



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 PM GMT

PDB ID : 4QU4
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

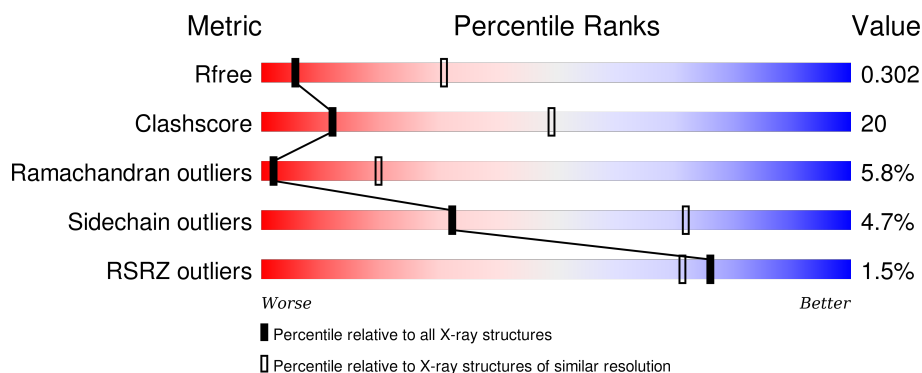
1 Overall quality at a glance ⓘ

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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div></div> <div>52%</div> <div>30%</div> <div>•</div> <div>15%</div> </div>

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:

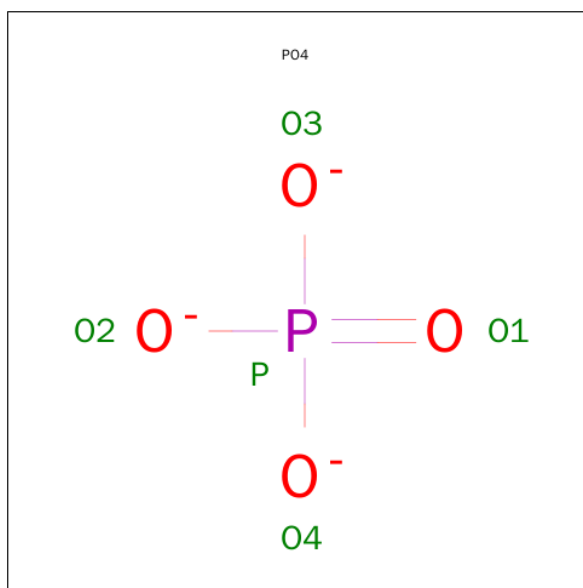
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	EXPRESSION TAG	UNP P47047
A	-33	HIS	-	EXPRESSION TAG	UNP P47047
A	-32	HIS	-	EXPRESSION TAG	UNP P47047
A	-31	HIS	-	EXPRESSION TAG	UNP P47047
A	-30	HIS	-	EXPRESSION TAG	UNP P47047
A	-29	HIS	-	EXPRESSION TAG	UNP P47047
A	-28	HIS	-	EXPRESSION TAG	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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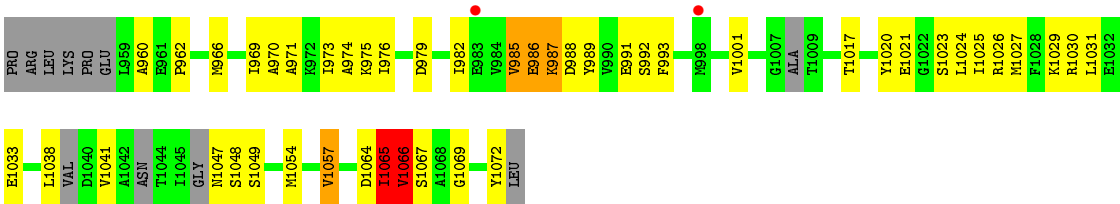
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P47047
A	-6	ILE	-	EXPRESSION TAG	UNP P47047
A	-5	ASP	-	EXPRESSION TAG	UNP P47047
A	-4	PRO	-	EXPRESSION TAG	UNP P47047
A	-3	PHE	-	EXPRESSION TAG	UNP P47047
A	-2	THR	-	EXPRESSION TAG	UNP P47047
A	-1	GLU	-	EXPRESSION TAG	UNP P47047
A	0	PHE	-	EXPRESSION TAG	UNP P47047

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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



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) 93.9 (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 0.263 , 0.302	Depositor DCC
R_{free} test set	1270 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	137.5	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 153.5	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26116 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.49	0/6777	0.71	3/9247 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	775	LEU	CA-CB-CG	7.66	132.91	115.30
1	A	735	LEU	CA-CB-CG	7.55	132.67	115.30
1	A	526	GLY	N-CA-C	5.93	127.93	113.10

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 ⓘ

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	252	0
2	A	15	0	0	0	0
All	All	6680	0	5969	252	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 20.

