Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 04:37 AM EDT

PDB ID	:	5N96
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with AGGGTTTTTT
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	:	2.72 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

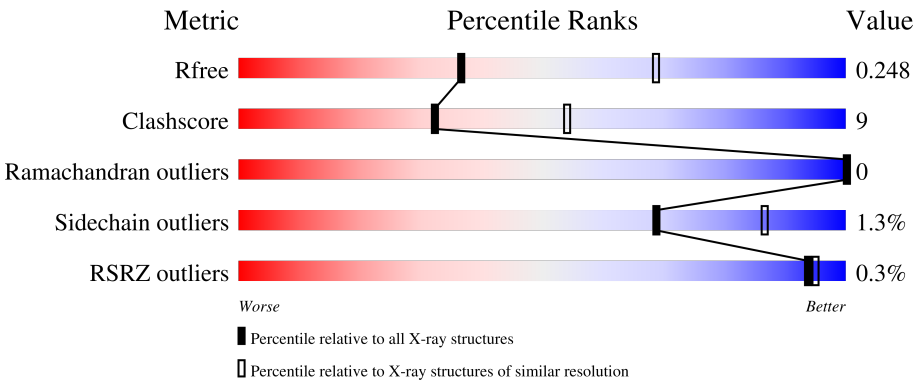
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	72% 17% • 10%
1	B	944	70% 18% • 10%
2	C	10	80% 20%
2	D	10	80% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14156 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
			Total	C	N	O	S			
1	A	849	6814	4304	1200	1265	45	0	0	0
1	B	851	6829	4312	1202	1270	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*AP*GP*GP*GP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	10	191	90	30	61	10	0	0	0
2	D	10	191	90	30	61	10	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is water.

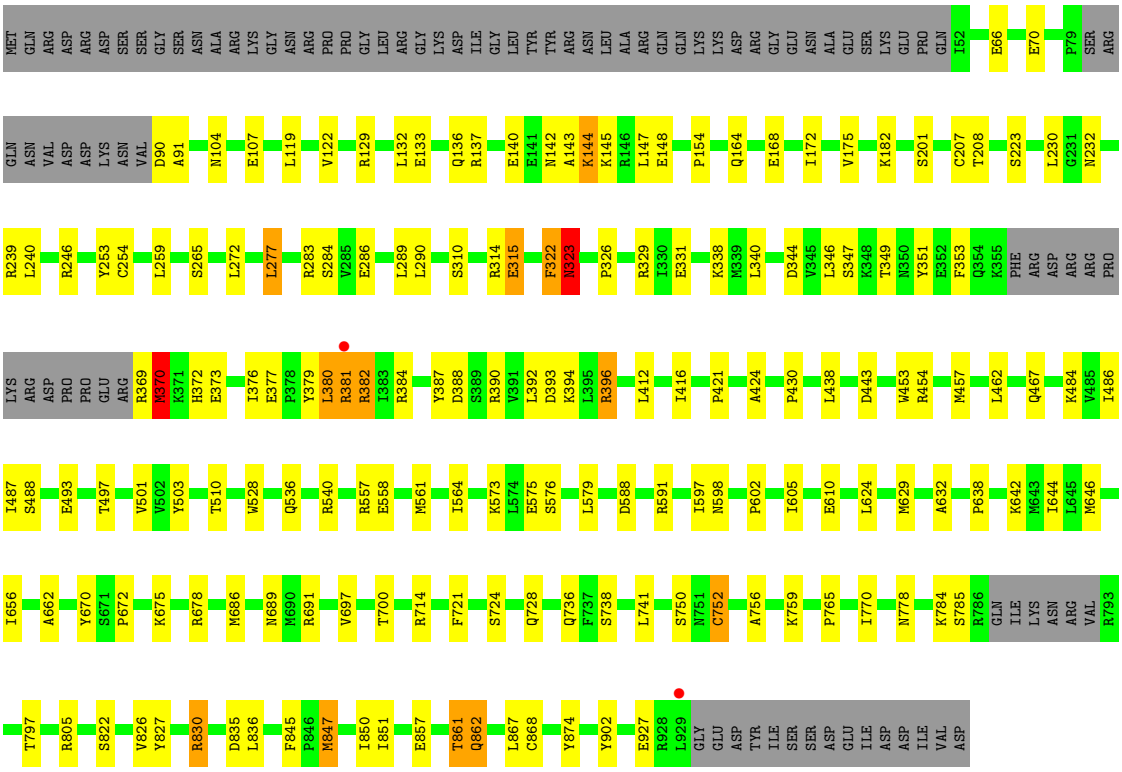
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	57	57	57	0	0
			Total	O		
4	B	67	67	67	0	0
			Total	O		
4	C	3	3	3	0	0
			Total	O		
4	D	2	2	2	0	0

3 Residue-property plots (i)

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.

