



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:39 PM UTC

PDB ID : 5N8U / pdb_00005n8u
Title : Crystal Structure of Drosophila DHX36 helicase in complex with CTCTCCT
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 : 2.62 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

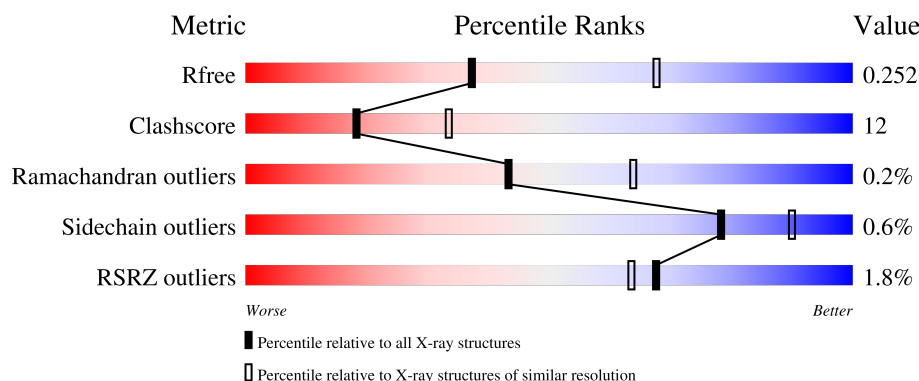
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	944	66% 24% • 10%
1	B	944	69% 20% • 10%
2	C	8	12% 62% 38%
2	D	8	25% 75% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14110 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	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			
1	B	849	Total	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			

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*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			155	75	21	51	8			
2	D	8	Total	C	N	O	P	0	0	0
			155	75	21	51	8			

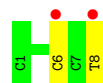
- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	B	80	Total	O	0	0
			80	80		
4	C	1	Total	O	0	0
			1	1		
4	D	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.37Å 51.29Å 164.10Å 90.00° 114.70° 90.00°	Depositor
Resolution (Å)	56.30 – 2.62 56.30 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.3 (56.30-2.62) 98.3 (56.30-2.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.182 , 0.249 0.184 , 0.252	Depositor DCC
R_{free} test set	3434 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14110	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	10/6933 (0.1%)	0.79	11/9353 (0.1%)
1	B	0.49	2/6933 (0.0%)	0.81	17/9353 (0.2%)
2	C	0.51	0/170	0.66	0/258
2	D	0.54	0/170	0.60	0/258
All	All	0.54	12/14206 (0.1%)	0.80	28/19222 (0.1%)

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	B	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	783	ARG	NE-CZ	-11.58	1.20	1.33
1	A	708	ARG	NE-CZ	-8.92	1.23	1.33
1	A	783	ARG	CZ-NH1	-8.71	1.20	1.32
1	A	434	LYS	CD-CE	-7.91	1.28	1.52
1	A	140	GLU	CD-OE1	-7.75	1.10	1.25
1	A	140	GLU	CD-OE2	-7.47	1.11	1.25
1	A	783	ARG	CD-NE	-6.88	1.36	1.46
1	A	783	ARG	CZ-NH2	-6.39	1.25	1.33
1	A	708	ARG	CZ-NH1	-6.24	1.24	1.32
1	B	92	LYS	CD-CE	-6.08	1.34	1.52
1	A	152	LYS	C-N	5.74	1.45	1.33
1	B	606	LYS	CD-CE	5.11	1.67	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	ASN	CA-C-N	10.81	136.64	121.61
1	A	863	ASN	C-N-CA	10.81	136.64	121.61
1	B	477	ARG	CG-CD-NE	-9.82	90.40	112.00
1	B	590	TYR	CA-CB-CG	-8.37	98.83	113.90
1	B	137	ARG	CB-CA-C	7.24	122.80	110.56
1	B	334	MET	CG-SD-CE	-7.18	85.10	100.90
1	B	477	ARG	CA-CB-CG	7.09	128.27	114.10
1	A	133	GLU	CB-CA-C	6.93	122.49	110.01
1	A	433	ASP	CA-C-N	-6.52	110.99	122.26
1	A	433	ASP	C-N-CA	-6.52	110.99	122.26
1	B	477	ARG	CD-NE-CZ	6.28	133.19	124.40
1	B	731	GLU	CA-C-N	-6.02	110.61	121.14
1	B	731	GLU	C-N-CA	-6.02	110.61	121.14
1	A	132	LEU	CA-C-N	-5.95	111.61	122.38
1	A	132	LEU	C-N-CA	-5.95	111.61	122.38
1	A	434	LYS	CG-CD-CE	-5.85	97.84	111.30
1	A	434	LYS	CA-CB-CG	-5.54	103.01	114.10
1	B	145	LYS	CB-CG-CD	5.51	123.98	111.30
1	B	477	ARG	NE-CZ-NH1	5.48	126.98	121.50
1	B	147	LEU	CA-C-N	-5.41	111.49	120.68
1	B	147	LEU	C-N-CA	-5.41	111.49	120.68
1	B	145	LYS	CG-CD-CE	5.32	123.54	111.30
1	B	146	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	543	ARG	N-CA-CB	-5.23	102.47	110.26
1	B	137	ARG	CD-NE-CZ	-5.16	117.18	124.40
1	A	708	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	B	136	GLN	CA-C-N	-5.03	114.60	122.65
1	B	136	GLN	C-N-CA	-5.03	114.60	122.65

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	137	ARG	Peptide
1	B	142	ASN	Peptide
1	B	143	ALA	Peptide
1	B	784	LYS	Peptide
1	B	862	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	6814	0	6913	188	0
1	B	6814	0	6913	146	0
2	C	155	0	92	4	0
2	D	155	0	92	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	77	0	0	11	0
4	B	80	0	0	10	0
4	C	1	0	0	0	0
4	D	4	0	0	1	0
All	All	14110	0	14010	337	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 12.

