WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:09 AM EDT

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PDB ID	:	5N8Z
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with CTCTCC-CTT
Authors	:	Chen, W.-F.; Rety, S.; Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on	:	2017-02-24
Resolution	:	3.48 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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
Rfree		0.272
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		3.0%

Worse *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
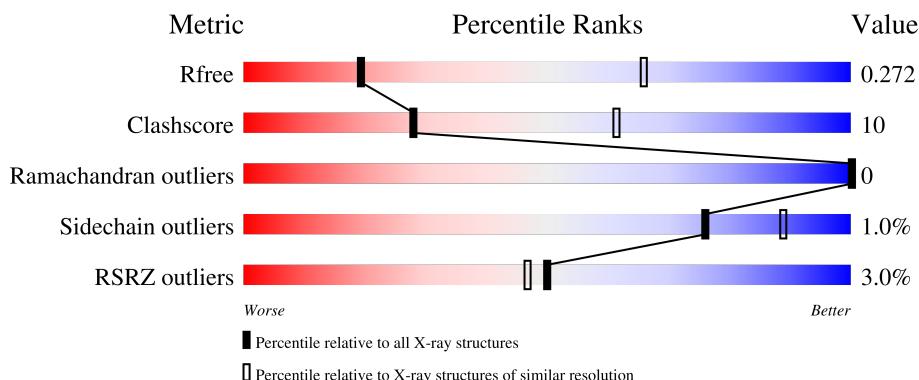
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	944	3% / 71% / 19% / 10%
1	B	944	3% / 66% / 24% / • 10%
2	C	9	11% / 33% / 33% / 33%
2	D	9	22% / 22% / 33% / 44%
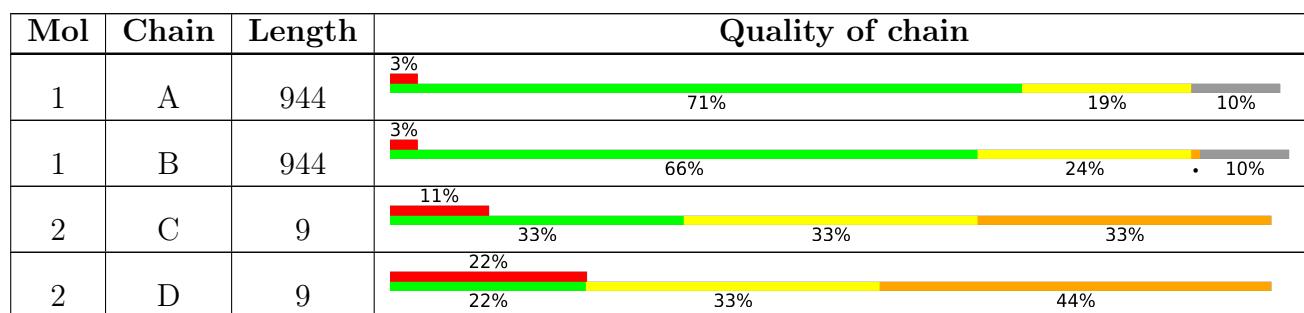
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13988 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 CG9323, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total 6814	C 4304	N 1200	O 1265	S 45	0	0	0
1	B	849	Total 6814	C 4304	N 1200	O 1265	S 45	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*TP*CP*TP*CP*CP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total 175	C 85	N 23	O 58	P 9	0	0	0
2	D	9	Total 175	C 85	N 23	O 58	P 9	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O2 ⊖O — P⊕ ═ O O1

P

O4
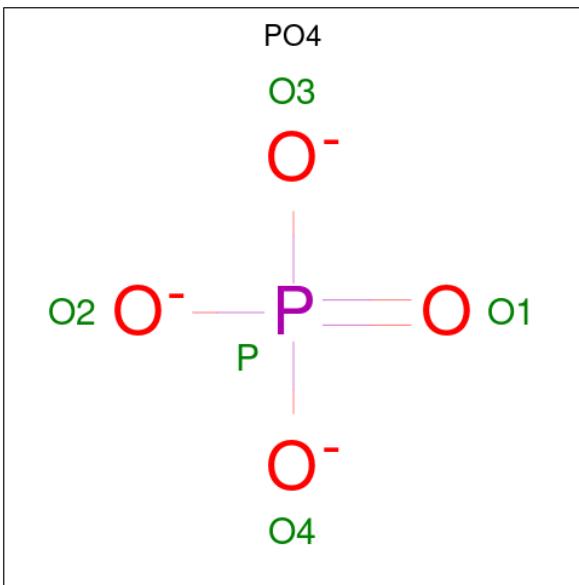
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0

