



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:09 PM EDT

PDB ID : 4QU4 / pdb_00004qu4
Title : Improved refinement of the Mtr4 apo crystal structure
Authors : Johnson, S.J.; Taylor, L.L.
Deposited on : 2014-07-10
Resolution : 3.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

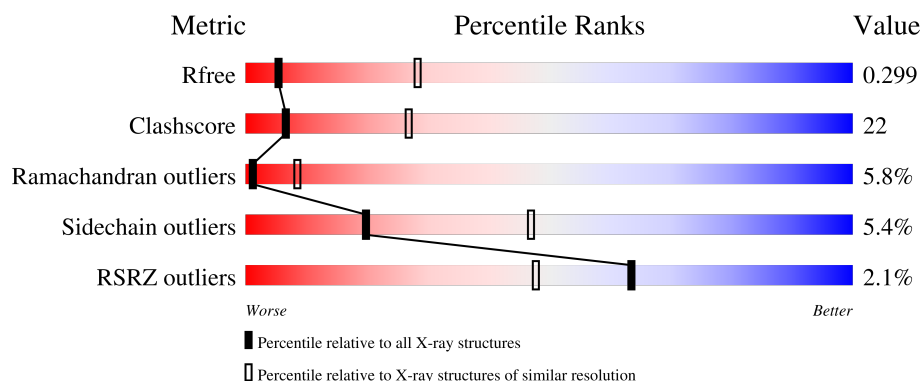
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1108	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6680 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 ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	942	6665	4259	1104	1266	36	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

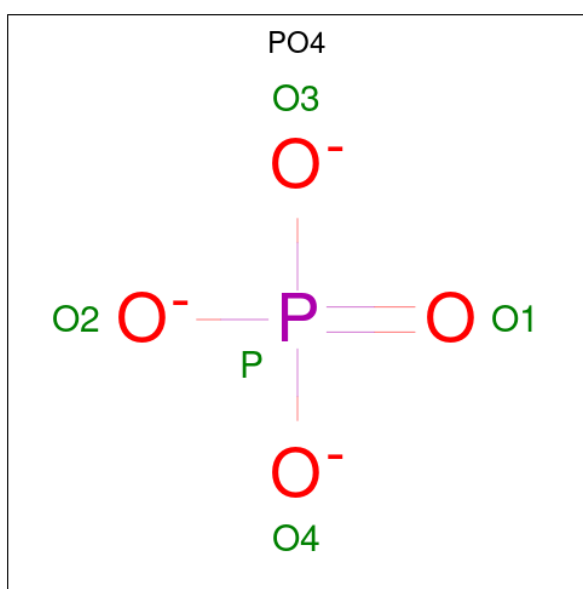
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	expression tag	UNP P47047
A	-33	HIS	-	expression tag	UNP P47047
A	-32	HIS	-	expression tag	UNP P47047
A	-31	HIS	-	expression tag	UNP P47047
A	-30	HIS	-	expression tag	UNP P47047
A	-29	HIS	-	expression tag	UNP P47047
A	-28	HIS	-	expression tag	UNP P47047
A	-27	GLY	-	expression tag	UNP P47047
A	-26	LYS	-	expression tag	UNP P47047
A	-25	PRO	-	expression tag	UNP P47047
A	-24	ILE	-	expression tag	UNP P47047
A	-23	PRO	-	expression tag	UNP P47047
A	-22	ASN	-	expression tag	UNP P47047
A	-21	PRO	-	expression tag	UNP P47047
A	-20	LEU	-	expression tag	UNP P47047
A	-19	LEU	-	expression tag	UNP P47047
A	-18	GLY	-	expression tag	UNP P47047
A	-17	LEU	-	expression tag	UNP P47047
A	-16	ASP	-	expression tag	UNP P47047
A	-15	SER	-	expression tag	UNP P47047
A	-14	THR	-	expression tag	UNP P47047
A	-13	GLU	-	expression tag	UNP P47047
A	-12	ASN	-	expression tag	UNP P47047
A	-11	LEU	-	expression tag	UNP P47047
A	-10	TYR	-	expression tag	UNP P47047
A	-9	PHE	-	expression tag	UNP P47047
A	-8	GLN	-	expression tag	UNP P47047

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P47047
A	-6	ILE	-	expression tag	UNP P47047
A	-5	ASP	-	expression tag	UNP P47047
A	-4	PRO	-	expression tag	UNP P47047
A	-3	PHE	-	expression tag	UNP P47047
A	-2	THR	-	expression tag	UNP P47047
A	-1	GLU	-	expression tag	UNP P47047
A	0	PHE	-	expression tag	UNP P47047