All (337) 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:142:ASN:O	1:A:146:ARG:NH2	1.73	1.21
1:A:52:ILE:N	4:A:1101:HOH:O	1.86	1.08
1:B:590:TYR:OH	1:B:606:LYS:HD3	1.61	1.01
1:A:515:TYR:OH	1:A:520:ASN:ND2	1.94	0.99
1:B:137:ARG:HA	1:B:140:GLU:OE1	1.69	0.92
1:A:590:TYR:OH	1:A:606:LYS:HG2	1.71	0.91
1:A:429:LEU:HB3	1:A:434:LYS:HE2	1.51	0.91
1:A:239:ARG:HG2	1:A:240:LEU:HG	1.52	0.91
1:A:149:ALA:HA	1:A:152:LYS:HE3	1.52	0.90
1:A:197:ARG:O	4:A:1102:HOH:O	1.89	0.89
1:A:401:GLU:OE1	4:A:1103:HOH:O	1.93	0.87
1:A:431:GLY:H	1:A:434:LYS:HZ1	1.16	0.87
1:A:285:VAL:HG23	1:A:568:GLU:HG3	1.55	0.87
1:A:146:ARG:HA	1:A:149:ALA:HB3	1.56	0.86
1:B:420:GLU:OE2	4:B:1101:HOH:O	1.95	0.83
1:A:567:PRO:HG2	1:A:598:ASN:HD22	1.42	0.83
1:B:369:ARG:NH2	4:B:1103:HOH:O	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:MET:HE1	1:B:663:LEU:HB2	1.61	0.81
1:B:239:ARG:HG2	1:B:240:LEU:HG	1.62	0.80
1:B:132:LEU:O	1:B:136:GLN:HG3	1.81	0.80
1:A:239:ARG:HB2	2:C:8:DT:H3'	1.64	0.80
1:A:141:GLU:OE2	1:A:144:LYS:HG2	1.82	0.79
1:A:470:GLU:OE2	1:A:670:TYR:OH	2.01	0.79
1:A:406:ILE:HD11	1:A:438:LEU:HB2	1.65	0.79
1:B:575:GLU:HG2	1:B:611:LEU:HD22	1.65	0.79
1:A:381:ARG:HA	1:A:384:ARG:HG2	1.66	0.78
1:B:188:GLN:HE21	1:B:226:ARG:HH11	1.28	0.78
1:A:431:GLY:H	1:A:434:LYS:NZ	1.82	0.77
1:B:90:ASP:HB2	1:B:92:LYS:HE3	1.66	0.77
1:A:472:GLN:NE2	4:A:1106:HOH:O	2.16	0.76
1:A:545:ARG:NH1	1:A:546:PRO:O	2.20	0.75
1:B:220:GLU:OE2	4:B:1102:HOH:O	2.04	0.75
1:A:430:PRO:HG2	1:A:434:LYS:HE3	1.68	0.74
1:B:142:ASN:O	1:B:146:ARG:NH1	2.20	0.74
1:A:137:ARG:HH21	1:A:227:CYS:HB2	1.52	0.74
1:B:145:LYS:HA	1:B:148:GLU:OE1	1.88	0.73
1:A:143:ALA:HA	1:A:146:ARG:HH21	1.52	0.73
1:A:430:PRO:CD	1:A:434:LYS:HE3	2.17	0.73
1:B:142:ASN:C	1:B:146:ARG:NH1	2.47	0.73
1:A:429:LEU:HB3	1:A:434:LYS:CE	2.19	0.72
1:B:142:ASN:C	1:B:146:ARG:HH12	1.98	0.71
1:A:146:ARG:O	1:A:150:ARG:N	2.17	0.70
1:B:406:ILE:CD1	1:B:441:ILE:HD12	2.21	0.70
1:A:137:ARG:HA	1:A:140:GLU:OE2	1.89	0.70
1:B:406:ILE:HD11	1:B:441:ILE:HD12	1.74	0.69
1:A:430:PRO:CG	1:A:434:LYS:HE3	2.22	0.69
1:A:431:GLY:N	1:A:434:LYS:HZ1	1.90	0.69
1:A:784:LYS:HG2	1:A:796:HIS:HA	1.73	0.69
1:B:283:ARG:NH1	4:B:1105:HOH:O	2.26	0.69
1:A:756:ALA:O	1:A:759:LYS:HE2	1.93	0.68
1:A:134:LEU:O	1:A:138:GLN:HG3	1.93	0.68
1:A:141:GLU:OE1	1:A:144:LYS:HB3	1.93	0.68
1:A:370:MET:HA	1:A:372:HIS:N	2.09	0.68
1:B:145:LYS:HE2	1:B:148:GLU:OE1	1.95	0.67
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.75	0.67
