1:A:330:ASN:HB3	2.51	0.40
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.82	0.40
1:C:86:VAL:HG22	1:C:164:TRP:CD1	2.55	0.40
1:A:247:GLU:HA	1:A:250:VAL:HG22	2.02	0.40
1:A:134:PRO:C	1:A:136:LYS:H	2.28	0.40
1:B:149:LYS:O	1:B:155:ALA:HB2	2.21	0.40
1:B:392:ARG:NH2	4:B:402:HOH:O	2.40	0.40
1:D:178:LEU:HD13	1:D:179:VAL:HG23	2.03	0.40
1:D:356:ALA:O	1:D:360:LEU:HB2	2.21	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)
4:C:487:HOH:O	4:C:527:HOH:O[6_566]	1.91	0.29

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	381/396 (96%)	356 (93%)	19 (5%)	6 (2%)	7	4
1	B	383/396 (97%)	359 (94%)	15 (4%)	9 (2%)	5	1
1	C	383/396 (97%)	363 (95%)	13 (3%)	7 (2%)	6	3
1	D	383/396 (97%)	358 (94%)	18 (5%)	7 (2%)	6	3
2	E	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	F	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	G	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
2	H	4/9 (44%)	3 (75%)	1 (25%)	0	100	100
All	All	1546/1620 (95%)	1448 (94%)	69 (4%)	29 (2%)	6	2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	A	276	GLU
1	B	4	PRO
1	B	179	VAL
1	B	239	LEU
1	B	255	ALA
1	B	274	LEU
1	C	4	PRO
1	C	179	VAL
1	C	241	ASN
1	C	255	ALA
1	C	267	ARG
1	C	270	ASP
1	C	273	GLU
1	D	179	VAL
1	D	238	HIS
1	D	270	ASP
1	D	275	GLY
1	D	277	LEU
1	A	4	PRO
1	A	255	ALA
1	A	273	GLU
1	B	243	LEU
1	D	4	PRO

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Mol	Chain	Res	Type
1	D	255	ALA
1	B	270	ASP
1	A	269	VAL
1	B	238	HIS
1	B	276	GLU

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	312/321 (97%)	287 (92%)	25 (8%)	11	8
1	B	314/321 (98%)	290 (92%)	24 (8%)	12	9
1	C	311/321 (97%)	290 (93%)	21 (7%)	14	12
1	D	314/321 (98%)	293 (93%)	21 (7%)	15	12
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	1259/1292 (97%)	1167 (93%)	92 (7%)	13	10

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	22	LEU
1	A	50	THR
1	A	77	GLN
1	A	116	LEU
1	A	133	MET
1	A	135	GLU
1	A	140	ARG
1	A	165	LEU
1	A	214	ARG

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Mol	Chain	Res	Type
1	A	228	GLU
1	A	239	LEU
1	A	240	THR
1	A	241	ASN
1	A	264	GLN
1	A	269	VAL
1	A	273	GLU
1	A	274	LEU
1	A	276	GLU
1	A	341	ARG
1	A	345	ILE
1	A	349	THR
1	A	360	LEU
1	A	377	LEU
1	A	378	ARG
1	B	1	MET
1	B	3	ARG
1	B	22	LEU
1	B	43	VAL
1	B	50	THR
1	B	71	VAL
1	B	77	GLN
1	B	133	MET
1	B	165	LEU
1	B	178	LEU
1	B	220	ASP
1	B	239	LEU
1	B	243	LEU
1	B	256	LEU
1	B	258	ASP
1	B	267	ARG
1	B	273	GLU
1	B	274	LEU
1	B	293	LEU
1	B	341	ARG
1	B	345	ILE
1	B	358	VAL
1	B	360	LEU
1	B	377	LEU
1	C	3	ARG
1	C	50	THR
1	C	146	GLU

