Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:05 AM EDT

PDB ID	:	5N9F
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with ssDNA CpG_A
Authors	:	Chen, W.-F.; Rety, S.; Hai-Lei Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on	:	2017-02-24
Resolution	:	2.97 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:

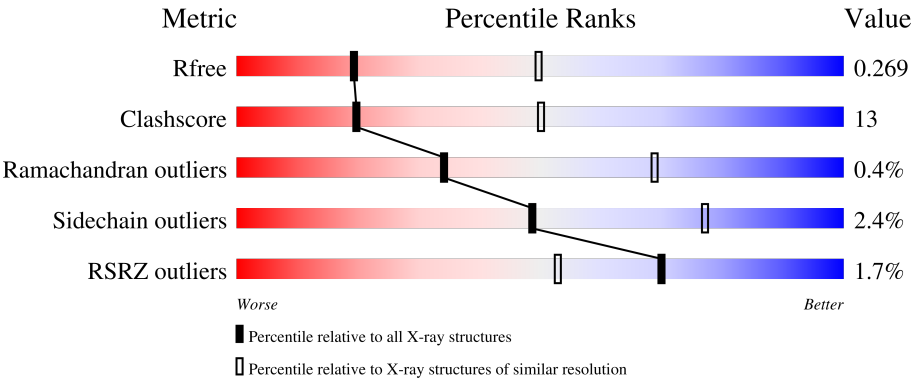
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.97 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	% 66% 24% • 9%
1	B	944	% 65% 25% • 9%
2	C	10	30% 50% 50%
2	D	10	40% 60% 40%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14133 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	859	Total	C	N	O	S	0	0	0
			6900	4357	1219	1279	45			
1	B	855	Total	C	N	O	S	0	0	0
			6844	4322	1206	1271	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(*GP*GP*GP*GP*AP*CP*GP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			192	89	40	54	9			
2	D	10	Total	C	N	O	P	0	0	0
			195	89	40	56	10			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

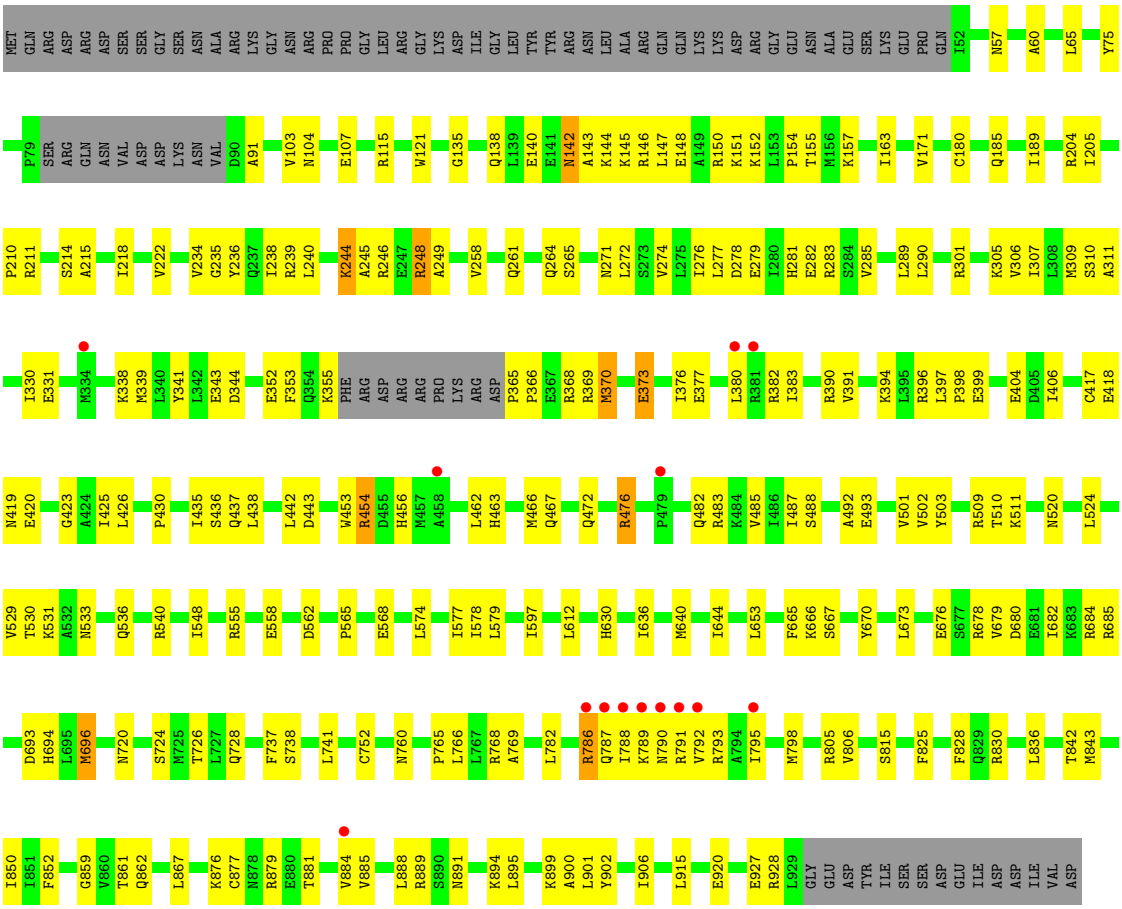
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

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.