1:A:432:TYR:OH	1:A:676:GLU:OE2	2.11	0.67
1:A:567:PRO:HG2	1:A:598:ASN:ND2	2.08	0.67
1:A:137:ARG:NH2	1:A:227:CYS:HB2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASP:OD1	4:A:1105:HOH:O	2.13	0.67
1:B:92:LYS:H	1:B:92:LYS:HD2	1.59	0.67
1:A:345:VAL:O	1:A:349:THR:HG22	1.95	0.66
1:A:694:HIS:HD2	1:A:842:THR:OG1	1.79	0.66
1:A:476:ARG:NH2	4:A:1110:HOH:O	2.28	0.65
1:B:197:ARG:NH2	4:B:1108:HOH:O	2.30	0.65
1:B:371:LYS:N	4:B:1107:HOH:O	2.28	0.65
1:A:482:GLN:NE2	4:A:1104:HOH:O	2.10	0.64
1:A:784:LYS:NZ	1:A:786:ARG:HB2	2.12	0.64
1:B:738:SER:OG	1:B:750:SER:O	2.15	0.64
1:B:821:ASP:CG	1:B:928:ARG:HH11	2.06	0.64
1:A:54:LEU:HD21	1:A:861:THR:HG21	1.80	0.63
1:B:283:ARG:NH2	1:B:598:ASN:OD1	2.21	0.63
1:A:387:TYR:HB2	1:A:392:LEU:HD21	1.78	0.63
1:A:857:GLU:HG2	1:A:868:CYS:SG	2.39	0.63
1:B:208:THR:HB	1:B:256:THR:HG22	1.80	0.63
1:B:65:LEU:HD21	1:B:881:THR:HG23	1.80	0.63
1:B:315:GLU:OE2	1:B:329:ARG:NH1	2.31	0.63
1:A:69:LYS:O	1:A:73:GLU:OE1	2.19	0.61
1:B:690:MET:HE2	1:B:695:LEU:HD13	1.81	0.61
1:B:134:LEU:O	1:B:138:GLN:HG3	2.00	0.61
1:A:246:ARG:NH1	4:A:1108:HOH:O	2.27	0.61
1:A:370:MET:HB3	1:A:373:GLU:H	1.65	0.60
1:A:519:THR:HG23	1:A:804:ARG:NH2	2.16	0.60
1:A:443:ASP:O	1:A:454:ARG:NH1	2.34	0.60
1:B:239:ARG:HB2	2:D:8:DT:H3'	1.83	0.60
1:B:285:VAL:HG23	1:B:568:GLU:HG2	1.84	0.60
1:A:343:GLU:OE2	1:A:379:TYR:OH	2.17	0.59
1:A:430:PRO:HD2	1:A:434:LYS:HE3	1.84	0.59
1:A:418:GLU:HG3	1:A:453:TRP:HZ2	1.68	0.59
1:A:730:LEU:HA	1:A:733:MET:HE3	1.85	0.58
1:B:369:ARG:N	4:B:1116:HOH:O	2.37	0.58
1:B:399:GLU:CD	1:B:399:GLU:H	2.13	0.57
1:A:240:LEU:HD12	1:A:729:GLN:NE2	2.20	0.57
1:B:104:ASN:OD1	1:B:107:GLU:HG3	2.04	0.57
1:A:143:ALA:CA	1:A:146:ARG:HH21	2.17	0.57
1:A:614:ARG:NH1	1:A:777:PRO:HG3	2.20	0.57
1:A:826:VAL:HG13	1:A:844:VAL:HG11	1.85	0.57
1:B:590:TYR:OH	1:B:606:LYS:CD	2.45	0.57
1:B:352:GLU:OE1	1:B:353:PHE:N	2.30	0.57
1:A:285:VAL:HG23	1:A:568:GLU:CG	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:ASN:HB3	1:B:827:TYR:CZ	2.40	0.57
1:B:908:GLU:OE1	1:B:913:LYS:HE2	2.04	0.57
1:A:370:MET:SD	1:A:370:MET:N	2.78	0.56
1:A:672:PRO:HG2	1:A:675:LYS:HB2	1.87	0.56
1:B:183:THR:HG21	1:B:218:ILE:HD13	1.87	0.56
1:B:715:ASP:OD2	1:B:719:LYS:NZ	2.36	0.56
1:B:387:TYR:HB2	1:B:392:LEU:HD21	1.88	0.56
1:B:672:PRO:HG2	1:B:675:LYS:HB2	1.87	0.56
1:B:523:SER:HB3	1:B:832:LYS:HE2	1.88	0.56
1:B:614:ARG:NH1	1:B:777:PRO:HG3	2.21	0.56
1:B:729:GLN:NE2	1:B:732:ARG:HE	2.03	0.56