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Mol	Chain	Res	Type
1	C	174	ASP
1	C	178	LEU
1	C	188	LEU
1	C	214	ARG
1	C	215	ARG
1	C	228	GLU
1	C	238	HIS
1	C	240	THR
1	C	256	LEU
1	C	269	VAL
1	C	287	VAL
1	C	293	LEU
1	C	345	ILE
1	C	353	LEU
1	C	358	VAL
1	C	360	LEU
1	C	370	LEU
1	C	377	LEU
1	D	22	LEU
1	D	71	VAL
1	D	92	LEU
1	D	135	GLU
1	D	140	ARG
1	D	148	LEU
1	D	240	THR
1	D	241	ASN
1	D	250	VAL
1	D	264	GLN
1	D	267	ARG
1	D	268	HIS
1	D	269	VAL
1	D	274	LEU
1	D	276	GLU
1	D	289	GLN
1	D	293	LEU
1	D	345	ILE
1	D	360	LEU
1	D	370	LEU
1	D	375	ARG
2	G	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	217	HIS
1	A	218	GLN
1	B	238	HIS
1	B	393	GLN
1	C	19	HIS
1	C	268	HIS
1	D	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues 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
2	MEA	G	5	2	11,12,13	1.05	1 (9%)	13,14,16	1.19	1 (7%)
2	MEA	F	5	2	11,12,13	1.03	1 (9%)	13,14,16	1.26	2 (15%)
2	DBB	E	2	2	4,5,6	0.51	0	1,5,7	1.65	0
2	DBB	H	2	2	4,5,6	0.44	0	1,5,7	0.65	0
2	MEA	H	5	2	11,12,13	1.02	1 (9%)	13,14,16	1.09	1 (7%)
2	DBB	F	2	2	4,5,6	0.56	0	1,5,7	1.69	0
2	DBB	G	2	2	4,5,6	0.42	0	1,5,7	0.12	0
2	MEA	E	5	2	11,12,13	1.07	1 (9%)	13,14,16	1.17	1 (7%)

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
2	MEA	G	5	2	-	3/5/8/10	0/1/1/1
2	MEA	F	5	2	-	4/5/8/10	0/1/1/1
2	DBB	E	2	2	-	1/3/4/6	-
2	DBB	H	2	2	-	0/3/4/6	-
2	MEA	H	5	2	-	3/5/8/10	0/1/1/1
2	DBB	F	2	2	-	0/3/4/6	-
2	DBB	G	2	2	-	1/3/4/6	-
2	MEA	E	5	2	-	4/5/8/10	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	MEA	CB-CG	2.53	1.57	1.51
2	G	5	MEA	CB-CG	2.49	1.57	1.51
2	F	5	MEA	CB-CG	2.49	1.57	1.51
2	H	5	MEA	CB-CG	2.41	1.57	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	MEA	C1-N-CA	3.06	122.86	113.70
2	E	5	MEA	C1-N-CA	3.00	122.66	113.70
2	F	5	MEA	C1-N-CA	2.94	122.48	113.70
2	H	5	MEA	C1-N-CA	2.82	122.12	113.70
2	F	5	MEA	CG-CB-CA	-2.25	110.31	113.51

