



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2026 – 09:15 AM EDT

PDB ID : 2ZAH / pdb_00002zah
Title : X-ray structure of Melon necrotic spot virus
Authors : Wada, Y.; Tsukihara, T.; Omura, T.
Deposited on : 2007-10-05
Resolution : 2.81 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

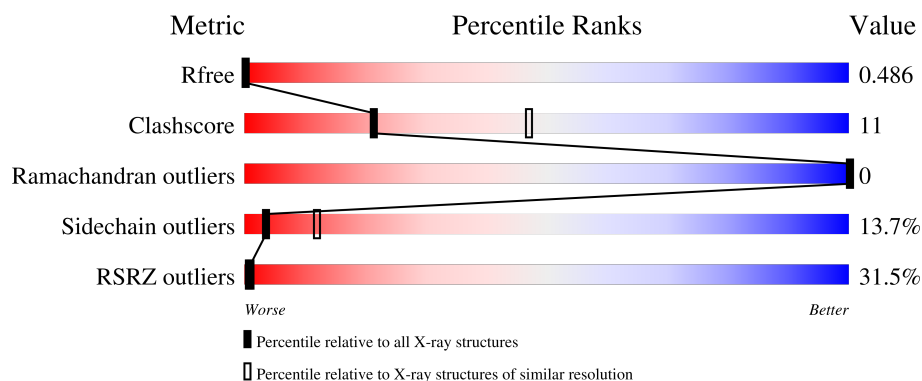
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	28% 70% 14% 5% 11%
1	B	331	27% 65% 20% • 11%
1	C	331	33% 78% 18% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7095 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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2261	1427	385	441	8			
1	B	296	Total	C	N	O	S	0	1	0
			2272	1433	389	442	8			
1	C	331	Total	C	N	O	S	0	0	0
			2518	1587	435	487	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	TYR	SER	SEE REMARK 999	UNP Q3LHM1
B	194	TYR	SER	SEE REMARK 999	UNP Q3LHM1
C	194	TYR	SER	SEE REMARK 999	UNP Q3LHM1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	X	0	0
			1	1		

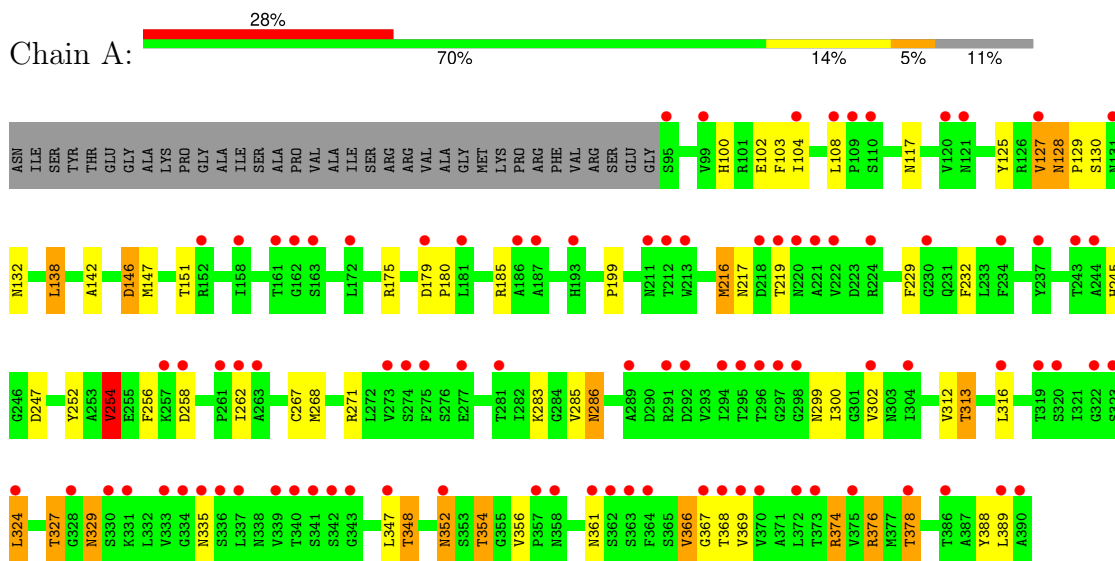
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	15	Total 15	O 15	0	0
4	C	10	Total 10	O 10	0	0