1:A:269:MET:C	1:A:301:ARG:HH12	2.13	0.56
1:B:171:VAL:HG22	1:B:306:VAL:HB	1.89	0.55
1:A:174:ILE:HD12	1:A:309:MET:HE2	1.87	0.55
1:A:418:GLU:HG3	1:A:453:TRP:CZ2	2.42	0.55
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.89	0.55
1:A:381:ARG:HG2	1:A:384:ARG:NH2	2.21	0.55
1:A:238:ILE:HG22	1:A:255:THR:HG23	1.88	0.55
1:B:821:ASP:OD1	1:B:928:ARG:NH1	2.39	0.55
1:A:142:ASN:C	1:A:146:ARG:NH2	2.60	0.54
1:B:793:ARG:HG2	1:B:794:ALA:N	2.22	0.54
1:A:431:GLY:O	1:A:434:LYS:NZ	2.41	0.54
1:A:778:ASN:HB3	1:A:827:TYR:CZ	2.42	0.54
1:B:370:MET:HA	1:B:372:HIS:N	2.23	0.54
1:A:91:ALA:HB2	1:A:902:TYR:CD1	2.42	0.54
1:B:678:ARG:HG2	1:B:721:PHE:HE2	1.73	0.54
1:A:212:ARG:NH1	4:A:1109:HOH:O	2.28	0.54
1:A:421:PRO:O	1:A:483:ARG:NH2	2.40	0.54
1:B:261:GLN:O	1:B:264:GLN:HG2	2.08	0.54
1:A:137:ARG:NH2	1:A:143:ALA:HB2	2.23	0.54
1:A:506:ASN:HD21	1:A:534:THR:HG22	1.73	0.54
1:A:784:LYS:HZ1	1:A:786:ARG:HB2	1.72	0.53
1:B:569:ILE:N	4:B:1110:HOH:O	2.32	0.53
1:A:735:ASN:O	1:A:739:GLU:HG3	2.09	0.53
1:A:354:GLN:NE2	1:A:355:LYS:HE3	2.24	0.53
1:A:461:PRO:HB2	1:A:466:MET:SD	2.49	0.53
1:B:188:GLN:HE21	1:B:226:ARG:NH1	2.01	0.52
1:A:730:LEU:HD23	1:A:733:MET:CE	2.40	0.52
1:A:321:TYR:CD1	1:A:597:ILE:HG12	2.44	0.52
1:B:509:ARG:HH21	1:B:526:GLU:HG2	1.75	0.52
1:B:148:GLU:O	1:B:152:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TRP:CE2	1:A:557:ARG:HD3	2.44	0.52
1:B:90:ASP:HB2	1:B:92:LYS:CE	2.38	0.52
1:A:146:ARG:O	1:A:150:ARG:HG3	2.10	0.52
2:C:6:DC:H5"	2:C:6:DC:H6	1.75	0.52
1:B:729:GLN:NE2	1:B:732:ARG:HH21	2.08	0.51
1:A:75:TYR:CE2	1:A:891:ASN:HB3	2.44	0.51
1:B:492:ALA:O	1:B:540:ARG:HD2	2.10	0.51
1:B:504:VAL:HG23	1:B:541:ALA:HB2	1.91	0.51
1:A:340:LEU:HB3	1:A:344:ASP:HB2	1.93	0.51
1:B:590:TYR:CD2	1:B:590:TYR:N	2.76	0.51
1:A:778:ASN:HB3	1:A:827:TYR:CE2	2.46	0.51
1:A:430:PRO:HB3	1:A:510:THR:CA	2.41	0.51
1:B:528:TRP:CZ2	1:B:557:ARG:HD3	2.46	0.51
1:B:544:VAL:HG23	1:B:545:ARG:HG2	1.91	0.51
1:A:335:PHE:HD2	1:A:545:ARG:N	2.08	0.51
1:A:283:ARG:HH22	1:A:598:ASN:ND2	2.08	0.50
1:B:146:ARG:O	1:B:150:ARG:HG3	2.11	0.50
1:B:500:ASP:OD1	1:B:500:ASP:N	2.34	0.50
1:A:795:ILE:O	1:A:796:HIS:CD2	2.64	0.50
1:B:778:ASN:HB3	1:B:827:TYR:CE1	2.47	0.50
1:A:222:VAL:O	1:A:226:ARG:HG2	2.12	0.50
1:A:590:TYR:HH	1:A:606:LYS:HG2	1.76	0.50
1:B:384:ARG:HG3	1:B:385:ASN:OD1	2.12	0.50
1:A:784:LYS:HD2	1:A:785:SER:N	2.26	0.50
1:A:258:VAL:HG23	2:C:8:DT:H5"	1.93	0.50
1:B:151:LYS:O	1:B:157:LYS:NZ	2.24	0.50