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

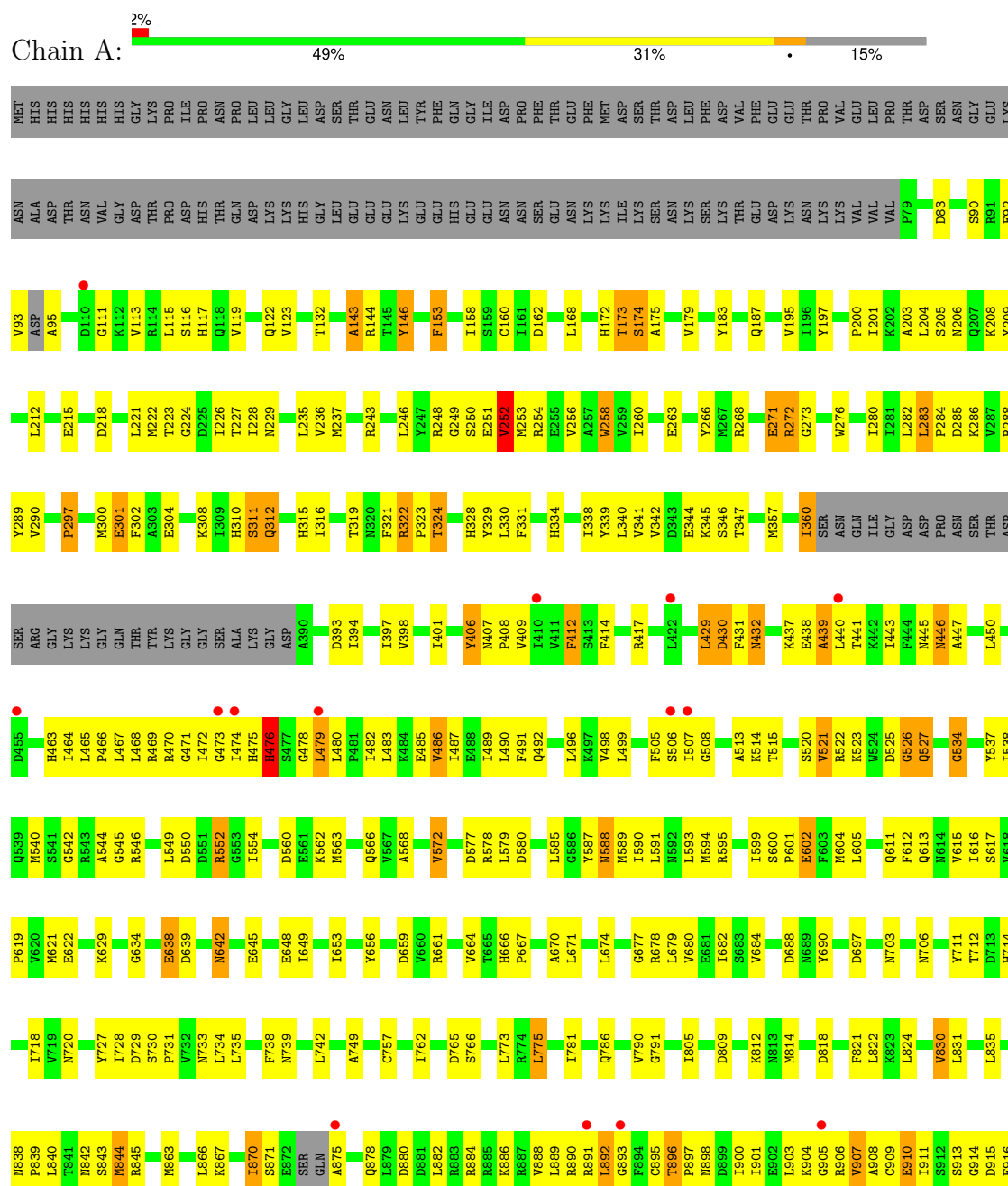


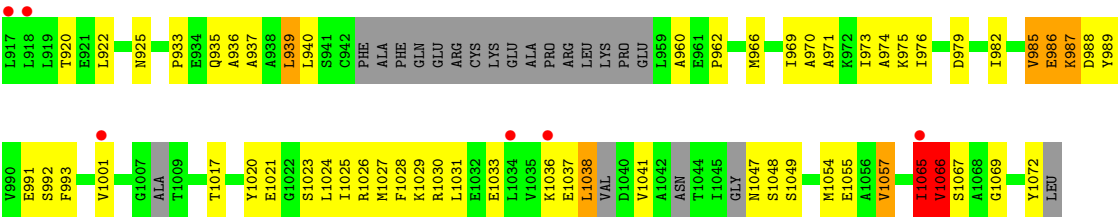
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

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: ATP-dependent RNA helicase DOB1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.52Å 133.52Å 190.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.76 – 3.39 28.76 – 3.39	Depositor EDS
% Data completeness (in resolution range)	93.8 (28.76-3.39) 93.7 (28.76-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.247 , 0.299 0.255 , 0.299	Depositor DCC
R_{free} test set	1270 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 182.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6680	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.67	0/6777	1.09	31/9247 (0.3%)