All (252) 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: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:513:ALA:HB1	1:A:545:GLY:H	1.56	0.71
1:A:258:TRP:CZ3	1:A:288:ARG:HB3	2.25	0.71
1:A:345:LYS:HB2	1:A:347:THR:H	1.56	0.71
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: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:223:THR:HG1	1:A:226:ILE:H	1.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:587:TYR:C	1:A:589:MET:H	2.03	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:939:LEU:HD13	1:A:993:PHE:HD1	1.65	0.61
1:A:482:ILE:HA	1:A:485:GLU:HG2	1.81	0.61
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:910:GLU:OE1	1:A:913:SER:OG	2.09	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: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:283:LEU:HD13	1:A:289:TYR:CE1	2.40	0.56
1:A:843:SER:C	1:A:845:ARG:H	2.09	0.56
1:A:969:ILE:O	1:A:973:ILE:HG13	2.05	0.56
1:A:727:TYR:HA	1:A:749:ALA:HB2	1.86	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:328:HIS:ND1	1:A:537:TYR:OH	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HG2	1:A:578:ARG:HA	1.88	0.55
1:A:936:ALA:CB	1:A:1031:LEU:HD11	2.37	0.55
1:A:679:LEU:HD13	1:A:805:ILE:HD13	1.89	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:158:ILE:HG23	1:A:183:TYR:CD1	2.44	0.53
1:A:939:LEU:HD13	1:A:993:PHE:CD1	2.43	0.53
1:A:445:ASN:C	1:A:447:ALA:H	2.12	0.53
1:A:470:ARG:O	1:A:472:ILE:HG13	2.08	0.53
1:A:971:ALA:O	1:A:975:LYS:N	2.42	0.52
1:A:117:HIS:CD2	1:A:321:PHE:HD1	2.28	0.52
1:A:252:VAL:O	1:A:254:ARG:N	2.43	0.52
1:A:162:ASP:HA	1:A:187:GLN:HE22	1.74	0.52
1:A:617:SER:O	1:A:621:MET:HG3	2.09	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:357:MET:HE3	1:A:360:ILE:HD12	1.91	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:437:LYS:C	1:A:439:ALA:H	2.14	0.50
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:443:ILE:O	1:A:446:ASN:HB2	2.12	0.50
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:206:ASN:OD1	1:A:221:LEU:HD21	2.12	0.49
1:A:971:ALA:HA	1:A:974:ALA:HB3	1.93	0.49
1:A:568:ALA:O	1:A:572:VAL:HG23	2.13	0.49
1:A:144:ARG:NH2	1:A:215:GLU:OE2	2.45	0.49
1:A:513:ALA:HB1	1:A:544:ALA:HA	1.95	0.49
1:A:330:LEU:O	1:A:338:ILE:HD12	2.12	0.49
1:A:92:GLU:HA	1:A:113:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ILE:O	1:A:593:LEU:HB2	2.12	0.49
1:A:284:PRO:C	1:A:286:LYS:H	2.16	0.49
1:A:482:ILE:O	1:A:486:VAL:HG12	2.13	0.49
1:A:331:PHE:CD2	1:A:397:ILE:HD11	2.47	0.49
1:A:688:ASP:HB3	1:A:690:TYR:CE2	2.48	0.48
1:A:263:GLU:HB3	1:A:266:TYR:HD2	1.77	0.48
1:A:429:LEU:O	1:A:431:PHE:N	2.39	0.48
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:588:ASN:N	1:A:916:GLU:OE2	2.37	0.48
1:A:414:PHE:HD2	1:A:523:LYS:HA	1.79	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:970:ALA:O	1:A:974:ALA:N	2.42	0.47
1:A:195:VAL:HG23	1:A:258:TRP:O	2.14	0.47
1:A:470:ARG:HB2	1:A:472:ILE:HD12	1.95	0.47
1:A:890:ARG:C	1:A:892:LEU:H	2.17	0.47
1:A:727:TYR:CE2	1:A:729:ASP:HB2	2.49	0.47
1:A:472:ILE:HG22	1:A:473:GLY:N	2.29	0.47
1:A:271:GLU:C	1:A:273:GLY:H	2.18	0.47
1:A:585:LEU:CG	1:A:605:LEU:HD21	2.44	0.47
1:A:414:PHE:CE2	1:A:523:LYS:HB3	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:809:ASP:OD2	1:A:812:LYS:N	2.35	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:843:SER:O	1:A:845:ARG:N	2.48	0.47
1:A:473:GLY:C	1:A:499:LEU:HD12	2.35	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:520:SER:OG	1:A:521:VAL:N	2.47	0.47
1:A:656:TYR:O	1:A:659:ASP:HB2	2.14	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:1026:ARG:O	1:A:1030:ARG:N	2.49	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:342:VAL:CG1	1:A:346:SER:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:CYS:SG	1:A:315:HIS:ND1	2.43	0.46