1:A:283:ARG:HH22	1:A:598:ASN:CG	2.20	0.49
1:B:341:TYR:OH	1:B:558:GLU:OE1	2.20	0.49
1:A:74:ASP:OD1	1:A:77:ARG:NH2	2.44	0.49
1:A:459:VAL:HG12	1:A:485:VAL:HB	1.93	0.49
1:B:238:ILE:HG22	1:B:255:THR:HG23	1.93	0.49
1:B:340:LEU:HB3	1:B:344:ASP:HB2	1.95	0.49
1:A:682:ILE:HD13	1:A:720:ASN:HA	1.95	0.49
1:A:73:GLU:O	1:A:77:ARG:HG3	2.12	0.49
1:A:94:GLN:HB2	1:A:901:LEU:HD22	1.95	0.49
1:A:105:PHE:O	1:A:108:PHE:HB3	2.12	0.49
1:A:430:PRO:HB3	1:A:510:THR:HA	1.93	0.49
1:A:830:ARG:HD2	1:A:836:LEU:HD21	1.95	0.49
1:B:665:PHE:HB2	1:B:733:MET:HE1	1.94	0.49
1:A:591:ARG:NH1	4:A:1111:HOH:O	2.29	0.48
1:A:143:ALA:HA	1:A:146:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:OD1	1:A:107:GLU:HG3	2.14	0.48
1:A:686:MET:HE2	1:A:700:THR:HA	1.94	0.48
1:B:463:HIS:HB3	1:B:466:MET:HG3	1.95	0.48
1:B:784:LYS:HG3	1:B:785:SER:H	1.77	0.48
1:A:566:THR:OG1	1:A:571:ARG:HD3	2.13	0.48
1:A:784:LYS:HD2	1:A:785:SER:H	1.79	0.48
1:B:775:LEU:HD12	1:B:826:VAL:HG23	1.94	0.48
1:A:482:GLN:CD	4:A:1104:HOH:O	2.54	0.48
1:A:144:LYS:H	1:A:146:ARG:HH21	1.59	0.48
1:A:658:SER:OG	1:A:698:HIS:HD2	1.97	0.48
1:A:430:PRO:HD2	1:A:434:LYS:CE	2.43	0.48
1:B:109:VAL:HG13	1:B:268:LEU:HD11	1.95	0.47
1:B:583:LEU:HD11	1:B:633:LYS:HG2	1.96	0.47
1:A:515:TYR:OH	1:A:607:MET:HE1	2.14	0.47
1:A:784:LYS:HE2	1:A:795:ILE:O	2.13	0.47
1:A:775:LEU:HD12	1:A:826:VAL:HG23	1.95	0.47
1:A:355:LYS:HE2	1:A:446:LYS:HZ1	1.78	0.47
1:A:270:HIS:HA	1:A:301:ARG:NH1	2.29	0.47
1:B:369:ARG:HB3	1:B:371:LYS:HB2	1.96	0.47
1:B:729:GLN:HE21	1:B:732:ARG:HH21	1.62	0.47
2:D:8:DT:O3'	4:D:101:HOH:O	2.03	0.47
1:A:315:GLU:OE2	1:A:329:ARG:NH1	2.48	0.47
1:A:592:PHE:O	1:A:595:THR:OG1	2.32	0.47
1:B:804:ARG:HD2	1:B:830:ARG:HH12	1.79	0.47
1:A:291:MET:HE1	1:A:318:PHE:CD1	2.50	0.46
1:A:355:LYS:CE	1:A:446:LYS:HZ1	2.29	0.46
1:A:314:ARG:HD3	1:A:564:ILE:HD13	1.97	0.46
1:A:523:SER:HB3	1:A:832:LYS:HD3	1.98	0.46
1:A:673:LEU:HD23	1:A:673:LEU:HA	1.65	0.46
1:B:640:MET:CE	1:B:660:ALA:HA	2.45	0.46
1:A:116:ASN:HB3	1:A:271:ASN:HD21	1.79	0.46
1:A:91:ALA:HB2	1:A:902:TYR:CE1	2.51	0.46
1:A:738:SER:HB2	1:A:752:CYS:HB3	1.97	0.46
1:B:738:SER:HB3	1:B:752:CYS:HB3	1.96	0.46
2:D:6:DC:H6	2:D:6:DC:H5''	1.80	0.46
1:B:388:ASP:HB3	1:B:391:VAL:HG23	1.97	0.46
1:B:830:ARG:HD2	1:B:836:LEU:HD21	1.98	0.46
1:A:240:LEU:HD12	1:A:729:GLN:HE21	1.81	0.46
1:B:690:MET:CE	1:B:695:LEU:HD13	2.45	0.46
1:A:236:TYR:HA	1:A:253:TYR:O	2.16	0.45