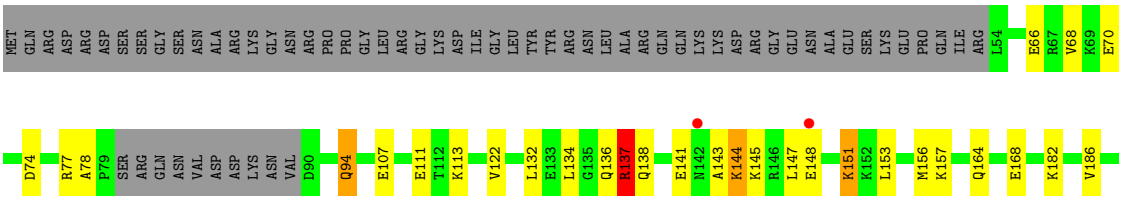
- Molecule 1: CG9323, isoform A

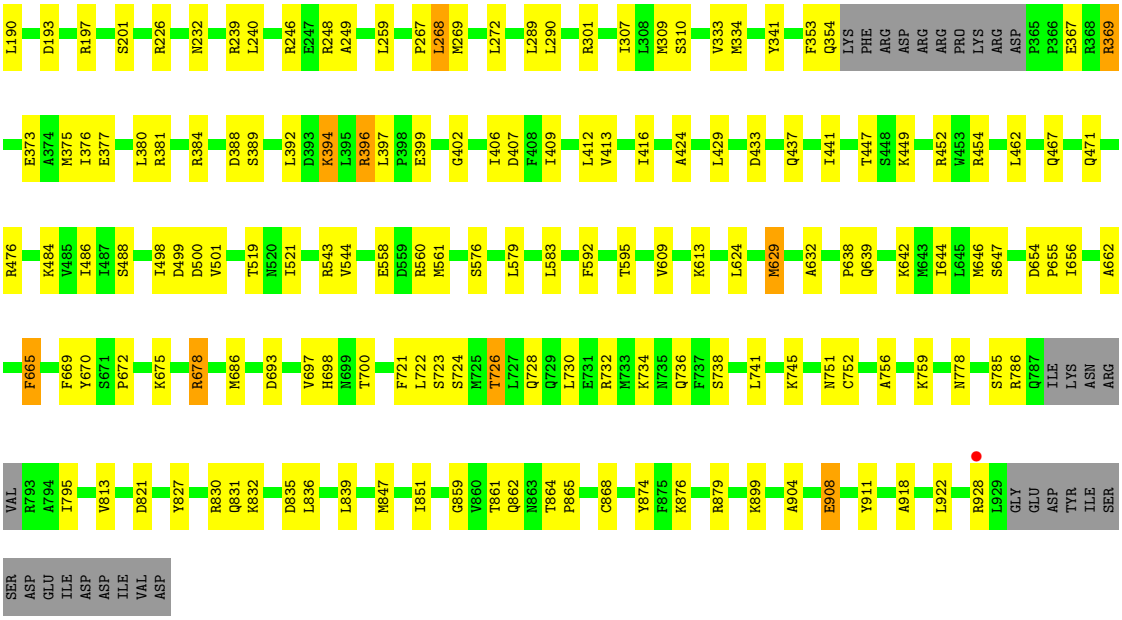
Chain A: 72% 17% • 10%



- Molecule 1: CG9323, isoform A

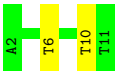
Chain B: 70% 18% • 10%





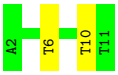
- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*TP*TP*TP*TP*T)-3')

Chain C:



- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*TP*TP*TP*TP*T)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	303.39Å 51.32Å 164.60Å 90.00° 114.57° 90.00°	Depositor
Resolution (Å)	56.65 – 2.72 149.70 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.65-2.72) 97.6 (149.70-2.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.73Å)	Xtriage
Refinement program	PHENIX (dev_2427: ???)	Depositor
R, R_{free}	0.180 , 0.248 0.180 , 0.248	Depositor DCC
R_{free} test set	3131 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14156	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG