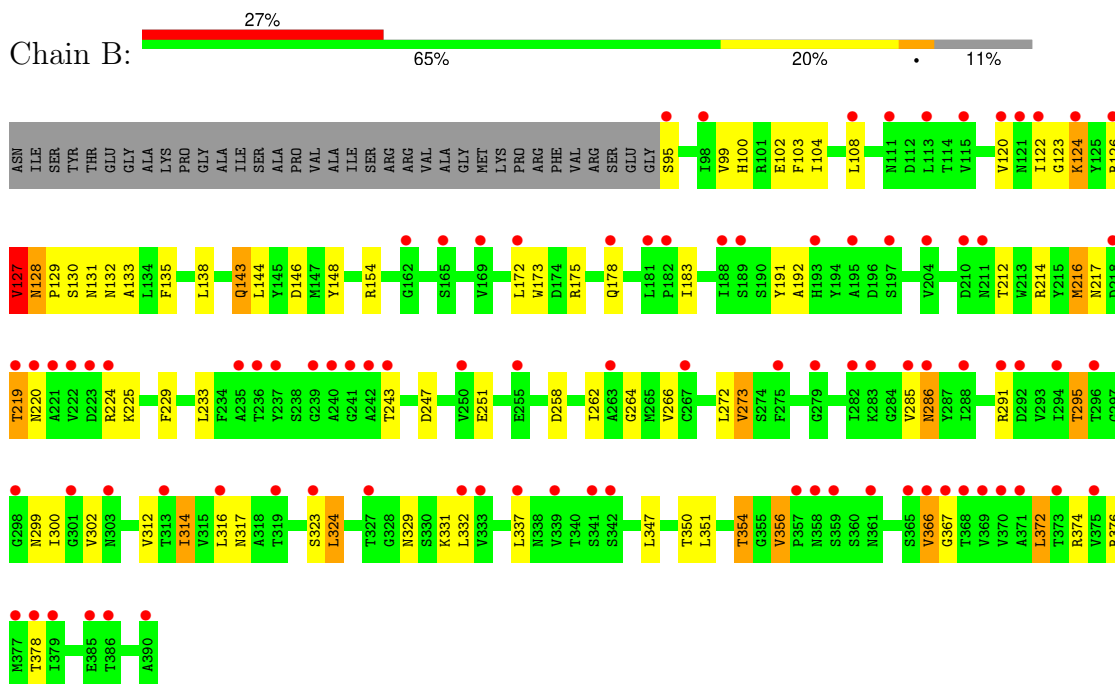
3 Residue-property plots [i](#)

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.

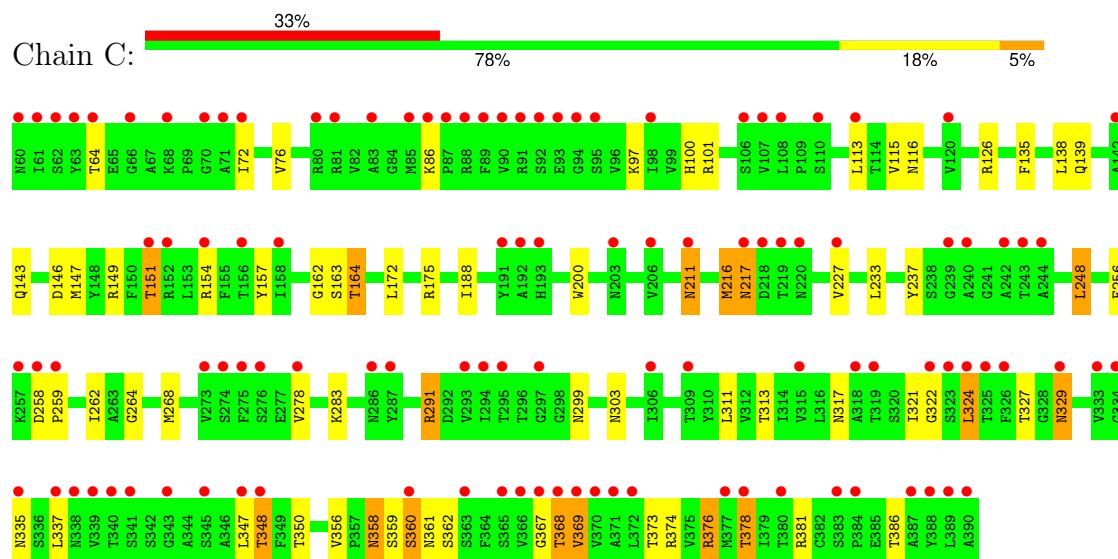
• Molecule 1: Coat protein



• Molecule 1: Coat protein



● Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	375.00Å 375.00Å 375.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	187.50 – 2.81 187.50 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (187.50-2.81) 99.2 (187.50-2.81)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.208 , 0.224 (Not available) , 0.486	Depositor DCC
R_{free} test set	10487 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	7095	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: CA, UNX