1:A:373:GLU:HA	1:A:376:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HG2	1:B:142:ASN:OD1	2.16	0.45
1:B:94:GLN:CG	1:B:901:LEU:HD11	2.46	0.45
1:B:784:LYS:HG3	1:B:785:SER:N	2.31	0.45
1:A:376:ILE:HD11	1:A:395:LEU:HB3	1.98	0.45
1:B:321:TYR:CD1	1:B:597:ILE:HG12	2.51	0.45
1:A:68:VAL:HG13	1:A:918:ALA:HB1	1.99	0.45
1:A:107:GLU:O	1:A:111:GLU:HG3	2.17	0.45
1:A:164:GLN:O	1:A:168:GLU:HG3	2.17	0.45
1:A:728:GLN:O	1:A:732:ARG:HG3	2.16	0.45
1:B:137:ARG:HD3	1:B:137:ARG:C	2.41	0.45
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.84	0.45
1:B:493:GLU:HG2	1:B:536:GLN:CG	2.47	0.45
1:B:765:PRO:HG2	1:B:927:GLU:HG2	1.97	0.45
1:B:499:ASP:O	1:B:544:VAL:HG13	2.17	0.45
1:A:850:ILE:O	1:A:889:ARG:HD2	2.18	0.45
1:A:380:LEU:HD22	1:A:392:LEU:HB3	1.99	0.44
1:A:417:CYS:HA	1:A:483:ARG:HH11	1.83	0.44
1:A:759:LYS:HB2	1:A:759:LYS:HE3	1.71	0.44
1:A:144:LYS:O	1:A:147:LEU:N	2.50	0.44
1:A:916:ILE:O	1:A:920:GLU:HG3	2.18	0.44
1:B:370:MET:C	4:B:1107:HOH:O	2.60	0.44
1:B:692:SER:HB2	1:B:842:THR:HG23	1.99	0.44
1:B:640:MET:HE2	1:B:640:MET:HB3	1.72	0.44
1:A:662:ALA:HB2	1:A:697:VAL:HG11	2.00	0.44
1:A:369:ARG:C	1:A:371:LYS:HB2	2.43	0.44
1:A:509:ARG:NH2	1:A:526:GLU:HG2	2.33	0.44
1:B:390:ARG:HE	1:B:390:ARG:HB2	1.53	0.44
1:B:862:GLN:HB3	1:B:864:THR:OG1	2.18	0.44
1:A:97:PHE:HD1	1:A:629:MET:HE3	1.83	0.44
1:A:301:ARG:HD2	1:A:301:ARG:HA	1.91	0.44
1:B:521:ILE:HD11	1:B:804:ARG:HD3	1.98	0.44
1:B:355:LYS:HB3	1:B:355:LYS:HE3	1.77	0.43
1:A:417:CYS:HB3	1:A:453:TRP:CZ3	2.53	0.43
1:A:419:ASN:HB2	1:A:420:GLU:HG2	2.00	0.43
1:B:73:GLU:OE2	1:B:77:ARG:NH1	2.51	0.43
1:B:94:GLN:HG2	1:B:901:LEU:HD11	2.00	0.43
1:B:133:GLU:O	1:B:137:ARG:HB3	2.18	0.43
1:B:54:LEU:HD23	1:B:874:TYR:HB3	2.01	0.43
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.53	0.43
1:B:107:GLU:O	1:B:111:GLU:HG3	2.17	0.43
1:B:424:ALA:HB3	1:B:501:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:CD	1:A:140:GLU:H	2.26	0.43
1:B:159:ALA:O	1:B:163:ILE:HG13	2.17	0.43
1:B:735:ASN:O	1:B:739:GLU:HG3	2.19	0.43
1:A:370:MET:HA	1:A:372:HIS:H	1.79	0.43
1:A:388:ASP:O	1:A:391:VAL:HG22	2.17	0.43
1:B:68:VAL:HG21	1:B:922:LEU:HG	2.01	0.43
1:A:144:LYS:H	1:A:146:ARG:NH2	2.16	0.43
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.99	0.43
1:B:64:VAL:HG13	1:B:921:LEU:HG	1.99	0.43
1:B:447:THR:O	1:B:451:GLN:HG2	2.18	0.43
1:B:65:LEU:HD11	1:B:881:THR:OG1	2.19	0.43
1:B:188:GLN:NE2	1:B:226:ARG:HH11	2.05	0.43
1:B:278:ASP:HA	1:B:309:MET:HB2	1.99	0.43
1:A:430:PRO:CD	1:A:434:LYS:CE	2.94	0.42