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: CG9323, isoform A
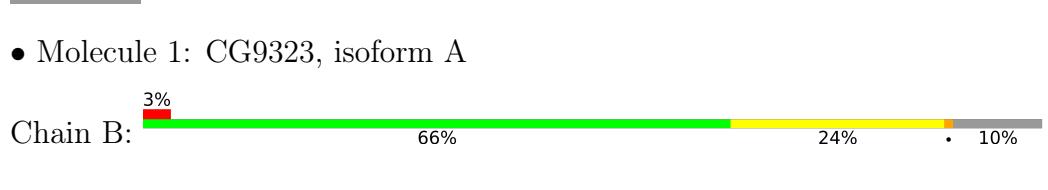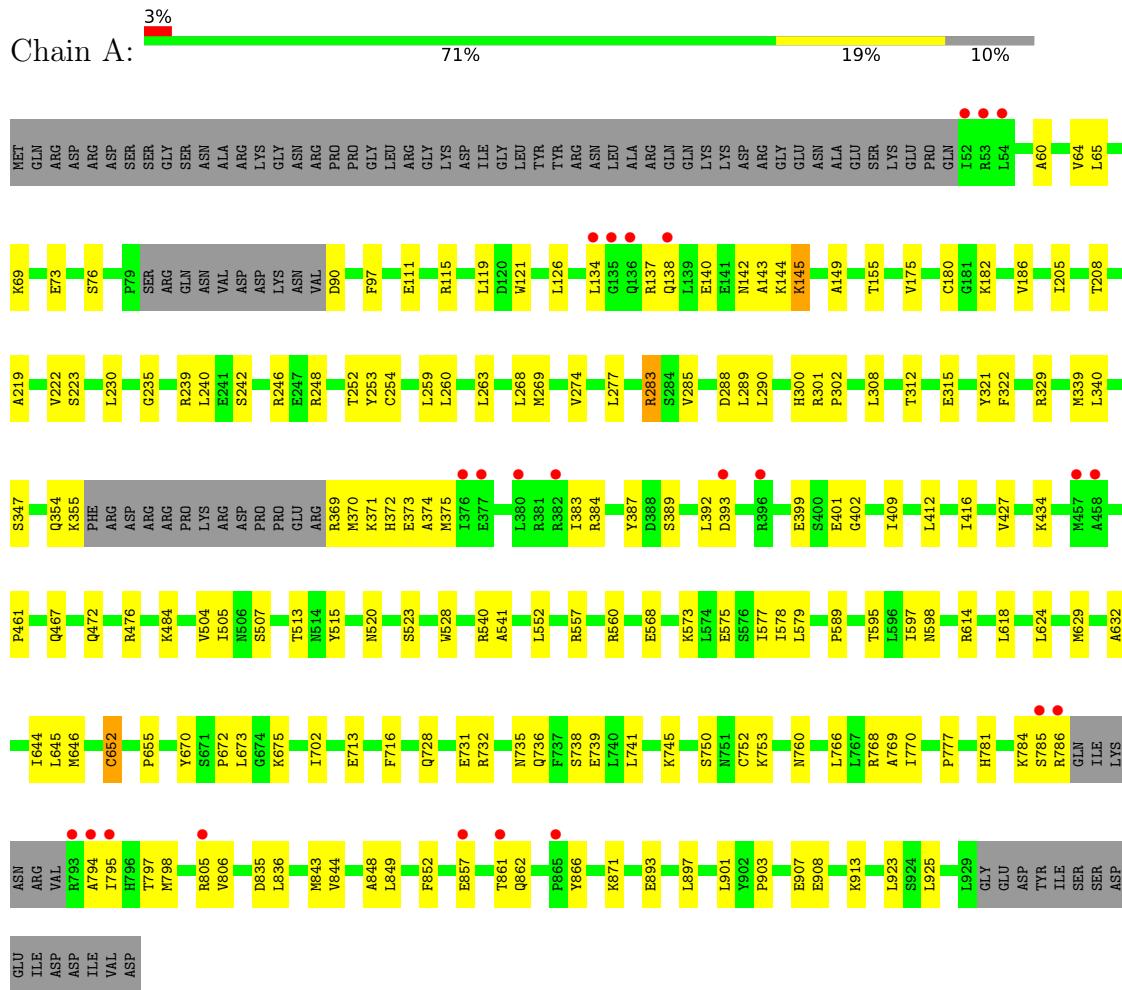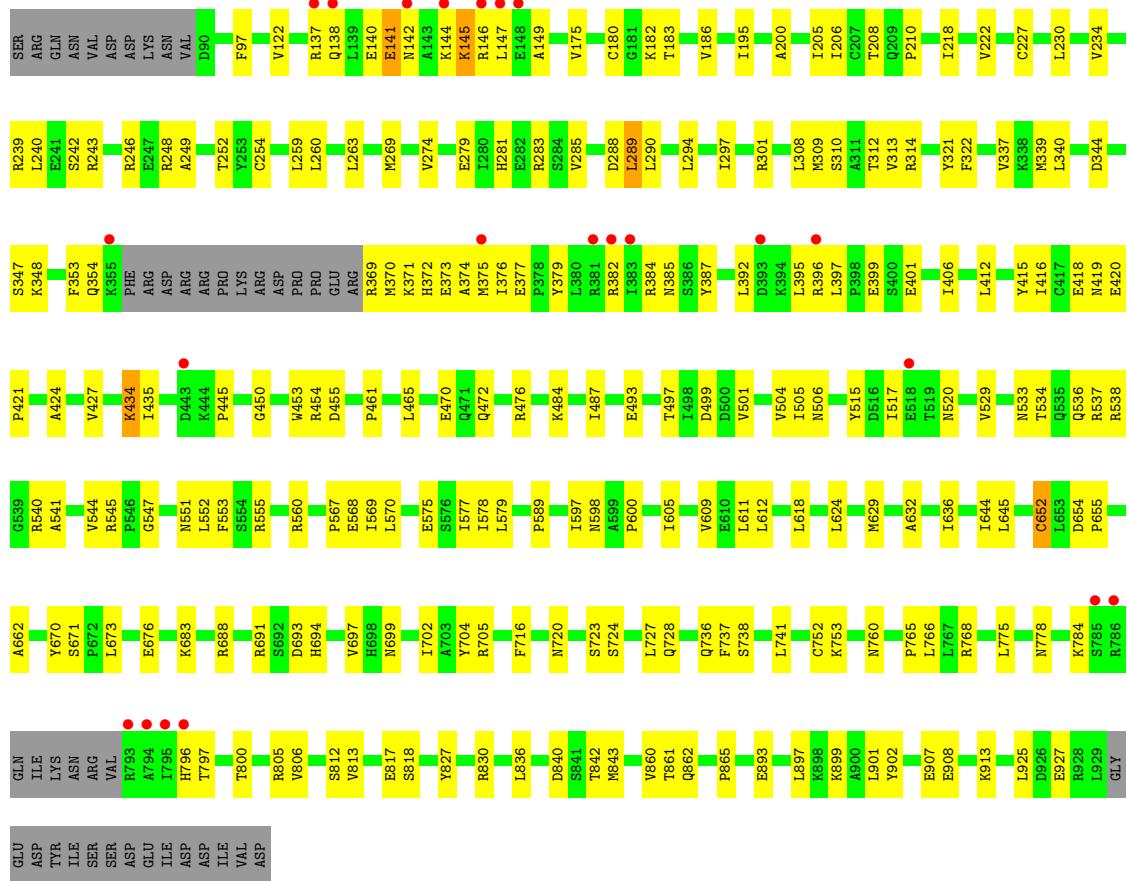
- Molecule 1: CG9323, isoform A