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	0.51	3/6933 (0.0%)	0.81	20/9353 (0.2%)
1	B	0.52	4/6950 (0.1%)	0.77	9/9378 (0.1%)
2	C	1.01	0/212	1.17	1/327 (0.3%)
2	D	1.07	0/212	1.21	1/327 (0.3%)
All	All	0.54	7/14307 (0.0%)	0.81	31/19385 (0.2%)

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	5
1	B	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	ARG	NE-CZ	10.88	1.47	1.33
1	A	396	ARG	CG-CD	-7.39	1.33	1.51
1	B	369	ARG	NE-CZ	6.77	1.41	1.33
1	B	396	ARG	NE-CZ	6.59	1.41	1.33
1	B	137	ARG	CB-CG	-5.72	1.37	1.52
1	B	369	ARG	CD-NE	5.58	1.55	1.46
1	A	752	CYS	CB-SG	-5.14	1.73	1.81

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	ARG	NE-CZ-NH2	16.39	128.50	120.30
1	A	396	ARG	NE-CZ-NH1	-13.46	113.57	120.30
1	A	382	ARG	NE-CZ-NH1	11.89	126.25	120.30
1	A	381	ARG	CA-CB-CG	-9.47	92.56	113.40
1	A	382	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	382	ARG	CD-NE-CZ	8.45	135.43	123.60
1	B	137	ARG	CG-CD-NE	-8.27	94.43	111.80
1	B	369	ARG	CG-CD-NE	-7.64	95.76	111.80
1	B	113	LYS	CA-CB-CG	7.04	128.90	113.40
1	A	323	ASN	C-N-CA	7.04	139.31	121.70
1	B	908	GLU	CA-CB-CG	-6.67	98.71	113.40
1	A	381	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	B	151	LYS	CB-CA-C	6.41	123.23	110.40
1	A	861	THR	C-N-CA	-6.34	105.85	121.70
1	A	322	PHE	C-N-CA	6.32	137.50	121.70
1	A	323	ASN	CA-C-N	6.03	130.47	117.20
1	A	847	MET	CG-SD-CE	5.98	109.76	100.20
2	C	6	DT	O4'-C4'-C3'	-5.95	102.12	104.50
1	A	396	ARG	CB-CG-CD	-5.85	96.40	111.60
1	B	144	LYS	CD-CE-NZ	5.73	124.89	111.70
1	B	629	MET	CG-SD-CE	5.71	109.33	100.20
1	A	380	LEU	CA-CB-CG	-5.64	102.33	115.30
1	B	268	LEU	CA-CB-CG	-5.63	102.36	115.30
1	A	323	ASN	N-CA-C	5.60	126.13	111.00
1	B	665	PHE	N-CA-CB	-5.56	100.59	110.60
1	A	382	ARG	CA-CB-CG	5.38	125.23	113.40
1	A	144	LYS	CA-CB-CG	5.37	125.20	113.40
1	A	382	ARG	CG-CD-NE	5.30	122.92	111.80
1	A	277	LEU	CB-CG-CD2	-5.21	102.14	111.00
2	D	6	DT	O4'-C4'-C3'	-5.19	102.42	104.50
1	A	370	MET	C-N-CA	5.11	134.47	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	PHE	Peptide
1	A	323	ASN	Peptide
1	A	353	PHE	Peptide
1	A	370	MET	Peptide
1	A	862	GLN	Peptide
1	B	665	PHE	Mainchain
1	B	861	THR	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	6814	0	6911	118	3
1	B	6829	0	6918	128	2
2	C	191	0	104	2	0
2	D	191	0	104	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	1	0
4	B	67	0	0	6	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
All	All	14156	0	14037	246	3

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 9.

