



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 04:56 PM 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

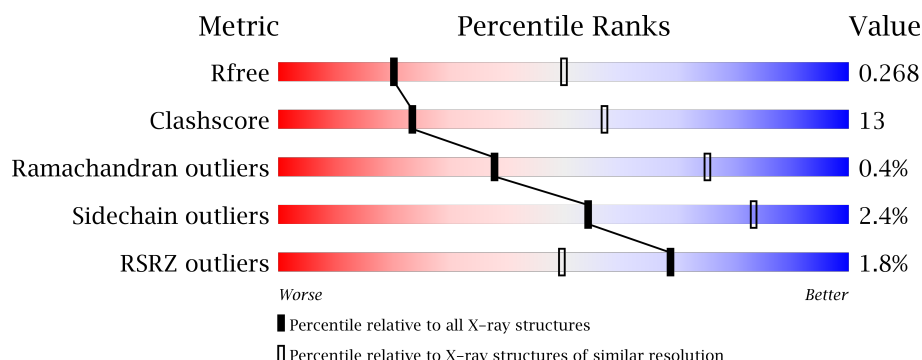
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	944	<div> <div>2%</div> <div>66%</div> <div>24%</div> <div>9%</div> </div>
1	B	944	<div> <div>%</div> <div>65%</div> <div>25%</div> <div>9%</div> </div>
2	C	10	<div> <div>30%</div> <div>50%</div> <div>50%</div> </div>
2	D	10	<div> <div>40%</div> <div>60%</div> <div>40%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	B	1001	-	-	-	X

## 2 Entry composition

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		

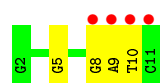
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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



- Molecule 1: CG9323, isoform A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11_2563: ???)	Depositor
R, $R_{free}$	0.214 , 0.270 0.213 , 0.268	Depositor DCC
$R_{free}$ test set	2298 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, CL

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 ⓘ

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:239:ARG:HG2	1:A:240:LEU:HD22	1.62	0.82
1:A:60:ALA:H	1:A:881:THR:HG21	1.45	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

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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:463:HIS:CD2	1:B:465:LEU:H	2.15	0.65
1:B:94:GLN:HE21	1:B:98:ARG:HE	1.45	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:NH1	1:B:454:ARG:O	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

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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:N	1:A:399:GLU:OE2	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:377:GLU:HA	1:A:380:LEU:HB2	1.87	0.55
1:A:376:ILE:O	1:A:380:LEU:N	2.39	0.55
1:B:143:ALA:C	1:B:145:LYS:H	2.10	0.55

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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:462:LEU:HD21	1:B:496:VAL:HG11	1.91	0.53
1:B:283:ARG:HH21	1:B:597:ILE:HB	1.71	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

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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:423:GLY:HA3	1:A:502:VAL:CG2	2.43	0.48
1:A:289:LEU:HD11	1:A:577:ILE:HG23	1.95	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:HG2	1:A:144:LYS:O	2.14	0.48
1:A:456:HIS:HA	1:A:482:GLN:HG2	1.95	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
1:B:321:TYR:CD1	1:B:597:ILE:HG12	2.48	0.48
1:A:511:LYS:HB2	2:C:5:DG:O4'	2.12	0.48

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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:895:LEU:HD22	1:A:915:LEU:HD23	1.96	0.47
1:A:574:LEU:O	1:A:578:ILE:HG12	2.14	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

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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:H	1:B:213:ILE:HD12	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:HA	1:A:836:LEU:HD12	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:HH11	1:A:382:ARG:C	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:867:LEU:HB2	1:A:877:CYS:SG	2.57	0.44
1:A:91:ALA:HB2	1:A:902:TYR:HD2	1.83	0.44
1:B:283:ARG:NH2	1:B:597:ILE:HB	2.32	0.44

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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:459:VAL:HA	1:B:485:VAL:O	2.18	0.44
1:B:97:PHE:HA	1:B:629:MET:HE3	2.00	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:108:PHE:O	1:B:112:THR:HG22	2.19	0.42
1:B:55:GLY:O	1:B:876:LYS:HG3	2.18	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:908:GLU:HA	1:B:913:LYS:HD3	2.01	0.42
1:B:513:THR:OG1	2:D:5:DG:O6	2.30	0.42
1:A:676:GLU:H	1:A:676:GLU:HG2	1.63	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:258:VAL:HG23	2:C:9:DA:H5"	2.02	0.42
1:A:338:LYS:HD2	1:A:338:LYS:N	2.34	0.42

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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:409:ILE:HG23	1:B:505:ILE:HG21	2.01	0.41
1:B:78:ALA:HA	1:B:79:PRO:HD3	1.94	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:OE1	1:B:472:GLN:N	2.52	0.41
1:A:107:GLU:H	1:A:107:GLU:HG2	1.75	0.41
1:A:103:VAL:HB	1:A:107:GLU:HG3	2.03	0.41
1:A:246:ARG:NH1	1:A:249:ALA:O	2.54	0.41
1:A:788:ILE:HG23	1:A:789:LYS:HB2	2.03	0.41
1:B:179:GLY:O	1:B:333:VAL:HG22	2.21	0.41
1:B:605:ILE:O	1:B:609:VAL:HG23	2.20	0.41
1:A:630:HIS:HE1	1:A:900:ALA:O	2.04	0.41
1:A:899:LYS:HE3	1:A:906:ILE:CG1	2.47	0.41
1:B:530:THR:HG21	1:B:564:ILE:HA	2.01	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:239:ARG:HB2	2:C:9:DA:O5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PRO:HB3	1:A:331:GLU:HG2	2.03	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:HA	1:B:119:LEU:HD23	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%)	38	75
1	B	849/944 (90%)	815 (96%)	30 (4%)	4 (0%)	32	71
All	All	1702/1888 (90%)	1635 (96%)	60 (4%)	7 (0%)	38	75

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 ⓘ

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%)	51	82
1	B	757/842 (90%)	740 (98%)	17 (2%)	57	85
All	All	1524/1684 (90%)	1487 (98%)	37 (2%)	54	83

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

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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

Some 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	859/944 (90%)	0.23	15 (1%) 70 51	33, 67, 119, 185	0
1	B	855/944 (90%)	0.14	10 (1%) 79 61	36, 69, 129, 191	0
2	C	10/10 (100%)	1.17	3 (30%) 1 0	81, 126, 156, 182	0
2	D	10/10 (100%)	1.96	4 (40%) 0 0	86, 128, 172, 194	0
All	All	1734/1908 (90%)	0.20	32 (1%) 69 50	33, 68, 128, 194	0

All (32) 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	4.3
2	D	11	DC	4.3
1	B	787	GLN	4.1
1	B	790	ASN	3.9
1	A	789	LYS	3.9
2	D	9	DA	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	795	ILE	2.6
1	A	380	LEU	2.5
1	B	791	ARG	2.4
2	C	11	DC	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	476	ARG	2.2
1	A	884	VAL	2.2
2	C	9	DA	2.1
1	B	371	LYS	2.1
1	A	479	PRO	2.1
1	A	792	VAL	2.1
1	B	391	VAL	2.1
2	C	10	DT	2.0
1	B	351	TYR	2.0
1	A	785	SER	2.0
1	B	785	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	B	1001	1/1	0.90	0.31	2.70	53,53,53,53	0
4	CL	B	1002	1/1	0.48	0.27	-	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.