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	0.61	0/2309	0.88	3/3155 (0.1%)
1	B	0.63	0/2320	0.87	3/3169 (0.1%)
1	C	0.60	0/2571	0.86	1/3508 (0.0%)
All	All	0.61	0/7200	0.87	7/9832 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ILE	CB-CA-C	-5.53	107.01	111.71
1	B	122	ILE	N-CA-C	5.42	116.19	110.72
1	B	104	ILE	CB-CA-C	-5.24	107.25	111.71
1	A	219	THR	N-CA-C	-5.22	103.83	111.30
1	B	127	VAL	CB-CA-C	5.20	119.81	111.29
1	C	216	MET	N-CA-C	-5.17	102.40	110.10
1	A	254	VAL	CB-CA-C	-5.01	102.67	110.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2261	0	2214	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2272	0	2226	59	0
1	C	2518	0	2482	42	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
4	A	14	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	0	0
All	All	7095	0	6922	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (152) 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:129:PRO:HB2	1:A:216:MET:HE3	1.22	1.09
1:A:313:THR:HB	1:A:348:THR:HG23	1.32	1.07
1:B:354:THR:HG23	1:B:356:VAL:HG13	1.39	1.02
1:A:129:PRO:HB2	1:A:216:MET:CE	1.92	1.00
1:B:144:LEU:HD22	1:B:262:ILE:HG22	1.46	0.95
1:A:142:ALA:HB1	1:A:216:MET:HE2	1.47	0.94
1:A:129:PRO:CB	1:A:216:MET:HE3	1.96	0.93
1:A:313:THR:HG23	1:A:378:THR:HG22	1.51	0.93
1:A:129:PRO:HB3	1:A:138:LEU:HD13	1.54	0.90
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.39	0.87
1:B:329:ASN:HB2	1:B:354:THR:HG22	1.59	0.84
1:A:142:ALA:CB	1:A:216:MET:HE2	2.06	0.83
1:A:128:ASN:HD22	1:A:130:SER:H	1.28	0.81
1:B:354:THR:CG2	1:B:356:VAL:HG13	2.11	0.80
1:A:100:HIS:HD2	1:A:102:GLU:OE1	1.70	0.75
1:A:354:THR:HG22	1:A:356:VAL:H	1.50	0.75
1:B:129:PRO:HG2	1:B:216:MET:HE1	1.71	0.72
1:C:216:MET:HE1	1:C:256:PHE:CD1	2.24	0.71
1:B:100:HIS:HD2	1:B:102:GLU:OE2	1.72	0.71
1:B:128:ASN:HD22	1:B:130:SER:H	1.37	0.71
1:B:354:THR:HG23	1:B:356:VAL:CG1	2.19	0.71
1:A:108:LEU:H	1:A:117:ASN:HD21	1.36	0.70
1:A:128:ASN:ND2	1:A:130:SER:H	1.91	0.69
1:B:178:GLN:HE21	1:B:225:LYS:H	1.41	0.69
1:B:129:PRO:HD2	1:B:216:MET:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:HD2	1:C:211:ASN:HA	1.75	0.67
1:B:295:THR:HG23	1:B:295:THR:O	1.95	0.66
1:A:175:ARG:NH1	1:B:258:ASP:OD1	2.23	0.66
1:B:317:ASN:HD21	1:B:376:ARG:HH21	1.42	0.66
1:A:216:MET:HE1	1:A:256:PHE:CZ	2.31	0.66
1:A:376:ARG:HG3	1:A:376:ARG:NH1	2.05	0.65
1:B:173:TRP:CH2	1:B:175:ARG:HB3	2.32	0.65
1:A:132:ASN:H	1:A:286:ASN:HD21	1.44	0.64
1:B:143:GLN:HE21	1:B:264:GLY:H	1.46	0.64
1:C:358:ASN:ND2	1:C:360:SER:H	1.95	0.63
1:B:175:ARG:NH1	1:C:258:ASP:OD2	2.27	0.63
1:A:129:PRO:CG	1:A:216:MET:HE3	2.28	0.63
1:C:139:GLN:NE2	1:C:381:ARG:HH21	1.96	0.63
1:A:300:ILE:HB	1:A:366:VAL:HG13	1.82	0.62
1:C:217:ASN:HB3	1:C:227:VAL:HG21	1.81	0.61
1:B:295:THR:O	1:B:295:THR:CG2	2.48	0.61
1:A:313:THR:HG23	1:A:378:THR:CG2	2.28	0.61
1:B:129:PRO:CG	1:B:216:MET:HE1	2.30	0.60
1:C:143:GLN:HE22	1:C:264:GLY:H	1.49	0.60
1:A:286:ASN:HD22	1:A:286:ASN:H	1.50	0.60
1:A:127:VAL:HG13	1:A:229:PHE:O	2.02	0.59
1:C:163:SER:HA	1:C:200:TRP:CG	2.37	0.59
1:C:358:ASN:HD22	1:C:360:SER:H	1.49	0.59
1:B:314:ILE:CD1	1:B:347:LEU:HB2	2.33	0.59
1:B:216:MET:HE3	1:B:216:MET:HA	1.85	0.58
1:A:313:THR:CB	1:A:348:THR:HG23	2.21	0.58
1:C:329:ASN:C	1:C:329:ASN:HD22	2.11	0.58
1:C:374:ARG:HG2	1:C:376:ARG:HD2	1.85	0.57
1:B:178:GLN:NE2	1:B:225:LYS:H	2.03	0.57
1:B:123:GLY:HA3	1:B:126[B]:ARG:CZ	2.35	0.56
1:B:127:VAL:HG22	1:B:229:PHE:HB3	1.87	0.56
1:B:132:ASN:H	1:B:286:ASN:HD21	1.53	0.56
1:A:376:ARG:HH11	1:A:376:ARG:CG	2.13	0.56
1:B:103:PHE:HE1	1:B:247:ASP:HB3	1.70	0.56
1:B:300:ILE:HB	1:B:366:VAL:HG13	1.87	0.56
1:B:103:PHE:CE1	1:B:247:ASP:HB3	2.40	0.56
1:A:327:THR:HG22	1:A:361:ASN:HB3	1.88	0.56
1:B:286:ASN:HD22	1:B:286:ASN:N	2.04	0.55
1:B:286:ASN:HD22	1:B:286:ASN:H	1.54	0.55
1:A:352:ASN:C	1:A:352:ASN:HD22	2.13	0.55
1:C:358:ASN:HD22	1:C:358:ASN:C	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:HB3	1:B:138:LEU:HB3	1.89	0.54
1:A:352:ASN:C	1:A:352:ASN:ND2	2.66	0.53
1:C:317:ASN:HD21	1:C:376:ARG:NH1	2.06	0.53
1:A:327:THR:CG2	1:A:361:ASN:OD1	2.56	0.53