1:A:629:MET:HE3	1:A:629:MET:HB2	1.81	0.42
1:B:379:TYR:OH	1:B:555:ARG:HD2	2.18	0.42
1:B:557:ARG:O	1:B:561:MET:HG3	2.18	0.42
1:A:417:CYS:HA	1:A:483:ARG:NH1	2.34	0.42
1:A:784:LYS:HZ2	1:A:786:ARG:HB2	1.80	0.42
1:A:544:VAL:HG23	1:A:545:ARG:HB3	2.01	0.42
1:B:180:CYS:HB2	1:B:330:ILE:HG22	2.02	0.42
1:A:381:ARG:HG2	1:A:384:ARG:CZ	2.50	0.42
1:A:462:LEU:HB3	1:A:488:SER:HB2	2.02	0.42
1:A:545:ARG:HH11	1:A:546:PRO:N	2.18	0.42
1:B:353:PHE:O	1:B:354:GLN:HB3	2.20	0.42
1:B:154:PRO:O	1:B:157:LYS:HG2	2.19	0.42
1:A:354:GLN:O	1:A:355:LYS:HB2	2.20	0.42
1:B:370:MET:HA	1:B:372:HIS:H	1.85	0.42
1:B:435:ILE:HG12	1:B:487:ILE:HG22	2.02	0.42
1:B:585:HIS:O	1:B:585:HIS:ND1	2.53	0.42
1:A:64:VAL:HG13	1:A:921:LEU:HG	2.01	0.41
1:B:885:VAL:O	1:B:889:ARG:HG3	2.20	0.41
1:A:370:MET:HA	1:A:371:LYS:C	2.46	0.41
1:A:643:MET:HG2	1:A:656:ILE:CG2	2.50	0.41
1:A:676:GLU:HG3	2:C:3:DC:H41	1.85	0.41
1:A:420:GLU:HA	1:A:421:PRO:HD3	1.89	0.41
1:A:522:GLN:O	1:A:831:GLN:HA	2.20	0.41
1:A:784:LYS:HE2	1:A:795:ILE:C	2.45	0.41
1:B:200:ALA:HB1	1:B:249:ALA:HB2	2.01	0.41
1:A:349:THR:OG1	1:A:411:ASP:OD2	2.38	0.41
1:A:496:VAL:O	1:A:540:ARG:NH1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ARG:CZ	4:B:1103:HOH:O	2.63	0.41
1:B:862:GLN:CG	1:B:863:ASN:H	2.33	0.41
1:B:186:VAL:CB	1:B:309:MET:HE1	2.51	0.41
1:B:922:LEU:HD23	1:B:922:LEU:HA	1.90	0.41
1:A:186:VAL:HB	1:A:309:MET:HE1	2.03	0.41
1:B:155:THR:OG1	1:B:180:CYS:O	2.39	0.41
1:B:190:LEU:HD11	1:B:307:ILE:CD1	2.51	0.41
1:B:414:TYR:CZ	1:B:450:GLY:HA2	2.55	0.41
1:B:687:ALA:HB2	1:B:696:MET:HG3	2.02	0.41
1:A:171:VAL:HG22	1:A:306:VAL:HB	2.02	0.41
1:A:597:ILE:H	1:A:597:ILE:HG13	1.72	0.41
1:A:835:ASP:HB3	1:A:837:PHE:CZ	2.55	0.41
1:A:899:LYS:HA	1:A:899:LYS:HD3	1.74	0.41
1:B:141:GLU:O	1:B:141:GLU:CG	2.67	0.41
1:B:850:ILE:O	1:B:889:ARG:HD2	2.21	0.41
1:A:62:SER:O	1:A:66:GLU:HG3	2.20	0.41
1:A:146:ARG:HA	1:A:149:ALA:CB	2.38	0.41
1:A:528:TRP:CZ2	1:A:557:ARG:HD3	2.56	0.41
1:A:769:ALA:HB1	1:A:852:PHE:CE2	2.56	0.41
1:A:885:VAL:O	1:A:889:ARG:HG3	2.21	0.41
1:B:164:GLN:HE21	1:B:168:GLU:CD	2.30	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.95	0.40
1:B:146:ARG:HD2	1:B:146:ARG:N	2.36	0.40
1:B:647:SER:HB3	1:B:656:ILE:HG21	2.03	0.40
1:A:243:ARG:NH1	1:A:243:ARG:HB3	2.36	0.40
1:B:449:LYS:HE2	1:B:449:LYS:HB2	1.80	0.40
1:B:452:ARG:HH11	1:B:452:ARG:HG2	1.86	0.40
1:A:105:PHE:O	1:A:109:VAL:HG23	2.21	0.40
1:A:399:GLU:CD	1:A:399:GLU:H	2.30	0.40