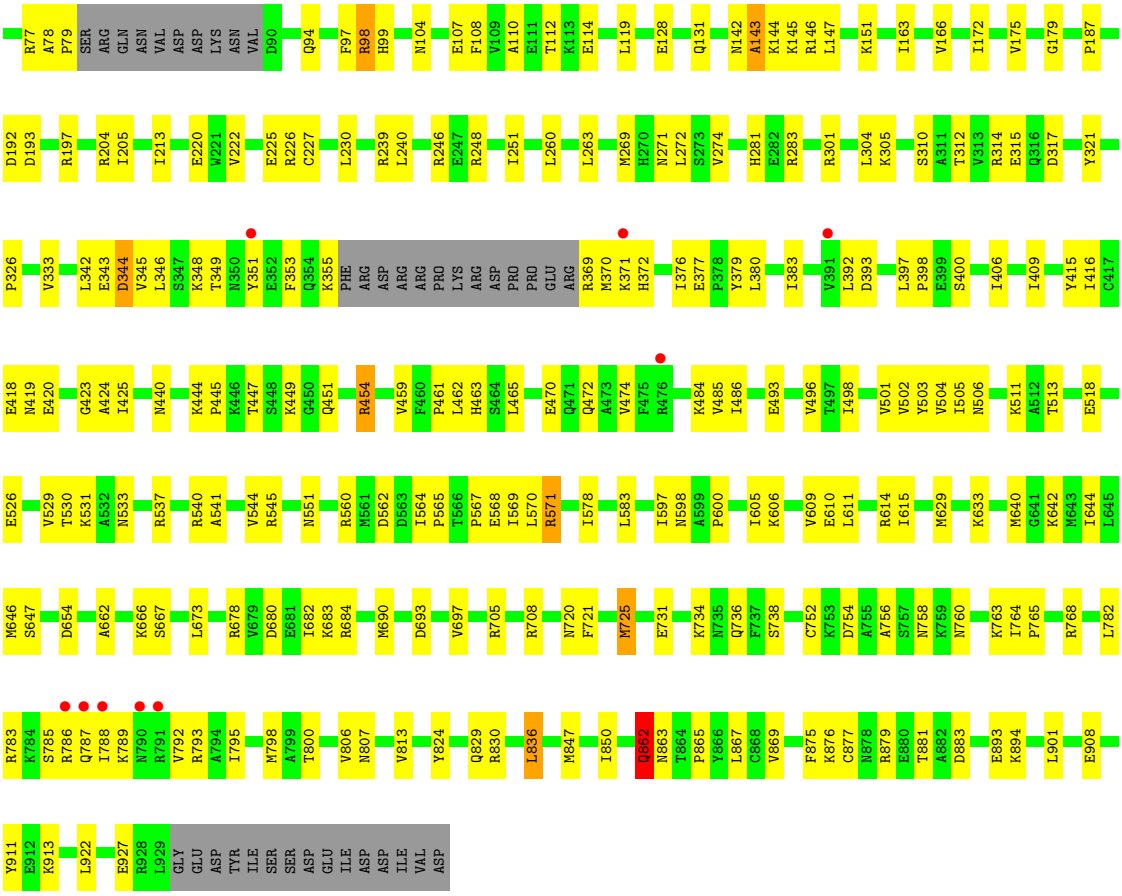
• Molecule 1: CG9323, isoform A

Chain A:



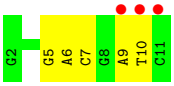
• Molecule 1: CG9323, isoform A

Chain B:



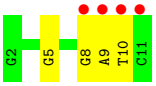
• Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*CP*GP*AP*TP*C)-3')

Chain C:



• Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*CP*GP*AP*TP*C)-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	306.68Å 51.31Å 164.86Å 90.00° 115.55° 90.00°	Depositor
Resolution (Å)	67.10 – 2.97 138.35 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (67.10-2.97) 95.4 (138.35-2.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11_2563: ???)	Depositor
R, R_{free}	0.214 , 0.270 0.215 , 0.269	Depositor DCC
R_{free} test set	2301 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14133	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

5.1 Standard geometry

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

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	0.27	0/7022	0.47	0/9474
1	B	0.27	0/6964	0.46	0/9398
2	C	0.56	0/216	0.81	0/334
2	D	0.48	0/219	0.82	0/338
All	All	0.28	0/14421	0.48	0/19544

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASN	Peptide
1	B	142	ASN	Peptide
1	B	862	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6900	0	7008	178	0
1	B	6844	0	6926	181	0
2	C	192	0	101	6	0
2	D	195	0	100	4	0
3	B	1	0	0	0	0
4	B	1	0	0	1	0
All	All	14133	0	14135	359	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 13.