1:C:188:ILE:HD11	1:C:237:TYR:HE1	1.74	0.53
1:C:317:ASN:HD22	1:C:374:ARG:HB3	1.73	0.53
1:C:317:ASN:HD21	1:C:376:ARG:HH11	1.56	0.52
1:A:147:MET:HE2	1:C:175:ARG:HD3	1.92	0.52
1:C:313:THR:OG1	1:C:348:THR:HG23	2.09	0.52
1:A:252:TYR:CD1	1:A:254:VAL:HG22	2.44	0.52
1:C:324:LEU:HG	1:C:347:LEU:HD13	1.91	0.52
1:A:252:TYR:HD1	1:A:254:VAL:HG22	1.75	0.51
1:A:329:ASN:C	1:A:329:ASN:HD22	2.18	0.51
1:C:100:HIS:CG	1:C:101:ARG:H	2.29	0.51
1:C:216:MET:HE1	1:C:256:PHE:HD1	1.74	0.51
1:A:108:LEU:H	1:A:117:ASN:ND2	2.08	0.50
1:B:314:ILE:HD12	1:B:347:LEU:HB2	1.93	0.50
1:A:327:THR:HG23	1:A:361:ASN:OD1	2.12	0.50
1:C:322:GLY:HA3	1:C:368:THR:HG23	1.93	0.50
1:B:148:TYR:CD2	1:B:216:MET:HE3	2.47	0.49
1:C:313:THR:HB	1:C:378:THR:HG22	1.93	0.49
1:A:146:ASP:OD2	1:A:217:ASN:ND2	2.46	0.49
1:A:267:CYS:HB2	1:A:285:VAL:O	2.11	0.49
1:A:216:MET:HE1	1:A:256:PHE:CE1	2.47	0.49
1:C:299:ASN:HD22	1:C:367:GLY:HA2	1.77	0.49
1:C:358:ASN:ND2	1:C:361:ASN:H	2.11	0.49
1:A:299:ASN:HD22	1:A:367:GLY:HA2	1.78	0.49
1:A:348:THR:HB	1:A:388:TYR:CE2	2.47	0.49
1:B:175:ARG:HD3	1:C:147:MET:SD	2.53	0.49
1:B:129:PRO:HB2	1:B:216:MET:HE2	1.94	0.48
1:B:299:ASN:HD22	1:B:367:GLY:HA2	1.77	0.48
1:A:100:HIS:CD2	1:A:102:GLU:OE1	2.59	0.48
1:B:123:GLY:O	1:B:124:LYS:C	2.57	0.48
1:B:286:ASN:H	1:B:286:ASN:ND2	2.11	0.48
1:B:131:ASN:HD21	1:B:133:ALA:HB3	1.78	0.48
1:C:268:MET:C	1:C:268:MET:SD	2.97	0.48
1:B:324:LEU:HG	1:B:347:LEU:HD22	1.95	0.48
1:A:138:LEU:HG	1:A:252:TYR:OH	2.14	0.47
1:C:216:MET:HE1	1:C:256:PHE:CE1	2.48	0.47
1:C:329:ASN:C	1:C:329:ASN:ND2	2.72	0.47
1:B:128:ASN:ND2	1:B:130:SER:H	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLN:HE21	1:C:381:ARG:HH21	1.61	0.45
1:A:125:TYR:HB2	1:A:232:PHE:O	2.16	0.45
1:A:271:ARG:O	1:A:374:ARG:HG2	2.16	0.45
1:B:143:GLN:NE2	1:B:264:GLY:H	2.13	0.45
1:B:172:LEU:HD22	1:B:233:LEU:HD13	1.98	0.45
1:B:219:THR:HA	1:B:224:ARG:HH22	1.81	0.45
1:B:128:ASN:HD22	1:B:128:ASN:C	2.24	0.45
1:A:299:ASN:ND2	1:A:367:GLY:HA2	2.32	0.45
1:B:323:SER:O	1:B:366:VAL:HA	2.18	0.44
1:A:324:LEU:HG	1:A:347:LEU:HD13	1.98	0.44
1:C:116:ASN:HD21	1:C:233:LEU:HA	1.83	0.44
1:A:348:THR:HG21	1:A:388:TYR:OH	2.18	0.44
1:B:262:ILE:O	1:B:262:ILE:HG13	2.17	0.44
1:C:321:ILE:HG22	1:C:369:VAL:HB	2.00	0.44
1:A:128:ASN:HD22	1:A:128:ASN:C	2.26	0.44
1:B:172:LEU:HD21	1:B:191:TYR:CG	2.53	0.44
1:A:354:THR:HG23	1:A:356:VAL:HG23	1.99	0.43
1:A:129:PRO:CB	1:A:216:MET:CE	2.74	0.43
1:C:135:PHE:HB3	1:C:138:LEU:HB3	1.99	0.43
1:A:146:ASP:HB2	1:A:258:ASP:HB2	2.00	0.43
1:A:262:ILE:O	1:A:262:ILE:HG13	2.18	0.43
1:B:314:ILE:HD13	1:B:347:LEU:HD13	2.00	0.43
1:B:273:VAL:HG11	1:B:372:LEU:HD13	1.99	0.43
1:A:175:ARG:HD2	1:B:258:ASP:OD1	2.19	0.43
1:B:100:HIS:CD2	1:B:102:GLU:OE2	2.63	0.42
1:B:129:PRO:HB2	1:B:216:MET:CE	2.49	0.42
1:C:143:GLN:NE2	1:C:264:GLY:H	2.13	0.42
1:C:97:LYS:NZ	1:C:151:THR:HG21	2.34	0.42
1:C:317:ASN:HB2	1:C:374:ARG:HB3	2.02	0.42
1:A:129:PRO:HG2	1:A:216:MET:HE3	2.02	0.42
1:B:129:PRO:HD2	1:B:216:MET:HE2	2.01	0.42
1:C:162:GLY:C	1:C:164:THR:H	2.28	0.42
1:C:157:TYR:HD1	1:C:248:LEU:HD13	1.85	0.42
1:B:129:PRO:CD	1:B:216:MET:CE	2.94	0.41
1:B:129:PRO:CG	1:B:216:MET:CE	2.97	0.41
1:A:199:PRO:HB3	1:A:245:HIS:CG	2.55	0.41
1:B:217:ASN:ND2	1:B:219:THR:H	2.19	0.41
1:C:291:ARG:C	1:C:291:ARG:HD3	2.44	0.41
1:A:103:PHE:CE1	1:A:247:ASP:HB3	2.56	0.41
1:A:179:ASP:HA	1:A:180:PRO:HD3	1.93	0.41
1:B:192:ALA:HB2	1:C:259:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:THR:HA	1:B:224:ARG:NH2	2.36	0.40
1:C:303:ASN:ND2	1:C:362:SER:HA	2.36	0.40
1:C:358:ASN:HD22	1:C:360:SER:N	2.17	0.40
1:B:131:ASN:C	1:B:131:ASN:ND2	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/331 (89%)	286 (97%)	8 (3%)	0	100	100
1	B	295/331 (89%)	284 (96%)	11 (4%)	0	100	100
1	C	329/331 (99%)	320 (97%)	9 (3%)	0	100	100
All	All	918/993 (92%)	890 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/277 (91%)	222 (88%)	29 (12%)	5	17
1	B	252/277 (91%)	211 (84%)	41 (16%)	2	8
1	C	277/277 (100%)	240 (87%)	37 (13%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	780/831 (94%)	673 (86%)	107 (14%)	3 12