• Molecule 2: DNA (5'-D(P*CP*TP*CP*TP*CP*CP*CP*TP*T)-3')

Chain C:

• Molecule 2: DNA (5'-D(P*CP*TP*CP*TP*CP*CP*CP*TP*T)-3')

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	306.25Å 51.17Å 165.18Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	40.00 – 3.48 42.46 – 3.48	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-3.48) 96.0 (42.46-3.48)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.198 , 0.274 0.199 , 0.272	Depositor DCC
R_{free} test set	1460 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 18.9	EDS
L-test for twinning[2]	$< |L| > = 0.42, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13988	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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 (i)

5.1 Standard geometry (i)

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	0.55	0/6933	0.77	1/9353 (0.0%)
1	B	0.54	1/6933 (0.0%)	0.74	1/9353 (0.0%)
2	C	2.37	8/192 (4.2%)	1.60	3/292 (1.0%)
2	D	2.00	3/192 (1.6%)	1.41	3/292 (1.0%)
All	All	0.64	12/14250 (0.1%)	0.79	8/19290 (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	2
1	B	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9	DT	C1'-N1	10.53	1.62	1.49
2	D	6	DC	C1'-N1	8.38	1.60	1.49
2	C	3	DC	C1'-N1	7.94	1.59	1.49
2	C	6	DC	C1'-N1	7.63	1.59	1.49
2	C	2	DT	C1'-N1	7.37	1.58	1.49
2	C	8	DT	C1'-N1	6.67	1.57	1.49
1	B	652	CYS	CB-SG	-6.23	1.71	1.82
2	D	8	DT	C1'-N1	5.91	1.56	1.49
2	D	8	DT	N1-C2	5.73	1.42	1.38
2	C	9	DT	N1-C6	5.63	1.42	1.38
2	C	8	DT	C3'-O3'	5.28	1.50	1.44
2	C	9	DT	N1-C2	5.09	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	DC	O4'-C4'-C3'	-7.30	101.58	104.50
2	C	3	DC	O4'-C4'-C3'	-6.54	101.88	104.50
2	C	3	DC	O4'-C1'-N1	6.30	112.41	108.00
2	D	5	DC	O4'-C4'-C3'	-5.85	102.16	104.50
1	B	289	LEU	CB-CG-CD2	-5.67	101.36	111.00
2	D	1	DC	O4'-C1'-N1	5.37	111.76	108.00
1	A	277	LEU	CA-CB-CG	5.04	126.89	115.30
2	D	3	DC	O4'-C1'-N1	5.01	111.51	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	LYS	Peptide
1	A	242	SER	Peptide
1	B	242	SER	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	6814	0	6912	121	0
1	B	6814	0	6913	154	0
2	C	175	0	104	5	0
2	D	175	0	104	6	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
All	All	13988	0	14033	278	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 10.

