Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 08:46 AM EDT

PDB ID	:	2ZAH
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 (i) symbol.

The types of validation reports are described at
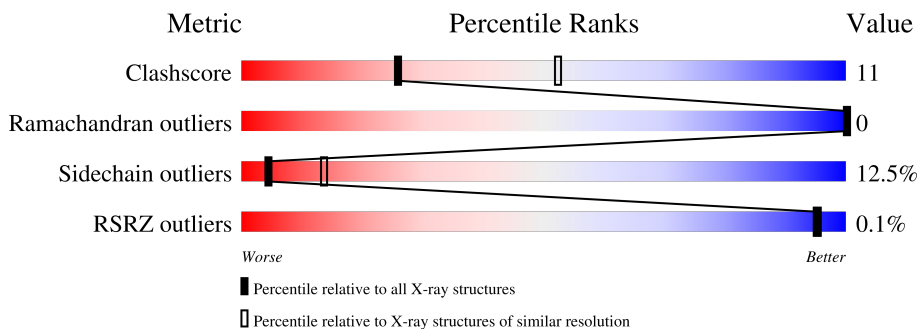http://www.wwpdb.org/validation/2017/FAQs#types.

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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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		12.5%
RSRZ outliers		0.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 <=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	70% 13% 6% 11%
1	B	331	67% 18% 5% 11%
1	C	331	81% 15% 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 (three-letter code: 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 (three-letter code: 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 ⓘ

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.
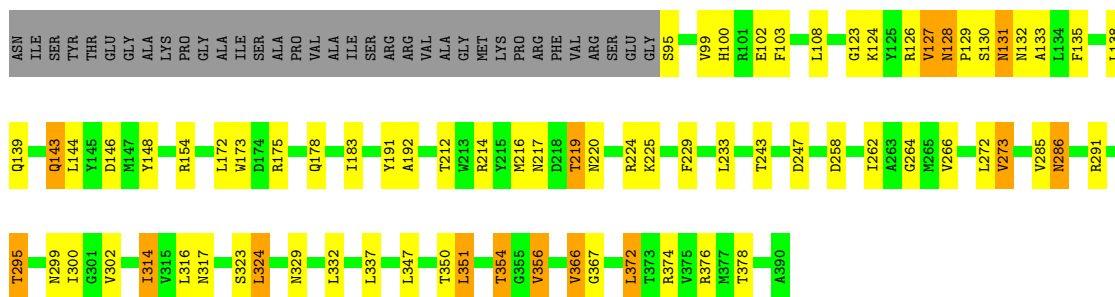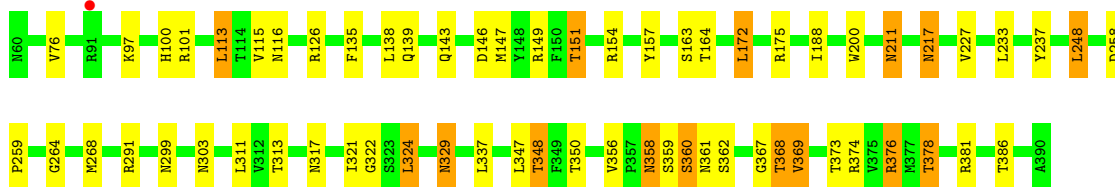
- Molecule 1: Coat protein

Chain A:
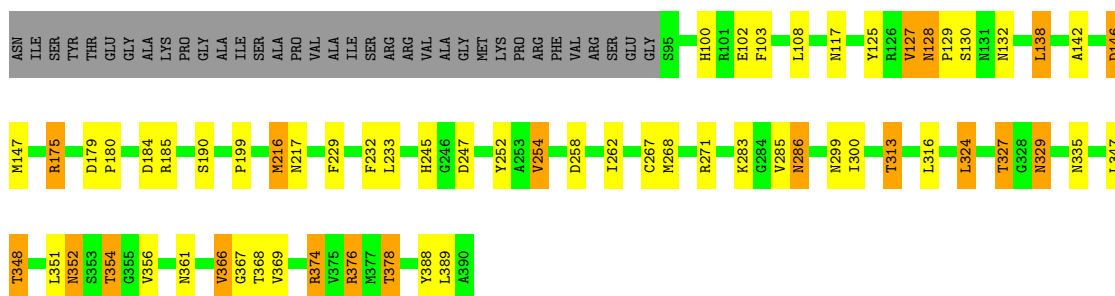
- Molecule 1: Coat protein

Chain B:

- Molecule 1: Coat protein

Chain C:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.34 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.3.0022	Depositor
R, R_{free}	0.208 , 0.224 (Not available) , (Not available)	Depositor DCC
R_{free} test set	10487 reflections (5.03%)	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)	0.32 , 17.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.89	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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UNX, CA

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	0.50	0/2309	0.65	0/3155
1	B	0.50	0/2320	0.67	1/3169 (0.0%)
1	C	0.49	0/2571	0.65	2/3508 (0.1%)
All	All	0.49	0/7200	0.66	3/9832 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	113	LEU	CA-CB-CG	6.50	130.25	115.30
1	B	351	LEU	CA-CB-CG	5.32	127.53	115.30
1	C	172	LEU	CA-CB-CG	5.20	127.25	115.30

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	2261	0	2214	58	0
1	B	2272	0	2226	58	0
1	C	2518	0	2482	37	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	147	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 (147) 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: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:A:129:PRO:HB2	1:A:216:MET:HE2	1.43	0.97
1:B:144:LEU:HD22	1:B:262:ILE:HG22	1.46	0.95
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: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:B:129:PRO:HG2	1:B:216:MET:HE1	1.67	0.76
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: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
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:B:129:PRO:CG	1:B:216:MET:HE1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:129:PRO:HB2	1:A:216:MET:HE3	1.78	0.61
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:C:143:GLN:HE22	1:C:264:GLY:H	1.49	0.60
1:A:129:PRO:HG2	1:A:216:MET:HE3	1.83	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:A:129:PRO:CB	1:A:216:MET:CE	2.74	0.58
1:A:129:PRO:CB	1:A:216:MET:HE3	2.32	0.58
1:A:313:THR:CB	1:A:348:THR:HG23	2.21	0.58
1:A:142:ALA:CB	1:A:216:MET:HE1	2.34	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:B:148:TYR:CD2	1:B:216:MET:HE3	2.42	0.55
1:B:135:PHE:HB3	1:B:138:LEU:HB3	1.89	0.54
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:329:ASN:C	1:C:329:ASN:HD22	2.11	0.53
1:C:317:ASN:HD21	1:C:376:ARG:HH11	1.56	0.52
1:C:313:THR:OG1	1:C:348:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TYR:CD1	1:A:254:VAL:HG22	2.44	0.52
1:B:216:MET:HE3	1:B:216:MET:HA	1.90	0.52
1:C:324:LEU:HG	1:C:347:LEU:HD13	1.91	0.52
1:A:147:MET:HE2	1:C:175:ARG:HD3	1.92	0.52
1:A:252:TYR:HD1	1:A:254:VAL:HG22	1.75	0.51
1:A:142:ALA:HB1	1:A:216:MET:CE	2.41	0.51
1:C:100:HIS:CG	1:C:101:ARG:H	2.29	0.51
1:A:129:PRO:CG	1:A:216:MET:HE3	2.41	0.50
1:A:352:ASN:C	1:A:352:ASN:HD22	2.13	0.50
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:C:358:ASN:HD22	1:C:358:ASN:C	2.15	0.50
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: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:A:352:ASN:C	1:A:352:ASN:ND2	2.66	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: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: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:A:329:ASN:C	1:A:329:ASN:HD22	2.18	0.46
1:B:128:ASN:ND2	1:B:130:SER:H	2.08	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:123:GLY:O	1:B:124:LYS:C	2.57	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:A:142:ALA:CB	1:A:216:MET:CE	2.96	0.43
1:B:314:ILE:HD13	1:B:347:LEU:HD13	2.00	0.43
1:C:268:MET:C	1:C:268:MET:SD	2.97	0.43
1:B:273:VAL:HG11	1:B:372:LEU:HD13	1.99	0.43
1:C:329:ASN:C	1:C:329:ASN:ND2	2.72	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: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:HB2	1:B:216:MET:HE2	2.01	0.41
1:A:199:PRO:HB3	1:A:245:HIS:CG	2.55	0.41
1:B:129:PRO:CG	1:B:216:MET:CE	2.97	0.41
1:B:217:ASN:ND2	1:B:219:THR:H	2.19	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:A:142:ALA:HB1	1:A:216:MET:HE2	2.03	0.41
1:B:129:PRO:CD	1:B:216:MET:HE1	2.51	0.41
1:B:192:ALA:HB2	1:C:259:PRO:HD2	2.03	0.40
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:A:142:ALA:HB1	1:A:216:MET:HE1	2.01	0.40
1:C:358:ASN:HD22	1:C:360:SER:N	2.17	0.40
1:B:128:ASN:HD22	1:B:128:ASN:C	2.24	0.40