All (359) 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:175:VAL:HG11	1:B:315:GLU:HG2	1.42	0.98
1:A:147:LEU:HD21	1:A:151:LYS:HE3	1.55	0.89
1:B:461:PRO:HG3	1:B:673:LEU:HD11	1.57	0.86
1:A:529:VAL:HG13	1:A:533:ASN:HB2	1.60	0.84
1:A:891:ASN:HA	1:A:894:LYS:HG2	1.61	0.82
1:B:346:LEU:HA	1:B:349:THR:HG22	1.59	0.82
1:B:143:ALA:O	1:B:145:LYS:N	2.12	0.82
1:A:60:ALA:H	1:A:881:THR:HG21	1.45	0.82
1:A:239:ARG:HG2	1:A:240:LEU:HD22	1.62	0.82
1:B:60:ALA:H	1:B:881:THR:HG21	1.42	0.81
1:B:850:ILE:HG22	1:B:869:VAL:HB	1.64	0.79
1:A:147:LEU:CD2	1:A:151:LYS:HE3	2.12	0.79
1:B:65:LEU:HD11	1:B:881:THR:HG22	1.62	0.79
1:B:830:ARG:HD2	1:B:836:LEU:HD21	1.63	0.78
1:A:418:GLU:HG2	1:A:453:TRP:HZ2	1.49	0.78
1:A:214:SER:O	1:A:218:ILE:HD12	1.84	0.77
1:B:240:LEU:HD21	1:B:736:GLN:HB2	1.67	0.77
1:A:65:LEU:HD11	1:A:881:THR:HG22	1.68	0.76
1:B:269:MET:HB3	1:B:272:LEU:HD21	1.66	0.76
1:B:654:ASP:H	1:B:758:ASN:ND2	1.84	0.75
1:A:636:ILE:HG12	1:A:640:MET:HG3	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASN:O	1:A:830:ARG:NH2	2.20	0.74
1:B:800:THR:HG23	1:B:806:VAL:HG11	1.70	0.73
1:B:447:THR:HG22	1:B:449:LYS:H	1.52	0.72
1:B:611:LEU:HD23	1:B:615:ILE:HD13	1.73	0.71
1:B:850:ILE:HD12	1:B:867:LEU:HD21	1.71	0.71
1:A:503:TYR:HE1	1:A:548:ILE:HD12	1.56	0.70
1:B:343:GLU:N	1:B:343:GLU:OE1	2.21	0.70
1:B:690:MET:O	1:B:768:ARG:NH2	2.24	0.70
1:A:154:PRO:HG2	1:A:180:CYS:HA	1.75	0.69
1:A:278:ASP:OD2	1:A:279:GLU:N	2.24	0.69
1:A:135:GLY:HA2	1:A:138:GLN:H	1.58	0.69
1:B:416:ILE:HD11	1:B:425:ILE:HD13	1.76	0.68
1:A:368:ARG:HE	1:A:398:PRO:HB3	1.59	0.68
1:A:369:ARG:NH1	1:B:393:ASP:OD2	2.28	0.67
1:B:459:VAL:HG23	1:B:485:VAL:HG23	1.76	0.67
1:B:246:ARG:HD2	1:B:248:ARG:O	1.94	0.66
1:A:171:VAL:HG22	1:A:306:VAL:HG13	1.77	0.66
1:B:416:ILE:CD1	1:B:425:ILE:HD13	2.27	0.65
1:B:94:GLN:HE21	1:B:98:ARG:HE	1.45	0.65
1:B:463:HIS:CD2	1:B:465:LEU:H	2.15	0.65
1:A:786:ARG:HH21	1:A:790:ASN:N	1.95	0.65
1:B:504:VAL:HG23	1:B:541:ALA:HB2	1.78	0.64
1:B:682:ILE:HD13	1:B:720:ASN:HA	1.77	0.64
1:A:899:LYS:HE3	1:A:906:ILE:HG12	1.78	0.64
1:A:155:THR:HG22	1:A:330:ILE:HD12	1.79	0.64
1:A:679:VAL:HA	1:A:682:ILE:HG22	1.78	0.64
1:A:417:CYS:HA	1:A:483:ARG:NH1	2.13	0.64
1:B:513:THR:O	1:B:571:ARG:NH1	2.31	0.64
1:B:786:ARG:HD3	1:B:787:GLN:N	2.13	0.64
1:B:146:ARG:NH1	1:B:227:CYS:SG	2.72	0.63
1:B:877:CYS:SG	1:B:881:THR:OG1	2.57	0.63
1:A:443:ASP:OD1	1:A:454:ARG:NH2	2.32	0.63
1:B:425:ILE:HD12	1:B:485:VAL:CG1	2.29	0.63
1:B:445:PRO:HG2	1:B:451:GLN:HG2	1.82	0.62
1:A:368:ARG:NH2	1:A:404:GLU:OE1	2.23	0.62
1:B:454:ARG:O	1:B:454:ARG:NH1	2.32	0.62
1:A:147:LEU:HA	1:A:150:ARG:HB2	1.82	0.62
1:A:214:SER:O	1:A:218:ILE:CD1	2.47	0.62
2:C:6:DA:H2"	2:C:7:DC:O5'	2.00	0.62
1:B:760:ASN:OD1	1:B:763:LYS:NZ	2.33	0.61
1:A:644:ILE:HG22	1:A:741:LEU:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:SER:HA	1:A:673:LEU:HD11	1.81	0.61
1:B:379:TYR:O	1:B:383:ILE:HG12	2.00	0.61
1:B:529:VAL:HG13	1:B:533:ASN:HB2	1.83	0.60
1:A:399:GLU:OE2	1:A:399:GLU:N	2.29	0.60
1:B:342:LEU:HA	1:B:345:VAL:HG12	1.81	0.60
1:B:654:ASP:H	1:B:758:ASN:HD21	1.47	0.60
1:B:806:VAL:HG12	1:B:836:LEU:CD2	2.32	0.60
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.83	0.59
1:B:60:ALA:HB3	1:B:65:LEU:HD21	1.82	0.59
1:B:94:GLN:NE2	1:B:98:ARG:HE	1.98	0.59
1:B:98:ARG:HH22	1:B:901:LEU:HD21	1.68	0.59
1:A:579:LEU:HD13	1:A:612:LEU:HD22	1.84	0.58
1:A:694:HIS:HD2	1:A:842:THR:OG1	1.85	0.58
1:B:312:THR:CA	1:B:315:GLU:OE2	2.51	0.58
1:A:786:ARG:HH21	1:A:790:ASN:H	1.50	0.58
1:A:406:ILE:HD11	1:A:438:LEU:HB2	1.85	0.57
1:B:380:LEU:HB3	1:B:392:LEU:HD21	1.86	0.57
1:A:151:LYS:O	1:A:157:LYS:NZ	2.27	0.57
1:B:312:THR:HB	1:B:315:GLU:OE2	2.03	0.57
1:B:447:THR:HG22	1:B:449:LYS:N	2.19	0.57
1:B:544:VAL:HG22	1:B:545:ARG:HG3	1.86	0.57
2:D:8:DG:H2"	2:D:9:DA:H5'	1.86	0.57
1:A:693:ASP:HA	1:A:696:MET:HG2	1.86	0.57
1:B:187:PRO:HB3	1:B:251:ILE:HD12	1.87	0.57
1:A:382:ARG:HD2	1:A:382:ARG:C	2.23	0.56
1:A:472:GLN:OE1	1:A:476:ARG:NH2	2.38	0.56
1:B:806:VAL:HG12	1:B:836:LEU:HD23	1.88	0.56
1:B:146:ARG:HD3	1:B:225:GLU:HA	1.88	0.56