All (278) 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:B:784:LYS:HB2	1:B:797:THR:H	1.37	0.89
1:B:269:MET:O	1:B:301:ARG:NH1	2.11	0.84
1:A:784:LYS:HB2	1:A:797:THR:H	1.44	0.82
1:B:145:LYS:H	1:B:145:LYS:HD2	1.46	0.80
1:A:283:ARG:NH1	1:A:288:ASP:OD2	2.14	0.80
1:B:283:ARG:NH2	1:B:598:ASN:OD1	2.17	0.76
1:A:515:TYR:OH	1:A:520:ASN:OD1	2.01	0.76
1:A:145:LYS:H	1:A:145:LYS:HD2	1.51	0.75
1:B:141:GLU:HA	1:B:145:LYS:HZ1	1.52	0.75
1:B:145:LYS:O	1:B:149:ALA:N	2.22	0.71
1:B:760:ASN:HB3	1:B:766:LEU:HD23	1.73	0.71
1:A:289:LEU:HD11	1:A:577:ILE:HG12	1.73	0.70
1:B:240:LEU:HD21	1:B:736:GLN:HB2	1.72	0.70
1:A:283:ARG:NH2	1:A:598:ASN:OD1	2.24	0.69
1:A:269:MET:O	1:A:301:ARG:NH1	2.26	0.68
1:A:738:SER:OG	1:A:752:CYS:HB3	1.94	0.68
1:A:646:MET:HB3	1:A:770:ILE:HD12	1.75	0.68
1:B:652:CYS:O	1:B:655:PRO:HD2	1.94	0.68
1:B:283:ARG:NH1	1:B:288:ASP:OD2	2.27	0.67
1:A:137:ARG:HA	1:A:140:GLU:HG3	1.79	0.65
1:A:844:VAL:HG21	1:A:849:LEU:HD21	1.78	0.64
1:A:64:VAL:HG11	1:A:925:LEU:HD11	1.77	0.64
1:A:573:LYS:HB3	1:A:575:GLU:OE1	1.98	0.64
1:B:137:ARG:HA	1:B:140:GLU:HG3	1.80	0.64
1:B:424:ALA:HB3	1:B:501:VAL:HA	1.80	0.63
1:B:570:LEU:HD21	1:B:598:ASN:HB3	1.80	0.63
1:A:240:LEU:HD21	1:A:736:GLN:HB2	1.81	0.63
1:A:259:LEU:HD23	1:A:290:LEU:HD11	1.81	0.62
1:B:418:GLU:HG2	1:B:453:TRP:HZ2	1.64	0.62
1:B:784:LYS:HB2	1:B:797:THR:N	2.12	0.62
1:B:670:TYR:CZ	1:B:723:SER:HB2	2.34	0.62
1:B:435:ILE:HG12	1:B:487:ILE:HG22	1.81	0.62
1:B:497:THR:HG22	1:B:540:ARG:HH22	1.65	0.62
1:B:195:ILE:HA	1:B:200:ALA:HB2	1.81	0.61
1:B:716:PHE:O	1:B:720:ASN:ND2	2.33	0.61
1:A:73:GLU:HA	1:A:76:SER:HB3	1.82	0.61
1:B:497:THR:HG22	1:B:540:ARG:NH2	2.15	0.61
1:A:652:CYS:O	1:A:655:PRO:HD2	2.01	0.61
1:A:504:VAL:HG23	1:A:541:ALA:HB2	1.82	0.60
1:B:371:LYS:O	1:B:374:ALA:N	2.32	0.60
1:B:901:LEU:HB3	1:B:902:TYR:CD2	2.38	0.59
1:A:781:HIS:O	1:A:798:MET:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:6:DC:H5"	2:C:6:DC:H6	1.67	0.58
1:B:738:SER:OG	1:B:752:CYS:HB3	2.04	0.58
1:B:694:HIS:ND1	1:B:842:THR:OG1	2.36	0.58
1:B:208:THR:HA	1:B:254:CYS:O	2.04	0.58
1:B:260:LEU:HD23	1:B:263:LEU:HD12	1.86	0.57
1:B:144:LYS:HA	1:B:147:LEU:HB3	1.85	0.57
1:A:97:PHE:HD1	1:A:629:MET:HE3	1.69	0.57
1:A:239:ARG:HG2	1:A:240:LEU:HG	1.86	0.57
1:A:321:TYR:CD1	1:A:597:ILE:HG12	2.40	0.57
1:B:605:ILE:O	1:B:609:VAL:HG23	2.05	0.57
1:B:520:ASN:O	1:B:830:ARG:NH2	2.38	0.57
1:A:370:MET:HB3	1:A:373:GLU:H	1.69	0.57
1:A:857:GLU:CD	1:A:871:LYS:HE2	2.26	0.56
1:A:371:LYS:O	1:A:374:ALA:N	2.33	0.56
1:A:786:ARG:HB3	1:A:795:ILE:H	1.70	0.56
1:A:401:GLU:HA	1:A:552:LEU:O	2.05	0.56
1:A:579:LEU:HG	1:A:632:ALA:HB2	1.86	0.56
1:B:97:PHE:HD1	1:B:629:MET:HE3	1.71	0.55
1:A:784:LYS:HG3	1:A:797:THR:HB	1.87	0.55
1:A:355:LYS:HG3	1:A:355:LYS:O	2.05	0.55
1:B:145:LYS:HD2	1:B:145:LYS:N	2.18	0.55
1:A:370:MET:HA	1:A:372:HIS:N	2.21	0.55
1:A:354:GLN:CD	1:A:355:LYS:H	2.10	0.55
1:B:504:VAL:HG23	1:B:541:ALA:HB2	1.88	0.54
1:B:60:ALA:HB3	1:B:65:LEU:HD21	1.88	0.54
1:B:676:GLU:HG2	2:D:3:DC:H42	1.72	0.54
1:A:739:GLU:HG2	1:A:750:SER:HB2	1.89	0.54
1:B:294:LEU:HD23	1:B:297:ILE:HD12	1.89	0.54
1:B:454:ARG:NH1	1:B:455:ASP:OD1	2.41	0.54
1:A:69:LYS:O	1:A:73:GLU:HG3	2.08	0.54
1:A:412:LEU:O	1:A:416:ILE:HG13	2.07	0.54