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
1	A	128	ASN
1	A	138	LEU
1	A	146	ASP
1	A	151	THR
1	A	185	ARG
1	A	216	MET
1	A	254	VAL
1	A	268	MET
1	A	283	LYS
1	A	286	ASN
1	A	302	VAL
1	A	312	VAL
1	A	313	THR
1	A	316	LEU
1	A	324	LEU
1	A	327	THR
1	A	329	ASN
1	A	335	ASN
1	A	348	THR
1	A	352	ASN
1	A	354	THR
1	A	366	VAL
1	A	368	THR
1	A	369	VAL
1	A	374	ARG
1	A	376	ARG
1	A	378	THR
1	A	389	LEU
1	B	95	SER
1	B	99	VAL
1	B	108	LEU
1	B	120	VAL
1	B	124	LYS
1	B	127	VAL
1	B	128	ASN
1	B	143	GLN

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Mol	Chain	Res	Type
1	B	146	ASP
1	B	154	ARG
1	B	183	ILE
1	B	212	THR
1	B	214	ARG
1	B	216	MET
1	B	219	THR
1	B	220	ASN
1	B	243	THR
1	B	251	GLU
1	B	266	VAL
1	B	272	LEU
1	B	273	VAL
1	B	285	VAL
1	B	286	ASN
1	B	291	ARG
1	B	295	THR
1	B	302	VAL
1	B	312	VAL
1	B	314	ILE
1	B	316	LEU
1	B	324	LEU
1	B	331	LYS
1	B	332	LEU
1	B	337	LEU
1	B	350	THR
1	B	351	LEU
1	B	354	THR
1	B	356	VAL
1	B	366	VAL
1	B	372	LEU
1	B	374	ARG
1	B	378	THR
1	C	64	THR
1	C	72	ILE
1	C	76	VAL
1	C	86	LYS
1	C	113	LEU
1	C	115	VAL
1	C	126	ARG
1	C	146	ASP
1	C	151	THR