1:B:531:LYS:HG3	1:B:562:ASP:O	2.06	0.56
1:B:850:ILE:HD12	1:B:867:LEU:CD2	2.36	0.56
1:A:75:TYR:HE2	1:A:891:ASN:HB3	1.71	0.56
1:A:467:GLN:HG3	1:A:670:TYR:CZ	2.40	0.55
1:A:786:ARG:HH11	1:A:795:ILE:CD1	2.18	0.55
1:A:204:ARG:HH22	1:A:244:LYS:NZ	2.04	0.55
1:A:859:GLY:HA2	1:A:879:ARG:HH22	1.71	0.55
1:A:368:ARG:HE	1:A:398:PRO:CB	2.18	0.55
1:A:768:ARG:NH1	1:A:843:MET:O	2.37	0.55
1:B:370:MET:HA	1:B:372:HIS:N	2.22	0.55
1:A:376:ILE:O	1:A:380:LEU:N	2.39	0.55
1:A:377:GLU:HA	1:A:380:LEU:HB2	1.87	0.55
1:B:143:ALA:C	1:B:145:LYS:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ILE:HD13	1:B:498:ILE:HD13	1.89	0.55
1:A:157:LYS:HD2	1:A:157:LYS:N	2.22	0.55
1:B:568:GLU:HA	1:B:571:ARG:HG2	1.88	0.55
1:B:425:ILE:HD12	1:B:485:VAL:HG12	1.89	0.55
1:A:765:PRO:HG2	1:A:927:GLU:HG2	1.90	0.54
1:B:569:ILE:HG23	1:B:570:LEU:HD12	1.88	0.54
1:A:146:ARG:HA	1:A:146:ARG:NE	2.23	0.54
1:A:884:VAL:O	1:A:888:LEU:N	2.39	0.54
1:A:685:ARG:NH2	1:A:720:ASN:OD1	2.41	0.53
1:B:283:ARG:HH21	1:B:597:ILE:HB	1.71	0.53
1:B:462:LEU:HD21	1:B:496:VAL:HG11	1.91	0.53
1:B:222:VAL:O	1:B:226:ARG:HG3	2.09	0.53
1:B:274:VAL:HG12	1:B:305:LYS:HB2	1.90	0.53
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.74	0.53
1:B:530:THR:HG21	1:B:564:ILE:CA	2.39	0.53
1:B:606:LYS:HE2	1:B:610:GLU:HG3	1.91	0.53
1:A:143:ALA:C	1:A:145:LYS:H	2.12	0.53
1:A:653:LEU:HD23	1:A:752:CYS:HA	1.90	0.53
1:B:569:ILE:HG13	1:B:600:PRO:HG3	1.91	0.53
1:A:215:ALA:HB3	1:A:238:ILE:HD11	1.91	0.53
1:A:382:ARG:HD2	1:A:382:ARG:O	2.08	0.53
1:A:463:HIS:HB3	1:A:466:MET:HG3	1.91	0.53
1:A:529:VAL:HG12	1:A:530:THR:O	2.09	0.53
1:A:861:THR:HG23	1:A:862:GLN:H	1.73	0.53
1:B:104:ASN:OD1	1:B:107:GLU:HG2	2.09	0.52
1:A:511:LYS:HB3	1:A:524:LEU:HD11	1.90	0.52
1:B:283:ARG:NH1	1:B:567:PRO:HB3	2.23	0.52
1:B:785:SER:HA	1:B:795:ILE:O	2.09	0.52
1:A:148:GLU:HA	1:A:151:LYS:HZ2	1.75	0.52
1:B:484:LYS:HD3	1:B:486:ILE:HD11	1.91	0.52
1:B:204:ARG:NH1	4:B:1002:CL:CL	2.80	0.52
1:B:786:ARG:HD2	1:B:788:ILE:O	2.09	0.52
1:A:406:ILE:HD13	1:A:437:GLN:HB2	1.91	0.52
1:A:274:VAL:HG23	1:A:305:LYS:HB2	1.92	0.51
1:A:239:ARG:HG3	2:C:10:DT:OP1	2.11	0.51
1:B:175:VAL:CG1	1:B:315:GLU:HG2	2.29	0.51
1:A:277:LEU:HD21	1:A:290:LEU:HD13	1.93	0.51
1:B:239:ARG:HG3	2:D:10:DT:OP1	2.10	0.51
1:A:881:THR:O	1:A:885:VAL:HG13	2.11	0.51
1:B:369:ARG:C	1:B:371:LYS:HB2	2.30	0.51
1:A:786:ARG:HH11	1:A:795:ILE:HD11	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:ASP:O	1:B:684:ARG:HG2	2.11	0.51
1:A:204:ARG:HH22	1:A:244:LYS:HZ2	1.57	0.50
1:A:462:LEU:HB3	1:A:488:SER:HB2	1.92	0.50
1:B:342:LEU:HD12	1:B:345:VAL:HG11	1.92	0.50
1:A:239:ARG:HG3	2:C:9:DA:H3'	1.92	0.50
1:A:425:ILE:HB	1:A:485:VAL:HG22	1.93	0.50
1:A:665:PHE:CG	1:A:666:LYS:N	2.69	0.50
1:B:470:GLU:HB3	1:B:725:MET:HE1	1.93	0.50
1:A:57:ASN:HA	1:A:876:LYS:O	2.12	0.50
1:B:502:VAL:HG23	1:B:503:TYR:CD2	2.46	0.50
1:A:376:ILE:HG13	1:A:380:LEU:HG	1.94	0.49
1:A:503:TYR:CE1	1:A:548:ILE:HD12	2.42	0.49
1:A:115:ARG:NH1	1:A:265:SER:O	2.45	0.49
1:B:220:GLU:HG3	1:B:230:LEU:HD22	1.93	0.49
1:A:530:THR:HG21	1:A:565:PRO:N	2.27	0.49
1:A:135:GLY:CA	1:A:138:GLN:H	2.26	0.49
1:A:222:VAL:HG12	1:A:234:VAL:HG21	1.93	0.49
1:B:260:LEU:HD23	1:B:263:LEU:HD12	1.95	0.49
1:A:365:PRO:N	1:A:366:PRO:HD3	2.28	0.49
1:B:193:ASP:O	1:B:197:ARG:HG3	2.13	0.49
1:A:239:ARG:CG	1:A:240:LEU:HD22	2.40	0.49
1:A:769:ALA:HB1	1:A:852:PHE:HE2	1.76	0.49
1:B:425:ILE:HD12	1:B:485:VAL:HG11	1.94	0.49
1:A:640:MET:HE1	1:A:828:PHE:CE1	2.48	0.49
1:A:285:VAL:HG23	1:A:568:GLU:HG3	1.95	0.48
1:B:415:TYR:O	1:B:418:GLU:HG3	2.13	0.48
1:A:274:VAL:HA	1:A:305:LYS:O	2.12	0.48
1:A:786:ARG:NH2	1:A:790:ASN:HB2	2.27	0.48
1:A:289:LEU:HD11	1:A:577:ILE:HG23	1.95	0.48
1:A:423:GLY:HA3	1:A:502:VAL:CG2	2.43	0.48
1:B:192:ASP:OD1	1:B:226:ARG:NH2	2.43	0.48
1:B:782:LEU:HA	1:B:798:MET:HB3	1.95	0.48
1:B:879:ARG:HD2	1:B:883:ASP:OD1	2.13	0.48
1:A:782:LEU:HB2	1:A:798:MET:HE2	1.96	0.48
1:B:416:ILE:HD12	1:B:425:ILE:HG12	1.95	0.48
1:A:144:LYS:O	1:A:144:LYS:HG2	2.14	0.48
1:A:456:HIS:HA	1:A:482:GLN:HG2	1.95	0.48
1:A:511:LYS:HB2	2:C:5:DG:O4'	2.12	0.48