1:B:175:VAL:HG12	1:B:312:THR:HG22	1.90	0.54
2:D:6:DC:H6	2:D:6:DC:H5"	1.73	0.54
1:A:427:VAL:HG22	1:A:505:ILE:HD12	1.89	0.53
1:A:731:GLU:O	1:A:735:ASN:ND2	2.41	0.53
1:B:239:ARG:HB2	2:D:8:DT:H5"	1.90	0.53
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.89	0.53
1:B:337:VAL:HG22	1:B:547:GLY:H	1.72	0.53
1:A:384:ARG:HA	1:A:392:LEU:HD11	1.90	0.53
1:A:513:THR:HA	1:A:523:SER:O	2.08	0.53
1:B:427:VAL:HG22	1:B:505:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:HG12	1:A:312:THR:HG22	1.89	0.53
1:B:146:ARG:NH1	1:B:227:CYS:SG	2.82	0.53
1:B:246:ARG:HG3	1:B:248:ARG:O	2.09	0.53
1:A:409:ILE:HG12	1:A:552:LEU:CD1	2.39	0.53
1:A:786:ARG:HB3	1:A:794:ALA:HA	1.90	0.53
1:A:760:ASN:HB3	1:A:766:LEU:HD23	1.91	0.52
1:A:208:THR:HA	1:A:254:CYS:O	2.09	0.52
1:B:281:HIS:HB3	1:B:310:SER:OG	2.09	0.52
1:A:893:GLU:O	1:A:897:LEU:HG	2.08	0.52
1:A:784:LYS:HE2	1:A:797:THR:OG1	2.09	0.52
1:B:421:PRO:HG2	1:B:545:ARG:NH2	2.24	0.52
1:B:222:VAL:HG12	1:B:234:VAL:HG21	1.91	0.52
1:B:370:MET:HA	1:B:372:HIS:N	2.24	0.52
1:A:614:ARG:NH1	1:A:777:PRO:HG3	2.25	0.52
1:A:315:GLU:OE2	1:A:329:ARG:NH1	2.37	0.51
1:B:339:MET:HE1	1:B:534:THR:CG2	2.40	0.51
1:B:353:PHE:O	1:B:354:GLN:HB2	2.11	0.51
1:A:806:VAL:HG12	1:A:836:LEU:HG	1.92	0.51
1:B:180:CYS:SG	1:B:182:LYS:HG2	2.51	0.51
1:B:205:ILE:HG12	1:B:274:VAL:HB	1.92	0.51
1:B:861:THR:HG23	1:B:862:GLN:H	1.75	0.51
1:A:145:LYS:O	1:A:149:ALA:N	2.33	0.51
1:B:285:VAL:HG23	1:B:568:GLU:HB3	1.93	0.50
1:A:205:ILE:HG12	1:A:274:VAL:HB	1.93	0.50
1:B:375:MET:SD	1:B:560:ARG:HD3	2.51	0.50
1:A:222:VAL:HG21	1:A:253:TYR:OH	2.10	0.50
1:B:476:ARG:O	1:B:484:LYS:HE2	2.12	0.50
1:A:908:GLU:O	1:A:913:LYS:HG2	2.11	0.50
1:A:145:LYS:HD2	1:A:145:LYS:N	2.22	0.50
1:A:861:THR:HG23	1:A:862:GLN:H	1.77	0.50
1:B:379:TYR:HD1	1:B:382:ARG:HH21	1.60	0.50
1:B:461:PRO:HG3	1:B:673:LEU:HD12	1.94	0.50
1:B:704:TYR:CD1	1:B:727:LEU:HD13	2.47	0.50
1:A:60:ALA:HB3	1:A:65:LEU:HD21	1.93	0.49
1:A:97:PHE:CD1	1:A:629:MET:HE3	2.46	0.49
1:B:472:GLN:O	1:B:476:ARG:HG3	2.12	0.49
1:B:210:PRO:HG3	1:B:279:GLU:HB2	1.93	0.49
1:B:644:ILE:HG22	1:B:741:LEU:HD21	1.94	0.49
1:B:200:ALA:O	1:B:249:ALA:HB2	2.13	0.49
1:B:399:GLU:OE1	1:B:399:GLU:N	2.41	0.49
1:A:745:LYS:HB2	1:A:903:PRO:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HG12	1:B:600:PRO:HG3	1.94	0.49
1:B:688:ARG:HD3	1:B:699:ASN:ND2	2.28	0.49
1:B:379:TYR:HD1	1:B:382:ARG:NH2	2.10	0.48
1:A:672:PRO:HG2	1:A:675:LYS:HG3	1.95	0.48
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.95	0.48
1:B:308:LEU:HD11	1:B:322:PHE:CE2	2.48	0.48
1:B:370:MET:HA	1:B:372:HIS:H	1.78	0.48
1:B:578:ILE:HG23	1:B:589:PRO:HB3	1.94	0.48
1:B:64:VAL:HG11	1:B:925:LEU:HD11	1.96	0.48
1:B:230:LEU:HD13	1:B:243:ARG:HG3	1.94	0.48
1:B:421:PRO:HG2	1:B:545:ARG:HH21	1.77	0.48
1:A:246:ARG:HG3	1:A:248:ARG:O	2.14	0.48
1:A:768:ARG:HD3	1:A:843:MET:O	2.13	0.48
1:A:235:GLY:O	1:A:252:THR:HA	2.14	0.48
1:B:308:LEU:HD11	1:B:322:PHE:CD2	2.49	0.48
1:A:476:ARG:O	1:A:484:LYS:HE2	2.14	0.47
1:B:321:TYR:CD1	1:B:597:ILE:HG12	2.49	0.47
1:B:618:LEU:HD23	1:B:624:LEU:HA	1.95	0.47
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.95	0.47
1:A:308:LEU:HD11	1:A:322:PHE:CD2	2.49	0.47
1:B:370:MET:HE3	1:B:372:HIS:HB3	1.95	0.47