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
1	A	0	4

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1036	LYS	N-CA-C	8.54	120.58	108.54
1	A	526	GLY	N-CA-C	7.87	127.93	113.76
1	A	409	VAL	N-CA-C	7.17	118.45	108.12
1	A	486	VAL	N-CA-C	-6.95	103.70	110.72
1	A	224	GLY	N-CA-C	-6.39	105.06	112.73
1	A	322	ARG	CA-C-N	6.18	127.56	119.84
1	A	322	ARG	C-N-CA	6.18	127.56	119.84
1	A	666	HIS	CA-C-N	6.09	125.79	119.82
1	A	666	HIS	C-N-CA	6.09	125.79	119.82
1	A	258	TRP	CA-C-N	-6.02	115.72	123.19
1	A	258	TRP	C-N-CA	-6.02	115.72	123.19
1	A	521	VAL	N-CA-C	-6.01	107.43	113.20
1	A	174	SER	N-CA-C	-5.82	106.02	113.01
1	A	312	GLN	N-CA-C	5.76	113.32	108.13
1	A	1055	GLU	N-CA-C	-5.74	105.11	111.71
1	A	111	GLY	N-CA-C	-5.68	107.35	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	VAL	N-CA-C	-5.66	105.21	110.53
1	A	407	ASN	N-CA-C	5.63	120.58	113.25
1	A	132	THR	CA-C-N	5.61	126.85	119.84
1	A	132	THR	C-N-CA	5.61	126.85	119.84
1	A	1028	PHE	N-CA-C	-5.55	105.13	111.07
1	A	324	THR	CA-C-N	5.53	126.75	119.84
1	A	324	THR	C-N-CA	5.53	126.75	119.84
1	A	301	GLU	N-CA-C	-5.43	105.79	112.90
1	A	146	TYR	CA-C-N	5.33	124.51	118.97
1	A	146	TYR	C-N-CA	5.33	124.51	118.97
1	A	256	VAL	N-CA-C	5.32	116.41	108.54
1	A	229	ASN	CA-C-N	5.15	124.84	119.64
1	A	229	ASN	C-N-CA	5.15	124.84	119.64
1	A	534	GLY	N-CA-C	-5.12	106.56	112.50
1	A	412	PHE	N-CA-C	5.01	116.96	109.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	HIS	Peptide
1	A	406	TYR	Peptide
1	A	476	HIS	Peptide
1	A	527	GLN	Peptide

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	6665	0	5969	273	0
2	A	15	0	0	0	0
All	All	6680	0	5969	273	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 22.