1:B:321:TYR:CD1	1:B:597:ILE:HG12	2.48	0.48
1:B:419:ASN:HB3	1:B:420:GLU:HG2	1.95	0.48
1:B:578:ILE:HG21	1:B:609:VAL:HG22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:VAL:HG23	1:A:793:ARG:N	2.29	0.48
1:A:397:LEU:HB3	1:A:399:GLU:OE2	2.14	0.48
1:A:417:CYS:HA	1:A:483:ARG:HH11	1.79	0.48
1:B:344:ASP:OD2	1:B:344:ASP:N	2.46	0.48
1:B:738:SER:OG	1:B:752:CYS:HB3	2.14	0.48
1:A:391:VAL:O	1:A:394:LYS:HB2	2.14	0.48
1:A:724:SER:O	1:A:728:GLN:HG3	2.14	0.48
1:A:236:TYR:HD1	1:A:238:ILE:HD13	1.78	0.48
1:B:312:THR:HA	1:B:315:GLU:OE2	2.13	0.48
1:B:353:PHE:CD2	1:B:397:LEU:HD13	2.48	0.48
1:B:342:LEU:HA	1:B:345:VAL:CG1	2.43	0.47
1:B:463:HIS:CD2	1:B:465:LEU:HB2	2.48	0.47
1:B:705:ARG:HD3	1:B:731:GLU:OE2	2.13	0.47
1:A:830:ARG:HD2	1:A:836:LEU:HG	1.96	0.47
1:A:121:TRP:O	1:A:248:ARG:NH2	2.47	0.47
1:A:341:TYR:H	1:A:344:ASP:HB2	1.79	0.47
1:A:370:MET:HA	1:A:373:GLU:HB3	1.95	0.47
1:A:261:GLN:O	1:A:264:GLN:HG2	2.14	0.47
1:A:435:ILE:HG12	1:A:487:ILE:HG22	1.95	0.47
1:B:416:ILE:CD1	1:B:425:ILE:CD1	2.92	0.47
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.50	0.47
1:A:492:ALA:O	1:A:540:ARG:HD2	2.15	0.47
1:A:574:LEU:O	1:A:578:ILE:HG12	2.14	0.47
1:A:895:LEU:HD22	1:A:915:LEU:HD23	1.96	0.47
1:B:416:ILE:HD12	1:B:425:ILE:CD1	2.45	0.47
1:A:406:ILE:HD11	1:A:438:LEU:N	2.29	0.47
1:B:493:GLU:HG3	1:B:537:ARG:HG2	1.97	0.47
1:A:142:ASN:O	1:A:146:ARG:HG2	2.15	0.47
1:A:861:THR:HG23	1:A:862:GLN:N	2.29	0.47
1:B:353:PHE:HD2	1:B:397:LEU:HD13	1.78	0.46
1:B:615:ILE:HG23	1:B:642:LYS:HD3	1.96	0.46
1:B:568:GLU:HA	1:B:571:ARG:CG	2.45	0.46
1:A:426:LEU:HB2	1:A:501:VAL:HG11	1.97	0.46
1:B:147:LEU:O	1:B:151:LYS:HG3	2.15	0.46
1:B:172:ILE:HG22	1:B:326:PRO:HG2	1.98	0.46
1:B:348:LYS:HB3	1:B:415:TYR:OH	2.15	0.46
1:B:564:ILE:HD12	1:B:565:PRO:O	2.16	0.46
1:A:75:TYR:CE2	1:A:891:ASN:HB3	2.51	0.46
1:A:769:ALA:HB1	1:A:852:PHE:CE2	2.51	0.46
1:B:314:ARG:NE	1:B:317:ASP:OD2	2.42	0.46
1:B:666:LYS:HG2	1:B:667:SER:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:ASP:OD1	1:B:756:ALA:N	2.49	0.46
1:B:788:ILE:HA	1:B:789:LYS:HA	1.69	0.46
1:A:285:VAL:HG23	1:A:568:GLU:CG	2.45	0.46
1:A:235:GLY:N	1:A:245:ALA:HB2	2.30	0.46
1:A:238:ILE:HG22	1:A:239:ARG:O	2.15	0.46
1:A:738:SER:OG	1:A:752:CYS:HB3	2.15	0.46
1:B:678:ARG:HG2	1:B:721:PHE:HE2	1.81	0.46
1:A:369:ARG:HD2	1:B:393:ASP:OD1	2.17	0.45
1:A:760:ASN:HB3	1:A:766:LEU:HG	1.97	0.45
1:B:213:ILE:HD12	1:B:213:ILE:H	1.82	0.45
1:B:239:ARG:HG2	1:B:240:LEU:HD12	1.99	0.45
1:B:342:LEU:HD12	1:B:345:VAL:CG1	2.47	0.45
1:B:420:GLU:HB3	1:B:503:TYR:CZ	2.52	0.45
1:B:511:LYS:HE3	1:B:526:GLU:HG3	1.99	0.45
1:B:764:ILE:O	1:B:768:ARG:HG3	2.17	0.45
1:B:654:ASP:OD2	1:B:705:ARG:NH2	2.48	0.45
1:B:654:ASP:N	1:B:758:ASN:HD21	2.13	0.45
1:A:806:VAL:HG12	1:A:836:LEU:HB3	1.99	0.45
1:A:283:ARG:NH2	1:A:597:ILE:HB	2.31	0.45
1:A:836:LEU:HD12	1:A:836:LEU:HA	1.69	0.45
1:B:204:ARG:HD3	1:B:271:ASN:O	2.16	0.45
1:B:283:ARG:NH2	1:B:598:ASN:OD1	2.49	0.45
1:A:382:ARG:C	1:A:382:ARG:HH11	2.21	0.45
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.99	0.45
1:A:531:LYS:HE3	1:A:558:GLU:O	2.17	0.45
1:B:380:LEU:HB3	1:B:392:LEU:HD11	1.99	0.45
1:B:98:ARG:NH2	1:B:901:LEU:HD21	2.32	0.44
1:A:145:LYS:HA	1:A:148:GLU:CD	2.38	0.44
1:A:281:HIS:CD2	1:A:311:ALA:H	2.35	0.44
1:A:339:MET:HE3	1:A:339:MET:HB3	1.86	0.44
1:B:301:ARG:NH2	1:B:304:LEU:HB2	2.33	0.44
1:B:372:HIS:NE2	1:B:398:PRO:HA	2.32	0.44
1:A:281:HIS:HB3	1:A:310:SER:OG	2.17	0.44
1:A:666:LYS:NZ	1:A:726:THR:HG21	2.33	0.44
1:B:312:THR:CB	1:B:315:GLU:OE2	2.65	0.44
1:B:786:ARG:HD3	1:B:787:GLN:H	1.80	0.44
1:A:406:ILE:HD11	1:A:438:LEU:CB	2.48	0.44
1:B:683:LYS:HB3	1:B:813:VAL:HG12	1.99	0.44
1:A:91:ALA:HB2	1:A:902:TYR:HD2	1.83	0.44
1:A:867:LEU:HB2	1:A:877:CYS:SG	2.57	0.44
1:B:283:ARG:NH2	1:B:597:ILE:HB	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASP:OD2	1:A:555:ARG:NH2	2.41	0.44
1:B:583:LEU:HD21	1:B:633:LYS:HG2	2.00	0.44
1:B:786:ARG:HD3	1:B:788:ILE:H	1.83	0.44
1:B:163:ILE:O	1:B:166:VAL:HG22	2.18	0.44
1:B:353:PHE:HE2	1:B:400:SER:HA	1.83	0.44
1:B:97:PHE:HA	1:B:629:MET:HE3	2.00	0.44