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Mol	Chain	Res	Type
1	C	154	ARG
1	C	164	THR
1	C	172	LEU
1	C	211	ASN
1	C	217	ASN
1	C	248	LEU
1	C	262	ILE
1	C	278	VAL
1	C	283	LYS
1	C	291	ARG
1	C	311	LEU
1	C	324	LEU
1	C	327	THR
1	C	329	ASN
1	C	335	ASN
1	C	337	LEU
1	C	348	THR
1	C	350	THR
1	C	356	VAL
1	C	358	ASN
1	C	359	SER
1	C	360	SER
1	C	368	THR
1	C	369	VAL
1	C	373	THR
1	C	376	ARG
1	C	378	THR
1	C	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	117	ASN
1	A	121	ASN
1	A	128	ASN
1	A	286	ASN
1	A	299	ASN
1	A	329	ASN
1	A	352	ASN
1	B	100	HIS
1	B	111	ASN

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Mol	Chain	Res	Type
1	B	128	ASN
1	B	131	ASN
1	B	143	GLN
1	B	178	GLN
1	B	217	ASN
1	B	231	GLN
1	B	286	ASN
1	B	299	ASN
1	B	305	ASN
1	B	317	ASN
1	B	338	ASN
1	B	361	ASN
1	C	116	ASN
1	C	121	ASN
1	C	139	GLN
1	C	143	GLN
1	C	217	ASN
1	C	299	ASN
1	C	303	ASN
1	C	305	ASN
1	C	317	ASN
1	C	329	ASN
1	C	352	ASN
1	C	358	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic and 1 is unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/331 (89%)	1.65	93 (31%)  	22, 31, 42, 49	0
1	B	296/331 (89%)	1.60	89 (30%)  	13, 32, 43, 49	1 (0%)
1	C	331/331 (100%)	1.68	109 (32%)  	24, 32, 45, 60	0
All	All	923/993 (92%)	1.64	291 (31%)  	13, 32, 43, 60	1 (0%)