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	DBB	O-C-CA-CB
2	E	5	MEA	O-C-CA-CB
2	F	5	MEA	O-C-CA-CB
2	F	5	MEA	C-CA-CB-CG
2	G	5	MEA	O-C-CA-CB
2	H	5	MEA	O-C-CA-CB
2	G	5	MEA	CA-CB-CG-CD2
2	H	5	MEA	CA-CB-CG-CD2
2	F	5	MEA	CA-CB-CG-CD2
2	E	5	MEA	CA-CB-CG-CD2
2	G	5	MEA	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
2	H	5	MEA	CA-CB-CG-CD1
2	E	5	MEA	CA-CB-CG-CD1
2	F	5	MEA	CA-CB-CG-CD1
2	E	2	DBB	N-CA-CB-CG
2	E	5	MEA	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	MEA	1	0
2	F	5	MEA	1	0
2	E	2	DBB	2	0
2	E	5	MEA	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	BG9	G	101	-	14,14,16	2.23	4 (28%)	16,16,20	1.71	4 (25%)
3	BG9	H	101	-	14,14,16	2.20	4 (28%)	16,16,20	1.77	3 (18%)
3	BG9	E	101	-	14,14,16	2.16	4 (28%)	16,16,20	1.46	3 (18%)
3	BG9	F	101	-	14,14,16	2.18	4 (28%)	16,16,20	1.69	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BG9	G	101	-	-	4/8/8/10	0/1/1/1
3	BG9	H	101	-	-	4/8/8/10	0/1/1/1
3	BG9	E	101	-	-	4/8/8/10	0/1/1/1
3	BG9	F	101	-	-	4/8/8/10	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	BG9	C4-C7	5.02	1.55	1.47
3	H	101	BG9	C4-C7	4.93	1.55	1.47
3	G	101	BG9	C3-C10	4.80	1.55	1.47
3	E	101	BG9	C4-C7	4.77	1.54	1.47
3	G	101	BG9	C4-C7	4.73	1.54	1.47
3	E	101	BG9	C3-C10	4.53	1.54	1.47
3	H	101	BG9	C3-C10	4.41	1.54	1.47
3	F	101	BG9	C3-C10	4.41	1.54	1.47
3	G	101	BG9	C11-C12	3.71	1.55	1.44
3	H	101	BG9	C11-C12	3.50	1.54	1.44
3	E	101	BG9	C11-C12	3.48	1.54	1.44
3	F	101	BG9	C11-C12	3.43	1.54	1.44
3	H	101	BG9	C9-C8	2.58	1.54	1.49
3	F	101	BG9	C9-C8	2.50	1.54	1.49
3	E	101	BG9	C9-C8	2.45	1.54	1.49
3	G	101	BG9	C9-C8	2.42	1.54	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	101	BG9	C3-C10-C11	-4.92	115.70	126.00
3	F	101	BG9	C3-C10-C11	-4.75	116.04	126.00
3	G	101	BG9	C3-C10-C11	-4.45	116.67	126.00
3	E	101	BG9	C3-C10-C11	-3.58	118.49	126.00
3	H	101	BG9	O2-C12-C11	-2.90	116.36	125.61
3	G	101	BG9	O2-C12-C11	-2.75	116.84	125.61
3	G	101	BG9	C4-C7-C8	-2.22	120.87	125.55
3	F	101	BG9	O2-C12-C11	-2.21	118.56	125.61
3	F	101	BG9	C9-C8-C7	-2.19	119.55	124.56
3	G	101	BG9	C9-C8-C7	-2.17	119.59	124.56
3	H	101	BG9	C9-C8-C7	-2.15	119.65	124.56
3	E	101	BG9	C4-C7-C8	-2.12	121.07	125.55
3	E	101	BG9	C9-C8-C7	-2.08	119.80	124.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	101	BG9	C10-C11-C12-O2
3	F	101	BG9	C10-C11-C12-O2
3	G	101	BG9	C10-C11-C12-O2
3	H	101	BG9	C7-C8-C9-O3
3	H	101	BG9	C10-C11-C12-O2
3	H	101	BG9	C5-C4-C7-C8
3	E	101	BG9	C3-C4-C7-C8
3	F	101	BG9	C3-C4-C7-C8
3	G	101	BG9	C3-C4-C7-C8
3	H	101	BG9	C3-C4-C7-C8
3	E	101	BG9	C5-C4-C7-C8
3	G	101	BG9	C5-C4-C7-C8
3	F	101	BG9	C5-C4-C7-C8
3	E	101	BG9	C7-C8-C9-O3
3	F	101	BG9	C7-C8-C9-O3
3	G	101	BG9	C7-C8-C9-O3