1:B:459:VAL:HA	1:B:485:VAL:O	2.18	0.44
1:B:893:GLU:OE1	1:B:894:LYS:NZ	2.50	0.44
1:A:210:PRO:HG3	1:A:279:GLU:HB2	2.00	0.43
1:A:390:ARG:O	1:A:394:LYS:HG3	2.18	0.43
1:A:423:GLY:HA3	1:A:502:VAL:HG21	2.00	0.43
1:B:474:VAL:O	1:B:484:LYS:NZ	2.37	0.43
1:A:185:GLN:O	1:A:189:ILE:HG13	2.18	0.43
1:A:442:LEU:HD12	1:A:487:ILE:HD11	2.00	0.43
1:A:786:ARG:HG2	1:A:787:GLN:N	2.32	0.43
1:A:737:PHE:O	1:A:741:LEU:HG	2.19	0.43
1:B:644:ILE:O	1:B:647:SER:OG	2.30	0.43
1:A:163:ILE:HD11	1:A:189:ILE:HG22	2.00	0.43
1:B:424:ALA:HB3	1:B:501:VAL:HA	2.01	0.43
1:B:765:PRO:HG2	1:B:927:GLU:HG2	2.01	0.43
1:A:215:ALA:CB	1:A:238:ILE:HD11	2.48	0.43
1:B:73:GLU:O	1:B:77:ARG:HG3	2.19	0.43
1:B:865:PRO:HB2	1:B:877:CYS:O	2.18	0.43
1:A:104:ASN:OD1	1:A:107:GLU:HG2	2.19	0.43
1:A:171:VAL:HA	1:A:306:VAL:O	2.19	0.43
1:A:343:GLU:OE2	1:A:555:ARG:NH1	2.52	0.43
1:B:380:LEU:HD22	1:B:392:LEU:HD21	2.01	0.43
1:A:352:GLU:HG3	1:A:353:PHE:N	2.34	0.42
1:A:430:PRO:HA	1:A:510:THR:HA	2.01	0.42
1:A:788:ILE:HA	1:A:789:LYS:HA	1.69	0.42
1:B:55:GLY:O	1:B:876:LYS:HG3	2.18	0.42
1:B:108:PHE:O	1:B:112:THR:HG22	2.19	0.42
1:A:885:VAL:O	1:A:889:ARG:HG3	2.18	0.42
1:B:370:MET:HA	1:B:372:HIS:H	1.84	0.42
1:B:513:THR:OG1	2:D:5:DG:O6	2.30	0.42
1:B:908:GLU:HA	1:B:913:LYS:HD3	2.01	0.42
1:A:676:GLU:H	1:A:676:GLU:HG2	1.63	0.42
1:A:258:VAL:HG23	2:C:9:DA:H5"	2.02	0.42
1:A:760:ASN:ND2	1:A:920:GLU:OE1	2.52	0.42
1:B:376:ILE:O	1:B:380:LEU:HG	2.20	0.42
1:A:338:LYS:HD2	1:A:338:LYS:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:HA	1:A:373:GLU:CB	2.50	0.42
1:B:506:ASN:HB3	1:B:551:ASN:HD22	1.85	0.42
1:B:862:GLN:HB2	1:B:863:ASN:H	1.72	0.42
1:A:140:GLU:O	1:A:144:LYS:HB3	2.20	0.42
1:B:406:ILE:HD12	1:B:406:ILE:HA	1.90	0.42
1:B:824:TYR:HH	1:B:875:PHE:HE1	1.67	0.42
1:A:531:LYS:HG3	1:A:562:ASP:O	2.20	0.42
1:A:680:ASP:O	1:A:684:ARG:HG3	2.20	0.42
1:A:825:PHE:CE2	1:A:843:MET:HB2	2.55	0.42
1:B:353:PHE:CE2	1:B:400:SER:HA	2.55	0.42
1:B:540:ARG:HA	1:B:540:ARG:HD2	1.93	0.42
1:B:128:GLU:HA	1:B:131:GLN:HB3	2.02	0.41
1:B:239:ARG:HB2	2:D:9:DA:O5'	2.20	0.41
1:B:642:LYS:O	1:B:646:MET:HG2	2.19	0.41
1:B:693:ASP:OD2	1:B:813:VAL:HG13	2.20	0.41
1:A:211:ARG:HH22	1:A:282:GLU:CD	2.24	0.41
1:B:377:GLU:HA	1:B:380:LEU:CD1	2.49	0.41
1:A:145:LYS:HA	1:A:148:GLU:OE2	2.20	0.41
1:B:349:THR:HG23	1:B:351:TYR:H	1.85	0.41
1:B:850:ILE:CG2	1:B:869:VAL:HB	2.44	0.41
1:A:278:ASP:HA	1:A:309:MET:HB2	2.02	0.41
1:B:78:ALA:HA	1:B:79:PRO:HD3	1.94	0.41
1:B:409:ILE:HG23	1:B:505:ILE:HG21	2.01	0.41
1:A:205:ILE:HG12	1:A:274:VAL:HG12	2.03	0.41
1:A:666:LYS:HE2	1:A:667:SER:O	2.21	0.41
1:A:204:ARG:HD3	1:A:271:ASN:O	2.20	0.41
1:B:847:MET:HE1	1:B:922:LEU:HD13	2.02	0.41
1:B:440:ASN:O	1:B:444:LYS:HG2	2.20	0.41
1:B:472:GLN:N	1:B:472:GLN:OE1	2.52	0.41
1:A:103:VAL:HB	1:A:107:GLU:HG3	2.03	0.41
1:A:107:GLU:HG2	1:A:107:GLU:H	1.75	0.41
1:A:246:ARG:NH1	1:A:249:ALA:O	2.54	0.41
1:A:630:HIS:HE1	1:A:900:ALA:O	2.04	0.41
1:A:788:ILE:HG23	1:A:789:LYS:HB2	2.03	0.41
1:A:899:LYS:HE3	1:A:906:ILE:CG1	2.47	0.41
1:B:179:GLY:O	1:B:333:VAL:HG22	2.21	0.41
1:B:530:THR:HG21	1:B:564:ILE:HA	2.01	0.41
1:B:605:ILE:O	1:B:609:VAL:HG23	2.20	0.41
1:B:731:GLU:HA	1:B:734:LYS:HD3	2.02	0.41
1:B:110:ALA:O	1:B:114:GLU:HG2	2.21	0.41
1:A:154:PRO:HB3	1:A:331:GLU:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HB2	2:C:9:DA:O5'	2.21	0.40
1:A:679:VAL:HA	1:A:682:ILE:CG2	2.48	0.40
1:B:281:HIS:HB3	1:B:310:SER:OG	2.21	0.40
1:A:850:ILE:HG21	1:A:867:LEU:HD21	2.03	0.40
1:A:238:ILE:CG2	1:A:239:ARG:N	2.84	0.40
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.81	0.40
1:B:205:ILE:HB	1:B:251:ILE:HD13	2.03	0.40
1:A:276:ILE:HG12	1:A:307:ILE:HG12	2.03	0.40
1:A:682:ILE:CD1	1:A:720:ASN:HA	2.52	0.40
1:B:423:GLY:HA3	1:B:502:VAL:HG21	2.04	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	853/944 (90%)	820 (96%)	30 (4%)	3 (0%)	34	69
1	B	849/944 (90%)	815 (96%)	30 (4%)	4 (0%)	29	64
All	All	1702/1888 (90%)	1635 (96%)	60 (4%)	7 (0%)	34	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	LYS
1	B	143	ALA
1	B	862	GLN
1	A	791	ARG
1	B	792	VAL
1	A	420	GLU
1	A	383	ILE