1:B:186:VAL:HB	1:B:309:MET:HE1	2.03	0.40
1:B:835:ASP:OD1	1:B:836:LEU:N	2.49	0.40
1:A:381:ARG:HA	1:A:384:ARG:CG	2.44	0.40
1:B:240:LEU:HD13	1:B:732:ARG:HG3	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%)	814 (97%)	27 (3%)	0	100	100
1	B	841/944 (89%)	819 (97%)	19 (2%)	3 (0%)	30	49
All	All	1682/1888 (89%)	1633 (97%)	46 (3%)	3 (0%)	43	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	LYS
1	B	862	GLN
1	B	420	GLU

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%)	751 (99%)	6 (1%)	73	87
1	B	757/842 (90%)	754 (100%)	3 (0%)	84	92
All	All	1514/1684 (90%)	1505 (99%)	9 (1%)	78	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	226	ARG
1	A	347	SER

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Mol	Chain	Res	Type
1	A	449	LYS
1	A	497	THR
1	A	898	LYS
1	B	327	MET
1	B	399	GLU
1	B	571	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	170	GLN
1	A	232	ASN
1	A	237	GLN
1	A	262	GLN
1	A	271	ASN
1	A	316	GLN
1	A	437	GLN
1	A	520	ASN
1	A	598	ASN
1	A	694	HIS
1	A	698	HIS
1	A	760	ASN
1	B	96	GLN
1	B	138	GLN
1	B	164	GLN
1	B	188	GLN
1	B	209	GLN
1	B	271	ASN
1	B	350	ASN
1	B	437	GLN
1	B	699	ASN
1	B	729	GLN
1	B	891	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1001	-	4,4,4	1.04	0	6,6,6	0.81	0
3	PO4	A	1001	-	4,4,4	1.07	0	6,6,6	0.67	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

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%)	-0.07	13 (1%) 72 68	37, 62, 99, 140	0
1	B	849/944 (89%)	-0.09	14 (1%) 70 67	39, 61, 96, 153	0
2	C	8/8 (100%)	0.82	1 (12%) 8 6	78, 92, 117, 117	0
2	D	8/8 (100%)	0.90	2 (25%) 2 1	66, 86, 113, 114	0
All	All	1714/1904 (90%)	-0.07	30 (1%) 67 63	37, 62, 99, 153	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	ALA	3.5
1	B	178	THR	3.3
1	B	333	VAL	3.2
1	A	143	ALA	3.1
1	B	146	ARG	2.8
1	A	795	ILE	2.7
1	A	90	ASP	2.7
1	B	377	GLU	2.7
1	A	785	SER	2.7
1	B	929	LEU	2.7
1	A	142	ASN	2.6
1	A	434	LYS	2.6
2	C	8	DT	2.6
1	A	73	GLU	2.5
1	B	142	ASN	2.4
1	A	146	ARG	2.4
1	B	132	LEU	2.3
1	B	473	ALA	2.3
1	A	929	LEU	2.3
1	B	334	MET	2.2
1	B	332	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	518	GLU	2.2
2	D	8	DT	2.2
1	B	91	ALA	2.1
1	B	606	LYS	2.1
1	A	520	ASN	2.1
1	B	355	LYS	2.1
1	A	141	GLU	2.0
1	A	376	ILE	2.0
2	D	6	DC	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	B	1001	5/5	0.69	0.21	126,139,143,155	0
3	PO4	A	1001	5/5	0.71	0.17	161,165,170,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.