All (273) 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:200:PRO:HG3	1:A:276:TRP:HZ2	1.43	0.83
1:A:1027:MET:HA	1:A:1030:ARG:HB3	1.59	0.83
1:A:974:ALA:HB1	1:A:985:VAL:HA	1.60	0.83
1:A:1054:MET:HA	1:A:1057:VAL:HB	1.61	0.81
1:A:986:GLU:O	1:A:988:ASP:N	2.15	0.79
1:A:174:SER:HB3	1:A:323:PRO:HG3	1.65	0.78
1:A:345:LYS:H	1:A:346:SER:HA	1.50	0.76
1:A:580:ASP:HA	1:A:613:GLN:HE22	1.51	0.76
1:A:521:VAL:HG11	1:A:563:MET:HE1	1.68	0.75
1:A:437:LYS:HG3	1:A:469:ARG:HA	1.67	0.75
1:A:513:ALA:HB3	1:A:546:ARG:HG3	1.69	0.73
1:A:645:GLU:O	1:A:649:ILE:HG13	1.89	0.73
1:A:463:HIS:O	1:A:465:LEU:N	2.20	0.72
1:A:414:PHE:HE1	1:A:540:MET:HE1	1.56	0.71
1:A:258:TRP:CZ3	1:A:288:ARG:HB3	2.25	0.71
1:A:513:ALA:HB1	1:A:545:GLY:H	1.56	0.71
1:A:345:LYS:HB2	1:A:347:THR:H	1.56	0.71
1:A:357:MET:HE2	1:A:563:MET:H	1.56	0.70
1:A:910:GLU:OE1	1:A:913:SER:OG	2.09	0.70
1:A:593:LEU:HD13	1:A:601:PRO:HA	1.73	0.69
1:A:667:PRO:HA	1:A:671:LEU:HD13	1.74	0.69
1:A:90:SER:HA	1:A:116:SER:HA	1.73	0.69
1:A:587:TYR:O	1:A:589:MET:N	2.27	0.68
1:A:283:LEU:HD13	1:A:289:TYR:HE1	1.58	0.67
1:A:587:TYR:C	1:A:589:MET:H	2.03	0.67
1:A:907:VAL:O	1:A:909:CYS:N	2.28	0.66
1:A:480:LEU:HB2	1:A:483:LEU:HB2	1.77	0.66
1:A:594:MET:HE2	1:A:898:ASN:HB3	1.77	0.65
1:A:249:GLY:O	1:A:251:GLU:N	2.30	0.65
1:A:204:LEU:HD11	1:A:508:GLY:H	1.61	0.65
1:A:490:LEU:HB3	1:A:496:LEU:HG	1.78	0.64
1:A:329:TYR:CZ	1:A:340:LEU:HD23	2.33	0.63
1:A:443:ILE:HD13	1:A:446:ASN:ND2	2.14	0.63
1:A:638:GLU:OE1	1:A:845:ARG:NH1	2.30	0.63
1:A:895:CYS:SG	1:A:897:PRO:HD2	2.39	0.62
1:A:330:LEU:HG	1:A:341:VAL:HG21	1.81	0.62
1:A:83:ASP:HB3	1:A:123:VAL:HG12	1.81	0.61
1:A:412:PHE:HE1	1:A:505:PHE:HE2	1.48	0.61
1:A:119:VAL:HG22	1:A:319:THR:HB	1.81	0.61
1:A:482:ILE:HA	1:A:485:GLU:HG2	1.81	0.61
1:A:843:SER:C	1:A:845:ARG:H	2.09	0.61
1:A:939:LEU:HD13	1:A:993:PHE:HD1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ASP:OD2	1:A:812:LYS:HB2	2.01	0.60
1:A:345:LYS:HB2	1:A:347:THR:N	2.17	0.60
1:A:513:ALA:HB1	1:A:545:GLY:N	2.15	0.60
1:A:922:LEU:HD23	1:A:969:ILE:HD12	1.84	0.60
1:A:344:GLU:OE2	1:A:552:ARG:HD3	2.03	0.59
1:A:197:TYR:HB3	1:A:236:VAL:HG22	1.83	0.59
1:A:674:LEU:HD23	1:A:678:ARG:HG2	1.85	0.59
1:A:322:ARG:HH22	1:A:542:GLY:HA2	1.68	0.58
1:A:258:TRP:CE3	1:A:288:ARG:HB3	2.38	0.58
1:A:445:ASN:C	1:A:447:ALA:H	2.12	0.58
1:A:975:LYS:O	1:A:979:ASP:N	2.35	0.57
1:A:718:ILE:HG21	1:A:738:PHE:HA	1.86	0.57
1:A:280:ILE:HA	1:A:283:LEU:HD12	1.87	0.56
1:A:505:PHE:O	1:A:507:ILE:N	2.38	0.56
1:A:527:GLN:HB2	1:A:739:ASN:HD21	1.69	0.56
1:A:762:ILE:HB	1:A:766:SER:HB2	1.87	0.56
1:A:328:HIS:ND1	1:A:537:TYR:OH	2.38	0.56
1:A:283:LEU:HD13	1:A:289:TYR:CE1	2.40	0.56
1:A:727:TYR:HA	1:A:749:ALA:HB2	1.86	0.56
1:A:969:ILE:O	1:A:973:ILE:HG13	2.05	0.56
1:A:712:THR:HG22	1:A:714:HIS:H	1.70	0.56
1:A:527:GLN:HB2	1:A:739:ASN:ND2	2.19	0.56
1:A:200:PRO:HG3	1:A:276:TRP:CZ2	2.33	0.56
1:A:489:ILE:HA	1:A:492:GLN:HB2	1.88	0.55
1:A:268:ARG:NH2	1:A:577:ASP:O	2.39	0.55
1:A:393:ASP:O	1:A:397:ILE:HG13	2.06	0.55
1:A:437:LYS:C	1:A:439:ALA:H	2.14	0.55
1:A:474:ILE:O	1:A:499:LEU:HD11	2.07	0.55
1:A:260:ILE:HG12	1:A:290:VAL:HB	1.87	0.55
1:A:297:PRO:HG2	1:A:578:ARG:HA	1.88	0.55
1:A:679:LEU:HD13	1:A:805:ILE:HD13	1.89	0.55
1:A:936:ALA:CB	1:A:1031:LEU:HD11	2.37	0.55
1:A:467:LEU:O	1:A:472:ILE:N	2.40	0.55
1:A:591:LEU:O	1:A:594:MET:N	2.40	0.54
1:A:271:GLU:O	1:A:273:GLY:N	2.40	0.54
1:A:866:LEU:O	1:A:870:ILE:HB	2.08	0.54
1:A:284:PRO:C	1:A:286:LYS:H	2.16	0.54
1:A:158:ILE:HG23	1:A:183:TYR:CD1	2.44	0.53
1:A:664:VAL:HG13	1:A:814:MET:HE1	1.90	0.53
1:A:357:MET:HE2	1:A:562:LYS:HA	1.89	0.53
1:A:939:LEU:HD13	1:A:993:PHE:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:O	1:A:472:ILE:HG13	2.08	0.53
1:A:117:HIS:CD2	1:A:321:PHE:HD1	2.28	0.52
1:A:971:ALA:O	1:A:975:LYS:N	2.42	0.52
1:A:162:ASP:HA	1:A:187:GLN:HE22	1.74	0.52
1:A:252:VAL:O	1:A:254:ARG:N	2.43	0.52
1:A:890:ARG:C	1:A:892:LEU:H	2.17	0.52
1:A:357:MET:HE2	1:A:563:MET:N	2.24	0.51
1:A:617:SER:O	1:A:621:MET:HG3	2.09	0.51
1:A:271:GLU:C	1:A:273:GLY:H	2.18	0.51