1:A:461:PRO:HG3	1:A:673:LEU:HD12	1.96	0.47
1:B:768:ARG:HD3	1:B:843:MET:O	2.15	0.47
1:A:401:GLU:HG3	1:A:528:TRP:CH2	2.50	0.47
1:A:784:LYS:HB2	1:A:797:THR:N	2.21	0.47
1:B:907:GLU:O	1:B:913:LYS:HB2	2.14	0.47
1:B:676:GLU:HG2	2:D:3:DC:N4	2.30	0.47
1:B:540:ARG:HA	1:B:540:ARG:HD3	1.64	0.47
1:A:134:LEU:O	1:A:138:GLN:HG3	2.15	0.47
1:A:219:ALA:O	1:A:223:SER:HB2	2.15	0.47
1:A:907:GLU:O	1:A:913:LYS:HB2	2.15	0.47
1:A:785:SER:O	1:A:786:ARG:HB2	2.16	0.46
1:B:321:TYR:CE1	1:B:597:ILE:HG12	2.50	0.46
1:B:691:ARG:NH2	1:B:818:SER:O	2.48	0.46
1:A:370:MET:HE1	1:A:373:GLU:HB2	1.98	0.46
1:B:206:ILE:HD13	1:B:252:THR:HB	1.97	0.46
1:A:399:GLU:OE1	1:A:399:GLU:N	2.48	0.46
1:B:575:GLU:HG2	1:B:611:LEU:HD22	1.97	0.46
1:B:806:VAL:HG12	1:B:836:LEU:HG	1.98	0.46
1:B:376:ILE:HG12	1:B:395:LEU:O	2.16	0.45
1:B:419:ASN:HB2	1:B:420:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HA	1:B:552:LEU:O	2.16	0.45
1:B:901:LEU:HD23	1:B:901:LEU:HA	1.58	0.45
1:B:705:ARG:CZ	1:B:753:LYS:HD3	2.46	0.45
1:A:835:ASP:OD1	1:A:836:LEU:N	2.45	0.45
1:B:765:PRO:HG2	1:B:927:GLU:HG3	1.98	0.45
1:B:340:LEU:HB3	1:B:344:ASP:HB2	1.97	0.45
1:B:412:LEU:O	1:B:416:ILE:HG13	2.16	0.45
1:A:401:GLU:HG3	1:A:528:TRP:HH2	1.81	0.45
1:A:540:ARG:HD3	1:A:540:ARG:HA	1.40	0.45
1:B:186:VAL:HB	1:B:309:MET:HE1	1.99	0.45
1:B:283:ARG:NH1	1:B:567:PRO:HB3	2.32	0.45
1:A:142:ASN:OD1	1:A:143:ALA:N	2.45	0.45
1:A:111:GLU:OE1	1:A:115:ARG:NH2	2.50	0.45
1:A:644:ILE:HG22	1:A:741:LEU:HD21	1.99	0.45
1:B:141:GLU:HA	1:B:145:LYS:NZ	2.27	0.44
1:B:337:VAL:O	1:B:538:ARG:NH2	2.49	0.44
1:A:285:VAL:CG2	1:A:568:GLU:HB3	2.47	0.44
1:B:370:MET:HB3	1:B:373:GLU:H	1.82	0.44
1:A:618:LEU:HD23	1:A:624:LEU:HA	1.99	0.44
1:B:339:MET:HE1	1:B:534:THR:HG22	1.99	0.44
1:B:397:LEU:HD22	1:B:399:GLU:OE2	2.17	0.44
2:C:6:DC:H5"	2:C:6:DC:C6	2.48	0.44
1:A:321:TYR:OH	1:A:595:THR:O	2.19	0.44
1:A:786:ARG:CB	1:A:795:ILE:H	2.29	0.44
1:A:467:GLN:HA	1:A:670:TYR:CE1	2.52	0.44
1:B:337:VAL:HG13	1:B:547:GLY:C	2.38	0.44
1:A:182:LYS:HA	1:A:186:VAL:HG23	1.99	0.44
1:A:239:ARG:HG3	2:C:9:DT:OP1	2.17	0.44
1:A:260:LEU:HD23	1:A:263:LEU:HD12	1.99	0.44
1:B:384:ARG:HG3	1:B:385:ASN:ND2	2.33	0.44
1:B:470:GLU:OE1	1:B:670:TYR:OH	2.26	0.44
1:B:645:LEU:HA	1:B:645:LEU:HD23	1.67	0.44
1:B:860:VAL:HG22	1:B:865:PRO:HA	2.00	0.44
1:A:409:ILE:HG12	1:A:552:LEU:HD11	1.99	0.43
1:B:636:ILE:HD12	1:B:737:PHE:CZ	2.53	0.43
1:B:260:LEU:HD21	1:B:290:LEU:HG	1.99	0.43
1:B:800:THR:HG23	1:B:806:VAL:HG21	1.98	0.43
1:B:899:LYS:HD2	1:B:899:LYS:HA	1.70	0.43
1:B:908:GLU:O	1:B:913:LYS:HG2	2.18	0.43
1:A:285:VAL:HG22	1:A:568:GLU:HB3	2.00	0.43
1:B:654:ASP:HB3	1:B:655:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:SER:O	1:A:393:ASP:HB2	2.19	0.43
1:B:515:TYR:HE2	1:B:517:ILE:HD12	1.84	0.43
1:B:694:HIS:NE2	1:B:840:ASP:OD2	2.48	0.43
1:B:348:LYS:HE3	1:B:415:TYR:OH	2.18	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.75	0.43
1:B:239:ARG:HG3	2:D:9:DT:OP1	2.19	0.43
1:B:796:HIS:NE2	1:B:817:GLU:O	2.48	0.43
1:A:119:LEU:HD12	1:A:248:ARG:CZ	2.49	0.43
1:B:893:GLU:O	1:B:897:LEU:HG	2.19	0.43
1:A:339:MET:O	1:A:340:LEU:HD23	2.19	0.42
1:A:848:ALA:HA	1:A:923:LEU:HD21	2.00	0.42
2:D:1:DC:H2"	2:D:2:DT:H71	2.01	0.42
1:A:786:ARG:HD2	1:A:786:ARG:O	2.19	0.42