There are no symmetry-related clashes.

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	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 ⓘ

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%)	220 (88%)	31 (12%)	4	14
1	B	252/277 (91%)	215 (85%)	37 (15%)	3	9
1	C	277/277 (100%)	248 (90%)	29 (10%)	7	20
All	All	780/831 (94%)	683 (88%)	97 (12%)	4	14

All (97) 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	175	ARG

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Mol	Chain	Res	Type
1	A	184	ASP
1	A	185	ARG
1	A	190	SER
1	A	216	MET
1	A	233	LEU
1	A	254	VAL
1	A	268	MET
1	A	283	LYS
1	A	286	ASN
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	351	LEU
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	127	VAL
1	B	128	ASN
1	B	131	ASN
1	B	139	GLN
1	B	143	GLN
1	B	146	ASP
1	B	154	ARG
1	B	183	ILE
1	B	212	THR
1	B	214	ARG
1	B	219	THR
1	B	220	ASN
1	B	243	THR

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Mol	Chain	Res	Type
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	314	ILE
1	B	316	LEU
1	B	324	LEU
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	76	VAL
1	C	113	LEU
1	C	115	VAL
1	C	126	ARG
1	C	146	ASP
1	C	151	THR
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	291	ARG
1	C	311	LEU
1	C	324	LEU
1	C	329	ASN
1	C	337	LEU
1	C	348	THR
1	C	350	THR
1	C	356	VAL
1	C	358	ASN

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Mol	Chain	Res	Type
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 (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	117	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	128	ASN
1	B	131	ASN
1	B	139	GLN
1	B	143	GLN
1	B	178	GLN
1	B	217	ASN
1	B	286	ASN
1	B	299	ASN
1	B	305	ASN
1	B	317	ASN
1	B	338	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

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Mol	Chain	Res	Type
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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	296/331 (89%)	0.07	0	100	100	22, 31, 42, 49	0
1	B	296/331 (89%)	0.08	0	100	100	23, 32, 43, 49	0
1	C	331/331 (100%)	0.19	1 (0%)	94	93	24, 32, 45, 60	0
All	All	923/993 (92%)	0.11	1 (0%)	95	95	22, 32, 43, 60	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	ARG	2.4

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 ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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(Å²)	Q<0.9
3	UNX	A	1	1/1	0.78	0.60	48,48,48,48	1
2	CA	B	2	1/1	0.86	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	4	1/1	0.90	0.12	43,43,43,43	1
2	CA	B	1	1/1	0.94	0.11	42,42,42,42	1
2	CA	B	3	1/1	0.97	0.08	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.