1:A:473:GLY:C	1:A:499:LEU:HD12	2.35	0.51
1:A:487:ILE:O	1:A:491:PHE:N	2.42	0.51
1:A:987:LYS:O	1:A:991:GLU:N	2.32	0.51
1:A:513:ALA:H	1:A:546:ARG:HD3	1.75	0.51
1:A:629:LYS:HA	1:A:863:MET:SD	2.51	0.51
1:A:526:GLY:N	1:A:527:GLN:HA	2.25	0.51
1:A:546:ARG:H	1:A:550:ASP:HB2	1.75	0.51
1:A:679:LEU:HD12	1:A:773:LEU:HB3	1.92	0.51
1:A:284:PRO:O	1:A:286:LYS:N	2.44	0.50
1:A:605:LEU:HD13	1:A:878:GLN:HB2	1.93	0.50
1:A:680:VAL:HG23	1:A:682:ILE:HD11	1.93	0.50
1:A:475:HIS:HB2	1:A:499:LEU:HD21	1.94	0.50
1:A:703:ASN:HB2	1:A:711:TYR:HE2	1.76	0.50
1:A:472:ILE:HG23	1:A:498:VAL:HG13	1.93	0.50
1:A:173:THR:C	1:A:175:ALA:H	2.18	0.50
1:A:443:ILE:O	1:A:446:ASN:HB2	2.12	0.50
1:A:206:ASN:OD1	1:A:221:LEU:HD21	2.12	0.49
1:A:412:PHE:HE1	1:A:505:PHE:CE2	2.30	0.49
1:A:563:MET:SD	1:A:568:ALA:HB2	2.51	0.49
1:A:144:ARG:NH2	1:A:215:GLU:OE2	2.45	0.49
1:A:568:ALA:O	1:A:572:VAL:HG23	2.13	0.49
1:A:971:ALA:HA	1:A:974:ALA:HB3	1.93	0.49
1:A:92:GLU:HA	1:A:113:VAL:O	2.13	0.49
1:A:330:LEU:O	1:A:338:ILE:HD12	2.12	0.49
1:A:513:ALA:HB1	1:A:544:ALA:HA	1.95	0.49
1:A:590:ILE:O	1:A:593:LEU:HB2	2.12	0.49
1:A:842:ASN:C	1:A:844:MET:H	2.20	0.49
1:A:331:PHE:CD2	1:A:397:ILE:HD11	2.47	0.49
1:A:482:ILE:O	1:A:486:VAL:HG12	2.13	0.49
1:A:263:GLU:HB3	1:A:266:TYR:HD2	1.77	0.48
1:A:688:ASP:HB3	1:A:690:TYR:CE2	2.48	0.48
1:A:429:LEU:O	1:A:431:PHE:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:GLY:HA2	1:A:775:LEU:HD22	1.94	0.48
1:A:612:PHE:CE2	1:A:616:ILE:HD11	2.48	0.48
1:A:906:ARG:O	1:A:920:THR:OG1	2.32	0.48
1:A:414:PHE:HD2	1:A:523:LYS:HA	1.79	0.48
1:A:588:ASN:N	1:A:916:GLU:OE2	2.37	0.48
1:A:90:SER:HB3	1:A:116:SER:HB3	1.95	0.48
1:A:174:SER:HB3	1:A:323:PRO:CG	2.39	0.48
1:A:622:GLU:CG	1:A:870:ILE:HD11	2.44	0.48
1:A:284:PRO:C	1:A:286:LYS:N	2.72	0.47
1:A:195:VAL:HG23	1:A:258:TRP:O	2.14	0.47
1:A:970:ALA:O	1:A:974:ALA:N	2.42	0.47
1:A:470:ARG:HB2	1:A:472:ILE:HD12	1.95	0.47
1:A:414:PHE:CE2	1:A:523:LYS:HB3	2.49	0.47
1:A:472:ILE:HG22	1:A:473:GLY:N	2.29	0.47
1:A:585:LEU:CG	1:A:605:LEU:HD21	2.44	0.47
1:A:727:TYR:CE2	1:A:729:ASP:HB2	2.49	0.47
1:A:880:ASP:HB3	1:A:884:ARG:CZ	2.45	0.47
1:A:172:HIS:O	1:A:174:SER:N	2.46	0.47
1:A:268:ARG:HB3	1:A:579:LEU:HD12	1.97	0.47
1:A:703:ASN:HB2	1:A:711:TYR:CE2	2.49	0.47
1:A:809:ASP:OD2	1:A:812:LYS:N	2.35	0.47
1:A:520:SER:OG	1:A:521:VAL:N	2.47	0.47
1:A:843:SER:O	1:A:845:ARG:N	2.48	0.47
1:A:1024:LEU:HD12	1:A:1025:ILE:N	2.30	0.47
1:A:1066:VAL:HB	1:A:1067:SER:H	1.46	0.47
1:A:656:TYR:O	1:A:659:ASP:HB2	2.14	0.46
1:A:146:TYR:OH	1:A:179:VAL:O	2.32	0.46
1:A:612:PHE:O	1:A:616:ILE:HG13	2.14	0.46
1:A:272:ARG:O	1:A:276:TRP:HD1	1.98	0.46
1:A:205:SER:HB3	1:A:221:LEU:HD11	1.95	0.46
1:A:221:LEU:O	1:A:227:THR:HA	2.15	0.46
1:A:1026:ARG:O	1:A:1030:ARG:N	2.49	0.46
1:A:93:VAL:O	1:A:95:ALA:N	2.48	0.46
1:A:160:CYS:SG	1:A:315:HIS:ND1	2.43	0.46
1:A:342:VAL:CG1	1:A:346:SER:HB3	2.45	0.46
1:A:653:ILE:HD12	1:A:835:LEU:HD22	1.96	0.46
1:A:939:LEU:O	1:A:939:LEU:HD12	2.15	0.46
1:A:329:TYR:HB3	1:A:338:ILE:HD11	1.98	0.46
1:A:447:ALA:O	1:A:450:LEU:N	2.44	0.46
1:A:616:ILE:O	1:A:619:PRO:HD2	2.15	0.46
1:A:1047:ASN:O	1:A:1049:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:HIS:CB	1:A:479:LEU:H	2.29	0.45
1:A:677:GLY:HA3	1:A:775:LEU:O	2.15	0.45
1:A:890:ARG:HD2	1:A:896:THR:HA	1.97	0.45
1:A:989:TYR:O	1:A:992:SER:HB3	2.16	0.45
1:A:534:GLY:O	1:A:538:ILE:HG13	2.16	0.45
1:A:222:MET:HG2	1:A:227:THR:HG23	1.98	0.45
1:A:282:LEU:HD21	1:A:604:MET:HE1	1.99	0.45
1:A:466:PRO:C	1:A:470:ARG:HG3	2.42	0.45
1:A:153:PHE:CD1	1:A:153:PHE:C	2.93	0.45
1:A:304:GLU:O	1:A:308:LYS:N	2.50	0.45
1:A:507:ILE:N	1:A:508:GLY:HA2	2.32	0.45
1:A:601:PRO:O	1:A:604:MET:N	2.49	0.45
1:A:821:PHE:O	1:A:824:LEU:HB3	2.16	0.45
1:A:893:GLY:HA2	1:A:903:LEU:HB2	1.98	0.45
1:A:645:GLU:HA	1:A:648:GLU:HG2	1.99	0.45
1:A:394:ILE:O	1:A:398:VAL:HG23	2.17	0.45
1:A:465:LEU:HA	1:A:468:LEU:HG	1.98	0.45
1:A:936:ALA:HB1	1:A:1031:LEU:HD11	1.99	0.45
1:A:397:ILE:O	1:A:401:ILE:HD12	2.17	0.44
1:A:487:ILE:HA	1:A:490:LEU:HB2	1.98	0.44