All (246) 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:380:LEU:HD13	1:B:396:ARG:NH1	1.91	0.85
1:A:784:LYS:HB3	1:A:797:THR:H	1.43	0.83
1:A:380:LEU:HD13	1:A:396:ARG:NH1	1.93	0.82
1:B:380:LEU:HD22	1:B:392:LEU:HB3	1.64	0.80
1:B:756:ALA:HA	1:B:759:LYS:HE2	1.65	0.79
1:B:406:ILE:HD13	1:B:441:ILE:HD12	1.65	0.79
1:A:90:ASP:N	4:A:1101:HOH:O	2.16	0.78
1:A:558:GLU:HA	1:A:561:MET:HG3	1.65	0.78
1:A:380:LEU:HD22	1:A:392:LEU:HB3	1.66	0.77
1:B:380:LEU:HD13	1:B:396:ARG:HH11	1.46	0.77
1:B:141:GLU:HB2	1:B:144:LYS:HZ3	1.51	0.75
1:B:353:PHE:O	4:B:1101:HOH:O	2.05	0.74
1:A:421:PRO:O	1:A:503:TYR:OH	2.05	0.73
1:B:745:LYS:NZ	4:B:1104:HOH:O	2.21	0.72
1:A:805:ARG:NH2	1:A:835:ASP:OD2	2.22	0.71
1:A:323:ASN:O	1:A:323:ASN:ND2	2.24	0.70
1:B:193:ASP:O	1:B:197:ARG:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:MET:O	1:A:851:ILE:HG13	1.93	0.69
1:B:381:ARG:HG3	1:B:384:ARG:HH11	1.58	0.69
1:A:373:GLU:HA	1:A:376:ILE:HG22	1.74	0.68
1:A:412:LEU:O	1:A:416:ILE:HG13	1.94	0.68
1:A:644:ILE:HG22	1:A:741:LEU:HD11	1.76	0.68
1:B:137:ARG:NH2	1:B:226:ARG:O	2.25	0.68
1:B:484:LYS:HD3	1:B:486:ILE:HD11	1.76	0.68
1:A:443:ASP:OD1	1:A:454:ARG:NH2	2.28	0.67
1:B:730:LEU:O	1:B:734:LYS:HG3	1.94	0.67
1:B:375:MET:HG3	1:B:560:ARG:HD3	1.76	0.67
1:A:66:GLU:O	1:A:70:GLU:HG3	1.94	0.67
1:A:624:LEU:HD21	1:A:629:MET:HB2	1.75	0.67
1:B:141:GLU:HB2	1:B:144:LYS:NZ	2.08	0.66
1:B:654:ASP:OD1	1:B:734:LYS:NZ	2.27	0.66
1:B:558:GLU:HA	1:B:561:MET:HG3	1.76	0.66
1:B:786:ARG:HB3	1:B:795:ILE:HG22	1.78	0.66
1:B:394:LYS:HA	1:B:397:LEU:HD12	1.78	0.66
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.79	0.64
1:A:381:ARG:HG2	1:A:384:ARG:HG2	1.79	0.64
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.77	0.64
1:B:141:GLU:HA	1:B:144:LYS:HG2	1.81	0.62
1:B:724:SER:O	1:B:728:GLN:HG3	2.01	0.61
1:B:399:GLU:N	1:B:399:GLU:OE1	2.34	0.61
1:A:283:ARG:NH2	1:A:598:ASN:OD1	2.25	0.61
1:B:153:LEU:O	1:B:157:LYS:NZ	2.33	0.61
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.82	0.61
1:A:379:TYR:HD1	1:A:382:ARG:NH2	1.99	0.60
1:B:66:GLU:O	1:B:70:GLU:HG3	2.02	0.60
1:B:376:ILE:HG23	1:B:380:LEU:HD12	1.84	0.60
1:B:462:LEU:HB3	1:B:488:SER:HB2	1.83	0.60
1:B:132:LEU:O	1:B:136:GLN:HG3	2.01	0.60
1:B:644:ILE:HG22	1:B:741:LEU:HD21	1.82	0.60
1:A:380:LEU:CD2	1:A:392:LEU:HB3	2.33	0.59
1:B:143:ALA:C	1:B:145:LYS:H	2.05	0.59
1:A:140:GLU:CD	1:A:142:ASN:H	2.06	0.58
1:A:579:LEU:HG	1:A:632:ALA:HB2	1.84	0.58
1:B:592:PHE:O	1:B:595:THR:HB	2.03	0.58
1:A:381:ARG:HG2	1:A:384:ARG:CG	2.32	0.58
1:B:232:ASN:O	1:B:246:ARG:HG2	2.02	0.58
1:B:137:ARG:HH22	1:B:226:ARG:C	2.08	0.57
1:B:723:SER:OG	1:B:726:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TRP:CZ2	1:A:557:ARG:HD3	2.40	0.57
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.40	0.57