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	385/396 (97%)	0.42	51 (13%) 7 6	26, 47, 106, 159	0
1	B	387/396 (97%)	0.66	59 (15%) 5 4	28, 50, 106, 175	0
1	C	387/396 (97%)	0.40	41 (10%) 11 10	29, 46, 112, 171	0
1	D	387/396 (97%)	0.38	44 (11%) 10 9	29, 45, 110, 170	0
2	E	4/9 (44%)	2.40	3 (75%) 0 0	66, 69, 72, 72	0
2	F	4/9 (44%)	3.99	4 (100%) 0 0	92, 94, 97, 99	0
2	G	4/9 (44%)	1.15	0 100 100	63, 64, 69, 70	0
2	H	4/9 (44%)	-0.14	0 100 100	39, 40, 45, 49	0
All	All	1562/1620 (96%)	0.48	202 (12%) 7 6	26, 47, 110, 175	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	71	VAL	10.8
1	C	236	GLY	6.4
1	C	271	ALA	6.4
1	D	239	LEU	5.7
1	B	271	ALA	5.6
1	D	271	ALA	5.5
1	C	240	THR	5.4
1	A	286	TRP	5.3
1	C	274	LEU	5.3
1	D	2	PRO	5.2
1	D	216	ALA	5.1
2	F	6	VAL	5.1
1	B	277	LEU	5.1
1	C	71	VAL	4.9
1	B	239	LEU	4.7
1	B	238	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	135	GLU	4.5
1	B	236	GLY	4.5
1	A	239	LEU	4.4
1	B	71	VAL	4.4
1	C	269	VAL	4.4
1	B	77	GLN	4.4
1	D	4	PRO	4.4
1	B	237	SER	4.3
1	B	213	GLY	4.3
1	C	2	PRO	4.3
1	D	238	HIS	4.1
1	B	235	LEU	4.0
2	F	7	GLY	4.0
1	C	216	ALA	4.0
1	C	213	GLY	4.0
1	A	237	SER	4.0
1	D	213	GLY	3.9
1	D	218	GLN	3.9
1	D	236	GLY	3.9
1	A	216	ALA	3.9
1	B	255	ALA	3.8
1	B	62	PRO	3.8
1	A	269	VAL	3.8
1	A	238	HIS	3.7
1	A	240	THR	3.7
1	B	278	PRO	3.7
1	D	277	LEU	3.7
1	D	237	SER	3.7
1	C	286	TRP	3.6
2	F	8	GLY	3.5
2	E	6	VAL	3.5
1	C	237	SER	3.5
1	A	226	GLY	3.5
1	D	219	GLY	3.5
1	D	275	GLY	3.5
1	A	274	LEU	3.5
1	A	271	ALA	3.4
1	C	218	GLN	3.4
1	B	269	VAL	3.3
1	C	275	GLY	3.3
1	D	276	GLU	3.3
1	B	348	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.3
1	C	241	ASN	3.3
1	B	345	ILE	3.3
1	C	15	ARG	3.3
1	A	236	GLY	3.2
1	B	219	GLY	3.2
1	B	15	ARG	3.2
1	D	135	GLU	3.2
2	F	4	VAL	3.2
1	C	238	HIS	3.2
1	D	274	LEU	3.2
1	D	225	ALA	3.2
1	D	324	ALA	3.2
1	C	268	HIS	3.1
1	D	217	HIS	3.1
1	B	274	LEU	3.1
1	C	217	HIS	3.1
1	C	270	ASP	3.1
1	A	72	THR	3.1
1	C	63	SER	3.1
1	C	324	ALA	3.1
1	A	348	VAL	3.1
1	D	257	PRO	3.1
1	D	240	THR	3.1
1	A	219	GLY	3.1
1	A	375	ARG	3.1
1	A	227	ALA	3.0
1	A	218	GLN	3.0
1	A	134	PRO	3.0
1	B	356	ALA	3.0
1	B	352	ARG	3.0
1	A	217	HIS	2.9
1	B	279	PRO	2.9
1	A	179	VAL	2.9
1	D	3	ARG	2.9
1	B	148	LEU	2.9
1	A	137	TYR	2.9
1	C	378	ARG	2.9
1	B	275	GLY	2.8
1	B	302	HIS	2.8
1	B	216	ALA	2.8
1	D	15	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	4	PRO	2.8
1	B	142	ALA	2.8
1	D	214	ARG	2.8
1	A	255	ALA	2.8
1	B	324	ALA	2.8
2	E	4	VAL	2.8
1	A	268	HIS	2.7
1	A	214	ARG	2.7
1	A	77	GLN	2.7
1	D	63	SER	2.7
1	D	286	TRP	2.7
1	A	15	ARG	2.7
1	A	213	GLY	2.7
1	D	255	ALA	2.7
1	D	72	THR	2.7
1	D	272	GLY	2.7
1	B	286	TRP	2.7
1	B	218	GLN	2.6