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	767/842 (91%)	747 (97%)	20 (3%)	46 75
1	B	757/842 (90%)	740 (98%)	17 (2%)	52 79
All	All	1524/1684 (90%)	1487 (98%)	37 (2%)	49 77

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LYS
1	A	244	LYS
1	A	248	ARG
1	A	272	LEU
1	A	301	ARG
1	A	355	LYS
1	A	370	MET
1	A	373	GLU
1	A	396	ARG
1	A	419	ASN
1	A	454	ARG
1	A	476	ARG
1	A	509	ARG
1	A	678	ARG
1	A	696	MET
1	A	786	ARG
1	A	805	ARG
1	A	815	SER
1	A	901	LEU
1	A	928	ARG
1	B	98	ARG
1	B	99	HIS
1	B	344	ASP
1	B	355	LYS
1	B	454	ARG
1	B	518	GLU
1	B	560	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	571	ARG
1	B	614	ARG
1	B	640	MET
1	B	708	ARG
1	B	725	MET
1	B	783	ARG
1	B	793	ARG
1	B	807	ASN
1	B	829	GLN
1	B	836	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	237	GLN
1	A	262	GLN
1	A	281	HIS
1	A	467	GLN
1	A	551	ASN
1	A	694	HIS
1	A	781	HIS
1	B	94	GLN
1	B	136	GLN
1	B	164	GLN
1	B	170	GLN
1	B	463	HIS
1	B	467	GLN
1	B	520	ASN
1	B	758	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no 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