1:A:164:GLN:HE21	1:A:168:GLU:CD	2.08	0.56
1:A:756:ALA:HA	1:A:759:LYS:HE2	1.87	0.56
1:A:380:LEU:CD1	1:A:396:ARG:NH1	2.67	0.56
1:A:784:LYS:HG3	1:A:785:SER:H	1.71	0.56
1:A:239:ARG:HG3	2:C:10:DT:OP1	2.06	0.56
1:B:447:THR:HG22	1:B:449:LYS:H	1.70	0.56
1:A:462:LEU:HB3	1:A:488:SER:HB2	1.87	0.55
1:A:373:GLU:HG3	1:A:377:GLU:HG3	1.88	0.55
1:B:409:ILE:O	1:B:413:VAL:HG23	2.06	0.55
1:A:381:ARG:O	1:A:384:ARG:HG3	2.05	0.55
1:A:91:ALA:HB2	1:A:902:TYR:HD1	1.71	0.55
1:A:277:LEU:HD21	1:A:290:LEU:HD13	1.89	0.55
1:A:784:LYS:HG3	1:A:785:SER:N	2.22	0.55
1:A:573:LYS:HG3	1:A:575:GLU:OE1	2.07	0.55
1:B:373:GLU:HG2	1:B:377:GLU:HG3	1.89	0.55
1:A:738:SER:HB3	1:A:750:SER:O	2.05	0.54
1:A:154:PRO:HB3	1:A:331:GLU:HG2	1.88	0.54
1:B:821:ASP:OD2	1:B:928:ARG:NH1	2.40	0.54
1:B:333:VAL:HG12	1:B:334:MET:N	2.21	0.54
1:A:140:GLU:OE2	1:A:142:ASN:N	2.40	0.54
1:A:259:LEU:HD23	1:A:290:LEU:HD11	1.88	0.54
1:B:148:GLU:HA	1:B:151:LYS:HB3	1.88	0.54
1:A:338:LYS:HG2	1:A:340:LEU:CD1	2.38	0.54
1:B:576:SER:HB2	1:B:638:PRO:HD3	1.89	0.54
1:B:908:GLU:CG	1:B:908:GLU:O	2.55	0.54
1:A:387:TYR:HB2	1:A:392:LEU:HD21	1.90	0.53
1:A:349:THR:HG23	1:A:351:TYR:H	1.72	0.53
1:B:406:ILE:HD12	1:B:407:ASP:N	2.24	0.53
1:A:672:PRO:HG2	1:A:675:LYS:HB2	1.89	0.53
1:B:182:LYS:NZ	1:B:310:SER:O	2.41	0.53
1:A:370:MET:HA	1:A:372:HIS:H	1.73	0.53
1:B:134:LEU:O	1:B:138:GLN:HG3	2.09	0.53
1:A:724:SER:O	1:A:728:GLN:HG3	2.08	0.53
1:B:156:MET:HB2	1:B:157:LYS:HZ2	1.74	0.53
1:B:678:ARG:HG2	1:B:721:PHE:HE2	1.74	0.52
1:A:424:ALA:HB3	1:A:501:VAL:HA	1.92	0.52
1:A:642:LYS:O	1:A:646:MET:HG2	2.10	0.52
1:A:240:LEU:HD21	1:A:736:GLN:HB2	1.92	0.52
1:A:172:ILE:HG22	1:A:326:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:HD13	1:A:867:LEU:HD23	1.92	0.52
1:B:424:ALA:HB3	1:B:501:VAL:HA	1.90	0.52
1:A:861:THR:HG23	1:A:862:GLN:HG2	1.91	0.51
1:B:583:LEU:HD21	1:B:629:MET:HG3	1.92	0.51
1:B:269:MET:O	1:B:301:ARG:NH1	2.43	0.51
1:A:738:SER:OG	1:A:752:CYS:HB3	2.10	0.51
1:B:156:MET:HB2	1:B:157:LYS:NZ	2.26	0.51
1:A:686:MET:HE2	1:A:700:THR:HA	1.93	0.51
1:B:373:GLU:CG	1:B:377:GLU:HG3	2.41	0.51
1:B:519:THR:OG1	1:B:521:ILE:HG12	2.10	0.51
1:A:868:CYS:HB3	1:A:874:TYR:CD2	2.46	0.50
1:B:141:GLU:HA	1:B:143:ALA:O	2.11	0.50
1:B:864:THR:HG21	1:B:876:LYS:HG2	1.93	0.50
1:B:137:ARG:HH22	1:B:226:ARG:CA	2.25	0.50
1:A:137:ARG:NH2	1:A:142:ASN:HD21	2.09	0.50
1:A:182:LYS:NZ	1:A:310:SER:O	2.45	0.50
1:B:388:ASP:OD1	1:B:389:SER:N	2.45	0.50
1:B:639:GLN:HG2	4:B:1148:HOH:O	2.12	0.49
1:B:908:GLU:O	1:B:908:GLU:HG3	2.12	0.49
1:A:686:MET:CE	1:A:700:THR:HA	2.42	0.49
1:B:830:ARG:HD2	1:B:836:LEU:HD21	1.93	0.49
1:B:240:LEU:HD21	1:B:736:GLN:HB2	1.93	0.49
1:A:314:ARG:HD3	1:A:564:ILE:HD13	1.95	0.49
1:A:430:PRO:HA	1:A:510:THR:HA	1.94	0.49
1:A:857:GLU:HG2	1:A:868:CYS:SG	2.53	0.49