1:A:838:ASN:C	1:A:840:LEU:H	2.25	0.44
1:A:867:LYS:O	1:A:870:ILE:HG22	2.18	0.44
1:A:122:GLN:O	1:A:316:ILE:HG22	2.18	0.44
1:A:223:THR:HG1	1:A:226:ILE:H	1.57	0.44
1:A:940:LEU:HD12	1:A:1030:ARG:HG3	1.98	0.44
1:A:271:GLU:C	1:A:273:GLY:N	2.75	0.44
1:A:339:TYR:O	1:A:341:VAL:HG23	2.17	0.44
1:A:933:PRO:C	1:A:935:GLN:H	2.26	0.44
1:A:1037:GLU:C	1:A:1038:LEU:HD23	2.42	0.44
1:A:143:ALA:HB3	1:A:183:TYR:CE2	2.53	0.44
1:A:566:GLN:H	1:A:566:GLN:CD	2.25	0.44
1:A:587:TYR:O	1:A:590:ILE:N	2.51	0.43
1:A:884:ARG:O	1:A:888:VAL:HG23	2.17	0.43
1:A:976:ILE:HA	1:A:979:ASP:HB2	1.99	0.43
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.34	0.43
1:A:589:MET:O	1:A:593:LEU:HG	2.18	0.43
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.80	0.43
1:A:922:LEU:HD21	1:A:966:MET:HA	2.01	0.43
1:A:1029:LYS:O	1:A:1033:GLU:HB2	2.18	0.43
1:A:757:CYS:SG	1:A:791:GLY:HA3	2.59	0.43
1:A:437:LYS:HA	1:A:440:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASP:C	1:A:432:ASN:N	2.77	0.43
1:A:622:GLU:HG2	1:A:870:ILE:HD11	2.01	0.43
1:A:119:VAL:HG22	1:A:319:THR:CB	2.47	0.43
1:A:505:PHE:C	1:A:507:ILE:H	2.26	0.43
1:A:890:ARG:HD3	1:A:898:ASN:OD1	2.18	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.82	0.42
1:A:886:LYS:HA	1:A:889:LEU:HB2	1.99	0.42
1:A:357:MET:O	1:A:360:ILE:HB	2.20	0.42
1:A:697:ASP:OD1	1:A:720:ASN:ND2	2.48	0.42
1:A:447:ALA:O	1:A:450:LEU:HB2	2.19	0.42
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.74	0.42
1:A:611:GLN:O	1:A:615:VAL:HG23	2.19	0.42
1:A:612:PHE:CZ	1:A:616:ILE:HD11	2.54	0.42
1:A:670:ALA:HB1	1:A:674:LEU:HD11	2.01	0.42
1:A:322:ARG:HA	1:A:323:PRO:HD2	1.70	0.42
1:A:684:VAL:CG1	1:A:688:ASP:HB2	2.49	0.42
1:A:703:ASN:OD1	1:A:706:ASN:HB3	2.20	0.42
1:A:830:VAL:HG12	1:A:831:LEU:HD12	2.01	0.42
1:A:123:VAL:HG23	1:A:315:HIS:HD2	1.83	0.42
1:A:288:ARG:HD2	1:A:288:ARG:HA	1.83	0.42
1:A:730:SER:HA	1:A:731:PRO:HD3	1.90	0.42
1:A:1020:TYR:O	1:A:1023:SER:HB2	2.19	0.42
1:A:679:LEU:HD12	1:A:773:LEU:CB	2.50	0.42
1:A:197:TYR:CE2	1:A:208:LYS:HG3	2.55	0.42
1:A:445:ASN:C	1:A:447:ALA:N	2.77	0.42
1:A:684:VAL:HG13	1:A:688:ASP:HB2	2.01	0.42
1:A:522:ARG:HD2	1:A:734:LEU:CD1	2.49	0.42
1:A:839:PRO:O	1:A:840:LEU:HD23	2.19	0.42
1:A:471:GLY:C	1:A:496:LEU:HA	2.45	0.41
1:A:684:VAL:HG23	1:A:766:SER:OG	2.20	0.41
1:A:406:TYR:O	1:A:515:THR:OG1	2.38	0.41
1:A:913:SER:OG	1:A:916:GLU:HB3	2.19	0.41
1:A:1031:LEU:HD12	1:A:1031:LEU:HA	1.63	0.41
1:A:115:LEU:HD22	1:A:344:GLU:O	2.20	0.41
1:A:310:HIS:O	1:A:312:GLN:HG2	2.20	0.41
1:A:639:ASP:O	1:A:642:ASN:N	2.53	0.41
1:A:168:LEU:HD22	1:A:302:PHE:CD2	2.56	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.78	0.41
1:A:661:ARG:NH2	1:A:765:ASP:O	2.52	0.41
1:A:414:PHE:CE1	1:A:540:MET:HE1	2.44	0.41
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HE2	1:A:237:MET:HB3	1.82	0.41
1:A:1065:ILE:O	1:A:1065:ILE:HG23	2.21	0.41
1:A:173:THR:C	1:A:175:ALA:N	2.77	0.41
1:A:818:ASP:HB2	1:A:821:PHE:HB2	2.03	0.41
1:A:201:ILE:HG22	1:A:203:ALA:H	1.86	0.41
1:A:870:ILE:O	1:A:871:SER:OG	2.29	0.41
1:A:263:GLU:O	1:A:266:TYR:HB2	2.21	0.41
1:A:301:GLU:O	1:A:612:PHE:HE2	2.04	0.41
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.76	0.40
1:A:679:LEU:HA	1:A:679:LEU:HD23	1.77	0.40
1:A:786:GLN:O	1:A:790:VAL:HG23	2.21	0.40
1:A:900:ILE:HG23	1:A:904:LYS:CB	2.51	0.40
1:A:985:VAL:O	1:A:986:GLU:C	2.64	0.40
1:A:122:GLN:HB3	1:A:300:MET:HE2	2.03	0.40
1:A:940:LEU:HB2	1:A:1031:LEU:HD13	2.02	0.40
1:A:818:ASP:O	1:A:822:LEU:HD23	2.21	0.40
1:A:914:GLY:HA3	1:A:940:LEU:HD21	2.03	0.40
1:A:937:ALA:HB2	1:A:1001:VAL:HB	2.03	0.40
1:A:203:ALA:O	1:A:206:ASN:N	2.55	0.40
1:A:602:GLU:H	1:A:602:GLU:CD	2.29	0.40
1:A:905:GLY:C	1:A:907:VAL:H	2.30	0.40
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.86	0.40
1:A:209:TYR:HB2	1:A:221:LEU:HD13	2.04	0.40
1:A:243:ARG:HH12	1:A:589:MET:HE2	1.87	0.40
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.79	0.40
1:A:611:GLN:CG	1:A:875:ALA:HA	2.51	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	924/1108 (83%)	771 (83%)	99 (11%)	54 (6%)	1 8