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.80	0.42
1:A:239:ARG:HH12	2:C:8:DT:H72	1.85	0.42
1:B:289:LEU:HA	1:B:289:LEU:HD23	1.80	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.79	0.42
1:B:387:TYR:HB2	1:B:392:LEU:HD21	2.01	0.42
1:B:544:VAL:HG23	1:B:545:ARG:H	1.84	0.42
1:A:239:ARG:HB2	2:C:8:DT:H5"	2.00	0.42
1:B:183:THR:HG21	1:B:218:ILE:HD13	2.01	0.42
1:B:399:GLU:H	1:B:399:GLU:CD	2.22	0.42
1:A:402:GLY:HA2	1:A:507:SER:O	2.19	0.42
1:A:528:TRP:CZ2	1:A:557:ARG:HD3	2.54	0.42
1:B:289:LEU:HD11	1:B:577:ILE:HG12	2.02	0.42
1:A:300:HIS:C	1:A:302:PRO:HD3	2.40	0.42
1:B:141:GLU:CA	1:B:145:LYS:HZ1	2.28	0.42
1:B:575:GLU:O	1:B:612:LEU:HD11	2.20	0.42
1:B:612:LEU:HD23	1:B:612:LEU:HA	1.86	0.42
1:A:268:LEU:O	1:A:301:ARG:HD3	2.20	0.41
1:B:379:TYR:CZ	1:B:555:ARG:HB2	2.55	0.41
1:A:121:TRP:HA	1:B:122:VAL:O	2.20	0.41
1:A:786:ARG:HB3	1:A:794:ALA:CA	2.49	0.41
1:B:64:VAL:HG21	1:B:925:LEU:HD11	2.01	0.41
1:B:529:VAL:HB	1:B:533:ASN:HB2	2.01	0.41
1:A:753:LYS:HE3	1:A:753:LYS:HB2	1.78	0.41
1:B:493:GLU:HG2	1:B:536:GLN:CG	2.51	0.41
1:A:399:GLU:CD	1:A:399:GLU:H	2.23	0.41
1:A:769:ALA:HB1	1:A:852:PHE:HE2	1.85	0.41
1:A:578:ILE:HG23	1:A:589:PRO:HB3	2.02	0.41
1:B:138:GLN:O	1:B:144:LYS:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ARG:HA	1:B:392:LEU:CD1	2.51	0.41
1:B:673:LEU:HD23	1:B:673:LEU:HA	1.79	0.41
1:B:724:SER:O	1:B:728:GLN:HG3	2.21	0.41
1:A:713:GLU:O	1:A:716:PHE:HB3	2.21	0.41
1:A:383:ILE:HD12	1:A:387:TYR:CD1	2.56	0.41
1:A:702:ILE:HD13	1:A:702:ILE:HA	1.84	0.41
1:B:183:THR:HB	3:B:1001:PO4:O2	2.21	0.41
1:B:313:VAL:O	1:B:314:ARG:C	2.57	0.41
1:A:155:THR:OG1	1:A:180:CYS:O	2.31	0.41
1:B:377:GLU:OE2	1:B:396:ARG:NE	2.44	0.41
1:B:465:LEU:O	1:B:671:SER:N	2.41	0.41
1:B:693:ASP:OD2	1:B:812:SER:OG	2.28	0.41
1:B:702:ILE:HD13	1:B:702:ILE:HA	1.73	0.41
1:A:738:SER:HB3	1:A:750:SER:O	2.20	0.41
1:B:142:ASN:N	1:B:145:LYS:HZ3	2.18	0.41
1:B:778:ASN:HB3	1:B:827:TYR:CE2	2.56	0.41
1:A:866:TYR:CD1	1:A:866:TYR:C	2.94	0.40
1:B:445:PRO:HG3	1:B:450:GLY:O	2.21	0.40
1:B:499:ASP:O	1:B:544:VAL:HG13	2.21	0.40
1:B:506:ASN:OD1	1:B:537:ARG:NH1	2.53	0.40
1:A:375:MET:SD	1:A:560:ARG:HD3	2.62	0.40
1:A:472:GLN:HG3	1:A:476:ARG:HG3	2.04	0.40
1:A:728:GLN:O	1:A:732:ARG:HG3	2.21	0.40
1:A:769:ALA:HB1	1:A:852:PHE:CE2	2.57	0.40
1:B:406:ILE:HD11	1:B:434:LYS:HG3	2.02	0.40
1:B:551:ASN:HB3	1:B:553:PHE:CE2	2.56	0.40
1:B:775:LEU:HA	1:B:775:LEU:HD23	1.84	0.40
1:A:370:MET:CE	1:A:373:GLU:HB2	2.52	0.40
1:A:528:TRP:CE2	1:A:557:ARG:HD3	2.57	0.40
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.76	0.40
1:B:683:LYS:HB3	1:B:813:VAL:HG12	2.03	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	841/944 (89%)	815 (97%)	26 (3%)	0	100	100
1	B	841/944 (89%)	815 (97%)	26 (3%)	0	100	100
All	All	1682/1888 (89%)	1630 (97%)	52 (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	757/842 (90%)	748 (99%)	9 (1%)	71	87
1	B	757/842 (90%)	751 (99%)	6 (1%)	81	92
All	All	1514/1684 (90%)	1499 (99%)	15 (1%)	76	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	145	LYS
1	A	283	ARG
1	A	347	SER
1	A	369	ARG
1	A	434	LYS
1	A	652	CYS
1	A	805	ARG
1	A	901	LEU
1	B	141	GLU
1	B	145	LYS
1	B	347	SER
1	B	369	ARG
1	B	434	LYS
1	B	805	ARG