1:A:93:VAL:O	1:A:95:ALA:N	2.48	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
1:A:677:GLY:HA3	1:A:775:LEU:O	2.15	0.45
1:A:476:HIS:CB	1:A:479:LEU:H	2.29	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:173:THR:C	1:A:175:ALA:H	2.18	0.45
1:A:507:ILE:N	1:A:508:GLY:HA2	2.32	0.45
1:A:304:GLU:O	1:A:308:LYS:N	2.50	0.45
1:A:601:PRO:O	1:A:604:MET:N	2.49	0.45
1:A:893:GLY:HA2	1:A:903:LEU:HB2	1.98	0.45
1:A:821:PHE:O	1:A:824:LEU:HB3	2.16	0.45
1:A:645:GLU:HA	1:A:648:GLU:HG2	1.99	0.45
1:A:936:ALA:HB1	1:A:1031:LEU:HD11	1.99	0.45
1:A:465:LEU:HA	1:A:468:LEU:HG	1.98	0.45
1:A:282:LEU:HD21	1:A:604:MET:HE1	1.99	0.45
1:A:394:ILE:O	1:A:398:VAL:HG23	2.17	0.45
1:A:487:ILE:HA	1:A:490:LEU:HB2	1.98	0.44
1:A:397:ILE:O	1:A:401:ILE:HD12	2.17	0.44
1:A:867:LYS:O	1:A:870:ILE:HG22	2.18	0.44
1:A:842:ASN:C	1:A:844:MET:H	2.20	0.44
1:A:122:GLN:O	1:A:316:ILE:HG22	2.18	0.44
1:A:940:LEU:HD12	1:A:1030:ARG:HG3	1.98	0.44
1:A:339:TYR:O	1:A:341:VAL:HG23	2.17	0.44
1:A:143:ALA:HB3	1:A:183:TYR:CE2	2.53	0.44
1:A:587:TYR:O	1:A:590:ILE:N	2.51	0.43
1:A:593:LEU:HD21	1:A:604:MET:HE3	1.98	0.43
1:A:976:ILE:HA	1:A:979:ASP:HB2	1.99	0.43
1:A:884:ARG:O	1:A:888:VAL:HG23	2.17	0.43
1:A:589:MET:O	1:A:593:LEU:HG	2.18	0.43
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.80	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
1:A:284:PRO:C	1:A:286:LYS:N	2.72	0.43
1:A:622:GLU:HG2	1:A:870:ILE:HD11	2.01	0.43
1:A:558:MET:HE3	1:A:558:MET:HB3	1.85	0.43
1:A:119:VAL:HG22	1:A:319:THR:CB	2.47	0.43
1:A:890:ARG:HD3	1:A:898:ASN:OD1	2.18	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD23	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:480:LEU:HD23	1:A:480:LEU:HA	1.74	0.42
1:A:447:ALA:O	1:A:450:LEU:HB2	2.19	0.42
1:A:670:ALA:HB1	1:A:674:LEU:HD11	2.01	0.42
1:A:612:PHE:CZ	1:A:616:ILE:HD11	2.54	0.42
1:A:611:GLN:O	1:A:615:VAL:HG23	2.19	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:357:MET:HE2	1:A:562:LYS:HA	2.01	0.42
1:A:703:ASN:OD1	1:A:706:ASN:HB3	2.20	0.42
1:A:414:PHE:HE1	1:A:540:MET:CE	2.32	0.42
1:A:830:VAL:HG12	1:A:831:LEU:HD12	2.01	0.42
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.83	0.42
1:A:123:VAL:HG23	1:A:315:HIS:HD2	1.83	0.42
1:A:1020:TYR:O	1:A:1023:SER:HB2	2.19	0.42
1:A:730:SER:HA	1:A:731:PRO:HD3	1.90	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: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:684:VAL:HG23	1:A:766:SER:OG	2.20	0.41
1:A:1031:LEU:HA	1:A:1031:LEU:HD12	1.63	0.41
1:A:913:SER:OG	1:A:916:GLU:HB3	2.19	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:661:ARG:NH2	1:A:765:ASP:O	2.52	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.78	0.41
1:A:168:LEU:HD22	1:A:302:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.86	0.41
1:A:1065:ILE:HG23	1:A:1065:ILE:O	2.21	0.41
1:A:818:ASP:HB2	1:A:821:PHE:HB2	2.03	0.41
1:A:870:ILE:O	1:A:871:SER:OG	2.29	0.41
1:A:201:ILE:HG22	1:A:203:ALA:H	1.86	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:679:LEU:HD23	1:A:679:LEU:HA	1.77	0.40
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.76	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:940:LEU:HB2	1:A:1031:LEU:HD13	2.02	0.40
1:A:914:GLY:HA3	1:A:940:LEU:HD21	2.03	0.40
1:A:818:ASP:O	1:A:822:LEU:HD23	2.21	0.40
1:A:937:ALA:HB2	1:A:1001:VAL:HB	2.03	0.40
1:A:466:PRO:C	1:A:470:ARG:HG3	2.42	0.40
1:A:203:ALA:O	1:A:206:ASN:N	2.55	0.40
1:A:153:PHE:CD1	1:A:153:PHE:C	2.93	0.40
1:A:283:LEU:HA	1:A:284:PRO:HD3	1.79	0.40
1:A:209:TYR:HB2	1:A:221:LEU:HD13	2.04	0.40
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.86	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%)	2 20