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	A	253	MET
1	A	283	LEU
1	A	476	HIS
1	A	588	ASN
1	A	908	ALA
1	A	960	ALA
1	A	987	LYS
1	A	1048	SER
1	A	1066	VAL
1	A	285	ASP
1	A	311	SER
1	A	429	LEU
1	A	446	ASN
1	A	506	SER
1	A	514	LYS
1	A	602	GLU
1	A	781	ILE
1	A	911	ILE
1	A	982	ILE
1	A	985	VAL
1	A	986	GLU
1	A	1069	GLY
1	A	173	THR
1	A	272	ARG
1	A	297	PRO
1	A	430	ASP
1	A	432	ASN
1	A	478	GLY
1	A	479	LEU
1	A	525	ASP
1	A	560	ASP
1	A	595	ARG
1	A	844	MET
1	A	891	ARG
1	A	915	ASP
1	A	1065	ILE
1	A	143	ALA

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Mol	Chain	Res	Type
1	A	248	ARG
1	A	438	GLU
1	A	464	ILE
1	A	907	VAL
1	A	910	GLU
1	A	925	ASN
1	A	1017	THR
1	A	1041	VAL
1	A	324	THR
1	A	439	ALA
1	A	892	LEU
1	A	1021	GLU
1	A	634	GLY
1	A	901	ILE
1	A	408	PRO
1	A	962	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	591/985 (60%)	559 (95%)	32 (5%)	20	47