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

Mol	Chain	Res	Type
1	A	471	GLN
1	B	261	GLN
1	B	264	GLN

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	PO4	A	1001	-	4,4,4	0.70	0	6,6,6	0.98	1 (16%)
3	PO4	B	1001	-	4,4,4	0.88	0	6,6,6	0.84	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	PO4	O3-P-O2	2.06	114.59	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	PO4	1	0

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(Å^2)	Q<0.9
1	A	849/944 (89%)	0.03	24 (2%)	53	49	30, 59, 93, 120	0
1	B	849/944 (89%)	0.07	24 (2%)	53	49	32, 63, 106, 135	0
2	C	9/9 (100%)	0.58	1 (11%)	5	7	69, 77, 93, 103	0
2	D	9/9 (100%)	1.12	2 (22%)	0	1	77, 87, 99, 113	0
All	All	1716/1906 (90%)	0.06	51 (2%)	50	47	30, 61, 98, 135	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	861	THR	5.0
1	A	52	ILE	5.0
1	A	795	ILE	4.5
2	D	1	DC	4.3
1	B	785	SER	3.8
2	C	1	DC	3.4
1	A	794	ALA	3.4
1	B	52	ILE	2.9
1	B	795	ILE	2.9
1	A	53	ARG	2.9
1	A	376	ILE	2.8
1	A	54	LEU	2.8
1	A	393	ASP	2.8
1	B	786	ARG	2.8
1	A	786	ARG	2.7
1	A	396	ARG	2.6
1	B	355	LYS	2.6
1	B	396	ARG	2.6
1	B	142	ASN	2.6
1	A	136	GLN	2.6
1	A	865	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	381	ARG	2.5
1	A	785	SER	2.5
1	A	793	ARG	2.5
1	B	375	MET	2.5
1	B	146	ARG	2.4
1	A	380	LEU	2.4
1	A	382	ARG	2.4
1	B	137	ARG	2.4
1	A	138	GLN	2.3
1	A	377	GLU	2.3
1	B	144	LYS	2.3
1	B	796	HIS	2.3
1	A	135	GLY	2.2
1	B	518	GLU	2.2
1	B	443	ASP	2.2
1	B	383	ILE	2.2
1	A	457	MET	2.2
1	B	393	ASP	2.2
1	B	138	GLN	2.2
1	B	793	ARG	2.1
1	B	53	ARG	2.1
1	B	794	ALA	2.1
1	A	134	LEU	2.1
1	B	147	LEU	2.1
1	B	148	GLU	2.1
2	D	9	DT	2.1
1	A	458	ALA	2.1
1	A	857	GLU	2.1
1	B	382	ARG	2.0
1	A	805	ARG	2.0

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(Å^2)	Q<0.9
3	PO4	A	1001	5/5	0.91	0.16	62,71,90,94	0
3	PO4	B	1001	5/5	0.96	0.14	64,64,81,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.