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ASN	9.3
1	A	323	SER	6.4
1	C	91	ARG	5.7
1	C	390	ALA	4.8
1	A	342	SER	4.7
1	A	339	VAL	4.6
1	C	309	THR	4.6
1	C	383	SER	4.5
1	C	95	SER	4.5
1	A	219	THR	4.4
1	C	70	GLY	4.4
1	B	385	GLU	4.3
1	C	62	SER	4.2
1	B	241	GLY	4.1
1	C	88	ARG	4.1
1	C	322	GLY	4.0
1	C	90	VAL	4.0
1	C	66	GLY	4.0
1	C	191	TYR	4.0
1	C	92	SER	3.9
1	C	324	LEU	3.8
1	B	319	THR	3.8
1	C	218	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	331	LYS	3.7
1	C	369	VAL	3.6
1	C	85	MET	3.6
1	A	162	GLY	3.6
1	A	369	VAL	3.5
1	A	370	VAL	3.5
1	A	108	LEU	3.5
1	C	337	LEU	3.5
1	B	370	VAL	3.5
1	C	203	ASN	3.5
1	C	61	ILE	3.5
1	A	375	VAL	3.5
1	A	320	SER	3.5
1	B	369	VAL	3.4
1	B	371	ALA	3.4
1	A	221	ALA	3.4
1	C	295	THR	3.4
1	A	275	PHE	3.3
1	A	364	PHE	3.3
1	A	368	THR	3.3
1	C	120	VAL	3.3
1	B	390	ALA	3.3
1	A	373	THR	3.3
1	B	358	ASN	3.2
1	A	99	VAL	3.2
1	A	357	PRO	3.2
1	A	218	ASP	3.2
1	A	95	SER	3.1
1	B	236	THR	3.1
1	B	282	ILE	3.1
1	B	275	PHE	3.1
1	B	283	LYS	3.1
1	B	240	ALA	3.0
1	A	274	SER	3.0
1	C	93	GLU	3.0
1	A	110	SER	3.0
1	A	335	ASN	3.0
1	B	368	THR	3.0
1	B	378	THR	3.0
1	B	122	ILE	3.0
1	C	72	ILE	3.0
1	C	81	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	340	THR	3.0
1	C	318	ALA	2.9
1	C	275	PHE	2.9
1	A	262	ILE	2.9
1	A	390	ALA	2.9
1	B	294	ILE	2.9
1	B	255	GLU	2.9
1	C	341	SER	2.9
1	B	120	VAL	2.9
1	C	319	THR	2.9
1	A	244	ALA	2.9
1	B	189	SER	2.9
1	C	89	PHE	2.9
1	A	243	THR	2.9
1	A	347	LEU	2.9
1	B	357	PRO	2.8
1	A	358	ASN	2.8
1	B	242	ALA	2.8
1	A	158	ILE	2.8
1	A	294	ILE	2.8
1	A	328	GLY	2.8
1	C	87	PRO	2.8
1	B	286	ASN	2.8
1	C	329	ASN	2.8
1	C	68	LYS	2.8
1	C	387	ALA	2.8
1	C	158	ILE	2.8
1	B	220	ASN	2.8
1	B	224	ARG	2.8
1	A	121	ASN	2.8
1	A	319	THR	2.8
1	B	296	THR	2.8
1	C	345	SER	2.8
1	A	273	VAL	2.7
1	B	333	VAL	2.7
1	A	161	THR	2.7
1	B	219	THR	2.7
1	B	218	ASP	2.7
1	B	108	LEU	2.7
1	C	388	TYR	2.7
1	A	152	ARG	2.7
1	A	322	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.7
1	C	60	ASN	2.7
1	C	325	THR	2.7
1	A	304	ILE	2.6
1	A	337	LEU	2.7
1	B	95	SER	2.7
1	C	211	ASN	2.6
1	A	127	VAL	2.6
1	A	291	ARG	2.6
1	C	219	THR	2.6
1	C	380	THR	2.6
1	B	366	VAL	2.6
1	C	220	ASN	2.6
1	B	292	ASP	2.6
1	C	367	GLY	2.6
1	A	340	THR	2.6
1	C	378	THR	2.6
1	C	338	ASN	2.6
1	C	326	PHE	2.6
1	C	315	VAL	2.6
1	C	348	THR	2.6
1	C	242	ALA	2.6
1	A	213	TRP	2.5
1	B	182	PRO	2.5
1	C	108	LEU	2.5
1	C	297	GLY	2.5
1	B	373	THR	2.5
1	B	263	ALA	2.5
1	C	240	ALA	2.5
1	B	126[A]	ARG	2.5
1	A	336	SER	2.5
1	C	86	LYS	2.5
1	A	104	ILE	2.5
1	B	221	ALA	2.5
1	B	121	ASN	2.5
1	C	286	ASN	2.5
1	C	389	LEU	2.5
1	B	162	GLY	2.5
1	C	94	GLY	2.5
1	C	156	THR	2.5
1	A	131	ASN	2.5
1	B	181	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	197	SER	2.5
1	C	259	PRO	2.5
1	B	285	VAL	2.5