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	PHE
1	A	218	ASP
1	A	228	ILE
1	A	252	VAL
1	A	271	GLU
1	A	311	SER
1	A	360	ILE
1	A	417	ARG
1	A	441	THR
1	A	549	LEU

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Mol	Chain	Res	Type
1	A	552	ARG
1	A	554	ILE
1	A	572	VAL
1	A	599	ILE
1	A	600	SER
1	A	638	GLU
1	A	642	ASN
1	A	728	ILE
1	A	733	ASN
1	A	735	LEU
1	A	742	LEU
1	A	775	LEU
1	A	830	VAL
1	A	870	ILE
1	A	882	LEU
1	A	896	THR
1	A	939	LEU
1	A	1038	LEU
1	A	1057	VAL
1	A	1065	ILE
1	A	1066	VAL
1	A	1072	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	187	GLN
1	A	352	ASN
1	A	475	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
2	PO4	A	1102	-	4,4,4	0.80	0	6,6,6	0.74	0
2	PO4	A	1101	-	4,4,4	1.00	0	6,6,6	0.55	0
2	PO4	A	1103	-	4,4,4	0.79	0	6,6,6	0.52	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	942/1108 (85%)	-0.09	20 (2%)	63 48	106, 158, 258, 324	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1034	LEU	4.1
1	A	474	ILE	3.8
1	A	1036	LYS	3.2
1	A	917	LEU	3.2
1	A	1065	ILE	3.1
1	A	473	GLY	3.1
1	A	422	LEU	3.0
1	A	455	ASP	2.8
1	A	506	SER	2.8
1	A	110	ASP	2.6
1	A	507	ILE	2.5
1	A	891	ARG	2.5
1	A	1001	VAL	2.3
1	A	479	LEU	2.3
1	A	905	GLY	2.2
1	A	918	LEU	2.2
1	A	893	GLY	2.1
1	A	875	ALA	2.1
1	A	440	LEU	2.1
1	A	410	ILE	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
2	PO4	A	1102	5/5	0.85	0.06	188,192,197,205	0
2	PO4	A	1103	5/5	0.89	0.06	190,197,203,204	0
2	PO4	A	1101	5/5	0.93	0.18	141,143,153,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.