1:B:476:ARG:O	1:B:484:LYS:NZ	2.39	0.49
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.94	0.49
1:B:137:ARG:NH1	1:B:226:ARG:O	2.44	0.49
1:A:122:VAL:HG13	1:A:201:SER:OG	2.12	0.49
1:B:373:GLU:HG2	1:B:373:GLU:O	2.12	0.49
1:B:141:GLU:CB	1:B:144:LYS:HZ3	2.23	0.48
1:B:670:TYR:CZ	1:B:723:SER:HB2	2.48	0.48
1:B:433:ASP:O	1:B:437:GLN:HG3	2.13	0.48
1:A:370:MET:HA	1:A:372:HIS:N	2.29	0.48
1:A:576:SER:HB2	1:A:638:PRO:HD3	1.96	0.48
1:A:338:LYS:HG2	1:A:340:LEU:HD11	1.94	0.48
1:B:246:ARG:NH1	1:B:249:ALA:O	2.46	0.48
1:B:239:ARG:HG3	2:D:10:DT:OP1	2.13	0.48
1:B:333:VAL:HG12	1:B:334:MET:O	2.13	0.48
1:A:765:PRO:HG2	1:A:927:GLU:CG	2.44	0.48
1:B:672:PRO:HG2	1:B:675:LYS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:CG	1:A:384:ARG:HG2	2.42	0.47
1:B:899:LYS:HE3	1:B:904:ALA:O	2.14	0.47
1:A:588:ASP:HB3	1:A:591:ARG:HG2	1.96	0.47
1:A:830:ARG:HD3	1:A:836:LEU:HD21	1.95	0.47
1:B:107:GLU:O	1:B:111:GLU:HG3	2.14	0.47
1:A:91:ALA:HB2	1:A:902:TYR:CD1	2.48	0.47
1:A:453:TRP:O	1:A:457:MET:HG3	2.15	0.47
1:A:351:TYR:O	1:A:394:LYS:HE3	2.15	0.47
1:B:122:VAL:HB	1:B:201:SER:OG	2.15	0.47
1:A:656:ILE:HG12	1:A:770:ILE:HG21	1.95	0.47
1:A:662:ALA:HB2	1:A:697:VAL:HG11	1.95	0.47
1:B:333:VAL:CG1	1:B:334:MET:N	2.77	0.47
1:B:147:LEU:CD1	1:B:151:LYS:HE3	2.45	0.47
1:A:346:LEU:HA	1:A:349:THR:HG22	1.96	0.46
1:B:402:GLY:O	4:B:1102:HOH:O	2.20	0.46
1:A:286:GLU:OE1	1:A:286:GLU:N	2.45	0.46
1:B:412:LEU:O	1:B:416:ILE:HG13	2.15	0.46
1:A:175:VAL:HG11	1:A:315:GLU:HG2	1.97	0.46
1:A:830:ARG:HD2	1:A:836:LEU:HD11	1.97	0.46
1:A:132:LEU:O	1:A:136:GLN:HG3	2.16	0.46
1:B:190:LEU:HD11	1:B:307:ILE:CD1	2.45	0.46
1:A:575:GLU:HG2	1:A:576:SER:N	2.31	0.46
1:B:447:THR:HG22	1:B:449:LYS:N	2.31	0.46
1:B:486:ILE:HD13	1:B:498:ILE:HD13	1.96	0.46
1:B:751:ASN:O	4:B:1103:HOH:O	2.20	0.46
1:A:388:ASP:O	1:A:392:LEU:HG	2.16	0.46
1:A:380:LEU:HD13	1:A:396:ARG:HH12	1.76	0.46
1:B:723:SER:CB	1:B:726:THR:HG23	2.46	0.46
1:A:778:ASN:O	1:A:826:VAL:HA	2.16	0.45
1:B:647:SER:HB3	1:B:656:ILE:HG21	1.98	0.45
1:A:340:LEU:HB3	1:A:344:ASP:HB2	1.98	0.45
1:A:315:GLU:OE2	1:A:329:ARG:NH2	2.49	0.45
1:B:669:PHE:CE2	1:B:722:LEU:HD21	2.52	0.45
1:A:380:LEU:HA	1:A:380:LEU:HD23	1.61	0.45
1:B:728:GLN:O	1:B:732:ARG:HG3	2.17	0.45
1:B:899:LYS:HA	1:B:899:LYS:HD2	1.61	0.45
1:A:467:GLN:HG3	1:A:670:TYR:CZ	2.52	0.45
1:B:734:LYS:HB3	1:B:734:LYS:HE2	1.59	0.45
1:A:778:ASN:HB3	1:A:827:TYR:CZ	2.52	0.45
1:B:409:ILE:HD13	1:B:429:LEU:HD21	1.98	0.45
1:B:186:VAL:HG21	1:B:309:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:TYR:OH	1:B:558:GLU:OE2	2.32	0.45
1:A:129:ARG:O	1:A:133:GLU:HG3	2.17	0.44
1:A:822:SER:HB2	1:A:845:PHE:CE1	2.53	0.44
1:B:376:ILE:HG23	1:B:380:LEU:CD1	2.47	0.44
1:A:393:ASP:HA	1:A:396:ARG:NE	2.32	0.44
1:B:500:ASP:OD1	1:B:500:ASP:N	2.50	0.44
1:B:738:SER:OG	1:B:752:CYS:HB3	2.17	0.44