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
1	A	248	ARG
1	A	438	GLU
1	A	464	ILE
1	A	907	VAL
1	A	910	GLU

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Mol	Chain	Res	Type
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%)	563 (95%)	28 (5%)	32 72

All (28) 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	417	ARG
1	A	441	THR
1	A	549	LEU
1	A	552	ARG
1	A	554	ILE
1	A	600	SER
1	A	638	GLU
1	A	642	ASN
1	A	675	GLN

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Mol	Chain	Res	Type
1	A	733	ASN
1	A	735	LEU
1	A	775	LEU
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	1064	ASP
1	A	1065	ILE
1	A	1066	VAL
1	A	1072	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	475	HIS
1	A	838	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1101	-	4,4,4	0.48	0	6,6,6	0.26	0
2	PO4	A	1102	-	4,4,4	0.35	0	6,6,6	0.29	0
2	PO4	A	1103	-	4,4,4	0.27	0	6,6,6	0.27	0

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	PO4	A	1101	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1102	-	-	0/0/0/0	0/0/0/0
2	PO4	A	1103	-	-	0/0/0/0	0/0/0/0

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%)	-0.24	14 (1%) 76 71	106, 158, 259, 324	3 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	705	ARG	4.8
1	A	440	LEU	4.0
1	A	507	ILE	3.3
1	A	506	SER	3.3
1	A	784	SER	3.2
1	A	80	VAL	2.9
1	A	998	MET	2.6
1	A	166	SER	2.6
1	A	473	GLY	2.6
1	A	205	SER	2.6
1	A	474	ILE	2.5
1	A	410	ILE	2.4
1	A	221	LEU	2.4
1	A	983	GLU	2.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	A	1101	5/5	0.89	0.22	-0.57	141,143,153,159	0
2	PO4	A	1102	5/5	0.93	0.09	-1.57	188,192,197,205	0
2	PO4	A	1103	5/5	0.79	0.14	-	190,197,203,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.