1	B	135	GLU	2.6
1	A	275	GLY	2.6
1	C	219	GLY	2.6
1	A	243	LEU	2.6
1	C	235	LEU	2.6
1	B	137	TYR	2.6
1	B	276	GLU	2.5
1	C	239	LEU	2.5
1	B	346	ALA	2.5
1	A	4	PRO	2.5
1	D	267	ARG	2.5
1	A	324	ALA	2.5
1	A	345	ILE	2.5
1	B	76	ALA	2.5
1	D	395	PRO	2.5
1	A	133	MET	2.4
1	C	280	ASN	2.4
1	A	16	GLY	2.4
1	A	136	LYS	2.4
1	B	259	TRP	2.4
1	A	277	LEU	2.4
1	D	280	ASN	2.4
2	E	7	GLY	2.4
1	B	265	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	217	HIS	2.4
1	D	62	PRO	2.4
1	A	346	ALA	2.4
1	B	254	ALA	2.4
1	C	254	ALA	2.4
1	C	302	HIS	2.4
1	D	178	LEU	2.3
1	B	272	GLY	2.3
1	C	266	GLY	2.3
1	D	235	LEU	2.3
1	D	266	GLY	2.3
1	B	179	VAL	2.3
1	B	158	TYR	2.3
1	A	281	VAL	2.3
1	B	326	ASP	2.2
1	A	224	PRO	2.2
1	A	272	GLY	2.2
1	C	392	ARG	2.2
1	C	225	ALA	2.2
1	B	253	PHE	2.2
1	D	268	HIS	2.2
1	A	225	ALA	2.2
1	C	277	LEU	2.2
1	B	144	VAL	2.2
1	A	241	ASN	2.2
1	A	270	ASP	2.2
1	B	4	PRO	2.2
1	C	272	GLY	2.2
1	A	254	ALA	2.2
1	B	378	ARG	2.2
1	D	273	GLU	2.2
1	B	268	HIS	2.2
1	B	72	THR	2.2
1	C	142	ALA	2.2
1	B	214	ARG	2.1
1	C	3	ARG	2.1
1	D	215	ARG	2.1
1	A	325	ASN	2.1
1	B	350	PRO	2.1
1	B	240	THR	2.1
1	B	280	ASN	2.1
1	B	250	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	2.1
1	B	155	ALA	2.1
1	B	379	ALA	2.1
1	D	254	ALA	2.1
1	D	242	GLN	2.1
1	D	270	ASP	2.1
1	C	179	VAL	2.1
1	A	220	ASP	2.0
1	B	134	PRO	2.0
1	C	62	PRO	2.0
1	C	214	ARG	2.0
1	D	269	VAL	2.0
1	A	276	GLU	2.0
1	C	72	THR	2.0
1	A	235	LEU	2.0
1	B	256	LEU	2.0
1	C	377	LEU	2.0
1	A	2	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DSG	E	3	8/9	0.64	0.19	79,83,84,85	0
2	DSG	G	3	8/9	0.77	0.17	72,76,84,84	0
2	DSG	F	3	8/9	0.78	0.12	101,103,107,114	0
2	DBB	E	2	6/7	0.79	0.16	86,88,90,95	0
2	DBB	F	2	6/7	0.81	0.14	120,122,138,150	0
2	MEA	F	5	12/13	0.85	0.19	88,89,94,94	0
2	DSG	H	3	8/9	0.86	0.14	45,50,64,65	0
2	DVA	F	9	7/8	0.87	0.22	93,95,98,98	0
2	DBB	G	2	6/7	0.89	0.12	66,70,71,72	0
2	MEA	E	5	12/13	0.90	0.12	49,54,65,65	0
2	DLE	G	10	9/9	0.90	0.16	56,58,62,62	0
2	DLE	E	10	9/9	0.91	0.16	56,61,73,81	0
2	DLE	F	10	9/9	0.91	0.21	86,94,115,125	0
2	DVA	G	9	7/8	0.91	0.13	63,65,66,67	0
2	MEA	G	5	12/13	0.92	0.13	64,64,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DLE	H	10	9/9	0.92	0.16	47,48,58,60	0
2	DVA	E	9	7/8	0.93	0.12	58,60,63,63	0
2	DVA	H	9	7/8	0.94	0.09	45,45,46,48	0
2	DBB	H	2	6/7	0.95	0.09	42,45,50,58	0
2	MEA	H	5	12/13	0.96	0.07	32,35,39,39	0

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
3	BG9	F	101	14/16	0.86	0.27	98,100,117,117	0
3	BG9	E	101	14/16	0.87	0.25	93,94,95,95	0
3	BG9	G	101	14/16	0.88	0.21	73,79,82,83	0
3	BG9	H	101	14/16	0.93	0.09	38,39,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.