1:B:778:ASN:HB3	1:B:827:TYR:CZ	2.52	0.44
1:A:765:PRO:HG2	1:A:927:GLU:HG3	1.99	0.44
1:B:333:VAL:CG1	1:B:334:MET:H	2.30	0.44
1:B:354:GLN:HB3	4:B:1101:HOH:O	2.17	0.44
1:B:859:GLY:O	1:B:865:PRO:HA	2.17	0.44
1:A:232:ASN:O	1:A:246:ARG:HG2	2.18	0.44
1:B:246:ARG:HD2	1:B:248:ARG:O	2.17	0.44
1:A:283:ARG:NH2	1:A:597:ILE:HG23	2.32	0.44
1:A:830:ARG:CD	1:A:836:LEU:HD11	2.47	0.43
1:A:104:ASN:OD1	1:A:107:GLU:HG2	2.18	0.43
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.77	0.43
1:A:778:ASN:HB3	1:A:827:TYR:CE2	2.54	0.43
1:A:784:LYS:CB	1:A:797:THR:H	2.24	0.43
1:A:208:THR:HA	1:A:254:CYS:O	2.19	0.43
1:B:381:ARG:HG3	1:B:384:ARG:NH1	2.29	0.43
1:B:847:MET:O	1:B:851:ILE:HG13	2.18	0.43
1:B:267:PRO:C	1:B:268:LEU:HD12	2.39	0.43
1:A:147:LEU:HD23	1:A:147:LEU:O	2.19	0.43
1:B:164:GLN:O	1:B:168:GLU:HG3	2.19	0.43
1:B:609:VAL:O	1:B:613:LYS:HG3	2.17	0.43
1:B:693:ASP:OD1	1:B:813:VAL:HG13	2.19	0.43
1:B:868:CYS:HB3	1:B:874:TYR:CD2	2.53	0.43
1:B:642:LYS:O	1:B:646:MET:HG2	2.19	0.43
1:B:655:PRO:HB3	1:B:698:HIS:CD2	2.54	0.43
1:B:74:ASP:O	1:B:77:ARG:HG2	2.19	0.43
1:A:678:ARG:HG2	1:A:721:PHE:HE2	1.83	0.43
1:B:832:LYS:HA	1:B:835:ASP:O	2.19	0.42
1:B:137:ARG:HH22	1:B:226:ARG:HB3	1.84	0.42
1:A:265:SER:HB3	2:C:10:DT:H3	1.85	0.42
1:B:94:GLN:HE21	1:B:94:GLN:HB3	1.60	0.42
1:A:323:ASN:O	1:A:323:ASN:CG	2.57	0.42
1:A:338:LYS:HE2	1:A:340:LEU:HD11	2.00	0.42
1:A:602:PRO:HA	1:A:605:ILE:HD12	2.00	0.42
1:B:467:GLN:HG3	1:B:471:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:LEU:HD23	1:B:922:LEU:HA	1.79	0.42
1:A:145:LYS:NZ	1:A:148:GLU:OE1	2.41	0.42
1:B:624:LEU:HD21	1:B:629:MET:HB2	2.00	0.42
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.83	0.42
1:A:207:CYS:O	1:A:253:TYR:HA	2.18	0.42
1:B:68:VAL:HG13	1:B:918:ALA:HB1	2.02	0.42
1:A:369:ARG:NE	1:A:369:ARG:HA	2.35	0.41
1:B:499:ASP:O	1:B:544:VAL:HG13	2.21	0.41
1:A:137:ARG:O	1:A:137:ARG:HG2	2.20	0.41
1:B:686:MET:CE	1:B:700:THR:HA	2.51	0.41
1:A:497:THR:HG23	1:A:540:ARG:NH1	2.35	0.41
1:A:143:ALA:O	1:A:144:LYS:HB3	2.21	0.41
1:B:137:ARG:CZ	1:B:226:ARG:O	2.69	0.41
1:B:147:LEU:HD13	1:B:151:LYS:HE3	2.03	0.41
1:B:839:LEU:HD23	1:B:839:LEU:HA	1.76	0.41
1:B:862:GLN:H	1:B:862:GLN:CD	2.25	0.41
1:A:438:LEU:HG	1:A:487:ILE:HD13	2.02	0.41
1:B:147:LEU:O	1:B:147:LEU:HD22	2.21	0.41
1:A:850:ILE:HG21	1:A:867:LEU:HD21	2.03	0.40
1:A:289:LEU:HA	1:A:289:LEU:HD12	1.82	0.40
1:B:499:ASP:OD2	1:B:543:ARG:NH1	2.55	0.40
1:A:484:LYS:HD3	1:A:486:ILE:HD11	2.03	0.40
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.84	0.40
1:A:145:LYS:HA	1:A:145:LYS:HD2	1.82	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLU:OE2	1:A:714:ARG:NH2[1_565]	2.04	0.16
1:A:390:ARG:NH2	1:B:367:GLU:OE2[3_555]	2.08	0.12
1:A:396:ARG:NE	1:B:369:ARG:NH1[3_555]	2.15	0.05