1	C	370	VAL	2.5
1	A	289	ALA	2.5
1	A	295	THR	2.5
1	B	316	LEU	2.4
1	C	347	LEU	2.4
1	B	367	GLY	2.4
1	C	142	ALA	2.4
1	B	115	VAL	2.4
1	A	330	SER	2.4
1	A	341	SER	2.4
1	C	335	ASN	2.4
1	A	224	ARG	2.4
1	C	368	THR	2.4
1	A	361	ASN	2.4
1	C	333	VAL	2.4
1	B	267	CYS	2.4
1	C	154	ARG	2.4
1	B	235	ALA	2.4
1	B	178	GLN	2.4
1	B	386	THR	2.4
1	B	111	ASN	2.3
1	C	217	ASN	2.3
1	C	278	VAL	2.3
1	C	339	VAL	2.3
1	B	298	GLY	2.3
1	A	292	ASP	2.3
1	C	244	ALA	2.3
1	C	227	VAL	2.3
1	A	230	GLY	2.3
1	B	211	ASN	2.3
1	B	332	LEU	2.3
1	C	106	SER	2.3
1	B	313	THR	2.3
1	C	64	THR	2.3
1	C	294	ILE	2.3
1	A	222	VAL	2.3
1	C	206	VAL	2.3
1	B	239	GLY	2.3
1	A	211	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	ASP	2.3
1	B	172	LEU	2.3
1	A	257	LYS	2.3
1	B	288	ILE	2.3
1	B	323	SER	2.3
1	C	98	ILE	2.3
1	C	63	TYR	2.3
1	A	186	ALA	2.3
1	C	83	ALA	2.3
1	C	113	LEU	2.3
1	A	193	HIS	2.3
1	A	386	THR	2.3
1	C	80	ARG	2.3
1	C	110	SER	2.3
1	C	107	VAL	2.3
1	A	298	GLY	2.3
1	A	343	GLY	2.3
1	B	113	LEU	2.2
1	A	212	THR	2.2
1	C	274	SER	2.2
1	C	323	SER	2.2
1	C	258	ASP	2.2
1	B	243	THR	2.2
1	B	250	VAL	2.2
1	A	363	SER	2.2
1	C	239	GLY	2.2
1	C	377	MET	2.2
1	A	302	VAL	2.2
1	B	341	SER	2.2
1	C	343	GLY	2.2
1	A	372	LEU	2.2
1	C	372	LEU	2.2
1	C	371	ALA	2.2
1	B	303	ASN	2.2
1	A	120	VAL	2.2
1	B	223	ASP	2.2
1	B	339	VAL	2.2
1	C	151	THR	2.2
1	B	124	LYS	2.2
1	A	234	PHE	2.2
1	A	362	SER	2.2
1	B	193	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	361	ASN	2.1
1	C	193	HIS	2.1
1	C	293	VAL	2.1
1	A	367	GLY	2.1
1	B	279	GLY	2.1
1	B	337	LEU	2.1
1	A	237	TYR	2.1
1	B	195	ALA	2.1
1	B	359	SER	2.1
1	B	291	ARG	2.1
1	A	109	PRO	2.1
1	B	210	ASP	2.1
1	A	172	LEU	2.1
1	A	263	ALA	2.1
1	C	71	ALA	2.1
1	C	287	TYR	2.1
1	A	277	GLU	2.1
1	B	98	ILE	2.1
1	B	365	SER	2.1
1	C	365	SER	2.1
1	A	333	VAL	2.1
1	A	352	ASN	2.1
1	B	204	VAL	2.1
1	B	222	VAL	2.1
1	B	377	MET	2.1
1	C	273	VAL	2.1
1	C	366	VAL	2.1
1	A	389	LEU	2.1
1	C	334	GLY	2.1
1	B	327	THR	2.1
1	B	188	ILE	2.1
1	A	163	SER	2.1
1	C	360	SER	2.1
1	C	363	SER	2.1
1	A	324	LEU	2.1
1	B	301	GLY	2.1
1	C	152	ARG	2.1
1	A	187	ALA	2.1
1	B	379	ILE	2.1
1	B	237	TYR	2.1
1	B	165	SER	2.0
1	B	342	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	257	LYS	2.0
1	C	276	SER	2.0
1	A	261	PRO	2.0
1	C	384	PRO	2.0
1	A	181	LEU	2.0
1	A	281	THR	2.0
1	A	296	THR	2.0
1	A	179	ASP	2.0
1	B	375	VAL	2.0
1	A	316	LEU	2.0
1	A	297	GLY	2.0
1	A	334	GLY	2.0
1	C	306	ILE	2.0
1	A	378	THR	2.0
1	C	192	ALA	2.0
1	C	243	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	A	1	1/1	0.21	1.16	48,48,48,48	1
2	CA	A	4	1/1	0.80	0.23	43,43,43,43	1
2	CA	B	2	1/1	0.86	0.12	49,49,49,49	0
2	CA	B	1	1/1	0.88	0.17	42,42,42,42	1
2	CA	B	3	1/1	0.94	0.08	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.