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, 95^{th} 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	859/944 (90%)	0.24	14 (1%) 72 55	33, 67, 119, 185	0
1	B	855/944 (90%)	0.14	9 (1%) 80 65	36, 69, 129, 191	0
2	C	10/10 (100%)	1.20	3 (30%) 0 0	81, 126, 156, 182	0
2	D	10/10 (100%)	1.99	4 (40%) 0 0	86, 128, 172, 194	0
All	All	1734/1908 (90%)	0.20	30 (1%) 70 53	33, 68, 128, 194	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	ARG	8.7
1	A	787	GLN	7.9
1	A	788	ILE	6.1
2	D	10	DT	4.5
2	D	11	DC	4.4
1	B	787	GLN	4.1
2	D	9	DA	4.0
1	A	789	LYS	3.9
1	B	790	ASN	3.9
1	A	381	ARG	3.9
1	A	790	ASN	3.6
1	B	788	ILE	3.5
2	D	8	DG	3.0
1	A	786	ARG	2.8
1	B	786	ARG	2.7
1	A	334	MET	2.6
1	A	458	ALA	2.6
1	A	380	LEU	2.5
1	A	795	ILE	2.5
2	C	11	DC	2.5
1	B	791	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	9	DA	2.2
1	B	476	ARG	2.2
1	A	884	VAL	2.2
1	B	371	LYS	2.1
2	C	10	DT	2.1
1	A	479	PRO	2.1
1	B	391	VAL	2.1
1	A	792	VAL	2.1
1	B	351	TYR	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 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, 95^{th} 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
4	CL	B	1002	1/1	0.48	0.27	94,94,94,94	0
3	NA	B	1001	1/1	0.90	0.31	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.