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	841/944 (89%)	825 (98%)	16 (2%)	0	100	100
1	B	843/944 (89%)	832 (99%)	11 (1%)	0	100	100
All	All	1684/1888 (89%)	1657 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	749 (99%)	8 (1%)	73	89
1	B	759/842 (90%)	748 (99%)	11 (1%)	67	85
All	All	1516/1684 (90%)	1497 (99%)	19 (1%)	69	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	272	LEU
1	A	284	SER
1	A	315	GLU
1	A	347	SER
1	A	689	ASN
1	A	691	ARG
1	A	830	ARG
1	B	94	GLN
1	B	137	ARG
1	B	272	LEU
1	B	394	LYS
1	B	452	ARG
1	B	454	ARG
1	B	678	ARG

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Mol	Chain	Res	Type
1	B	726	THR
1	B	785	SER
1	B	831	GLN
1	B	879	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	323	ASN
1	B	271	ASN
1	B	437	GLN
1	B	891	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	849/944 (89%)	-0.10	2 (0%)	95	96	30, 54, 95, 123	0
1	B	851/944 (90%)	-0.08	3 (0%)	92	93	30, 52, 91, 161	0
2	C	10/10 (100%)	-0.23	0	100	100	42, 67, 95, 104	0
2	D	10/10 (100%)	-0.08	0	100	100	41, 58, 96, 115	0
All	All	1720/1908 (90%)	-0.09	5 (0%)	94	95	30, 53, 93, 161	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	GLU	2.7
1	B	928	ARG	2.5
1	A	929	LEU	2.5
1	B	142	ASN	2.2
1	A	381	ARG	2.1

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 monosaccharides 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(Å^2)	Q<0.9
3	MG	A	1001	1/1	0.84	0.18	44,44,44,44	0
3	MG	B	1001	1/1	0.86	0.32	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.