



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2IS6  
Title : Crystal structure of UvrD-DNA-ADPMgF3 ternary complex  
Authors : Yang, W.; Lee, J.Y.  
Deposited on : 2006-10-16  
Resolution : 2.20 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

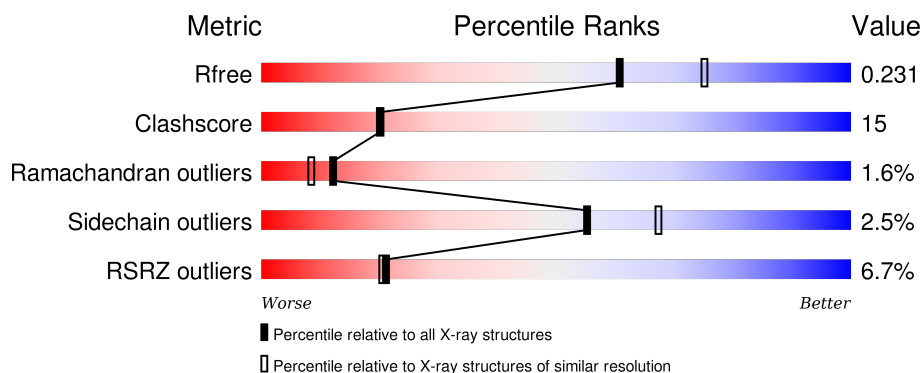
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	C	25	<div> <div>4%</div> <div>32% 60% 8%</div> </div>
1	D	25	<div> <div>4%</div> <div>32% 60% 8%</div> </div>
2	A	680	<div> <div>6%</div> <div>71% 23% . .</div> </div>
2	B	680	<div> <div>7%</div> <div>68% 26% . .</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11795 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 DNA chain called 5'-D(\*CP\*GP\*AP\*GP\*CP\*AP\*CP\*TP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*GP\*TP\*TP\*AP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			
1	D	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	654	Total	C	N	O	S	0	0	0
			5155	3224	939	966	26			
2	B	652	Total	C	N	O	S	0	0	0
			5127	3208	930	962	27			

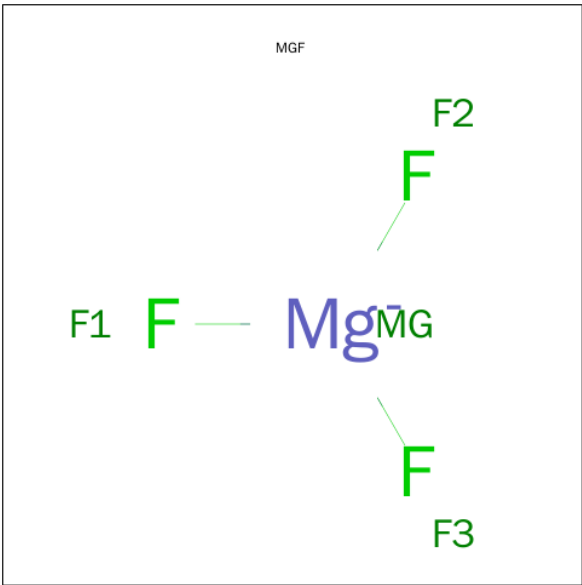
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

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

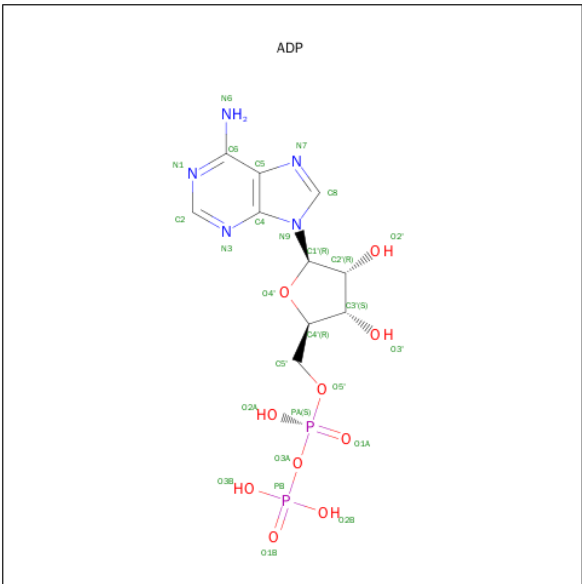
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F<sub>3</sub>Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	F	Mg	0	0
			4	3	1		
4	B	1	Total	F	Mg	0	0
			4	3	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

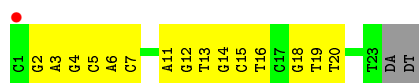
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	243	Total	O	0	0
			243	243		
7	B	239	Total	O	0	0
			239	239		
7	C	15	Total	O	0	0
			15	15		
7	D	10	Total	O	0	0
			10	10		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

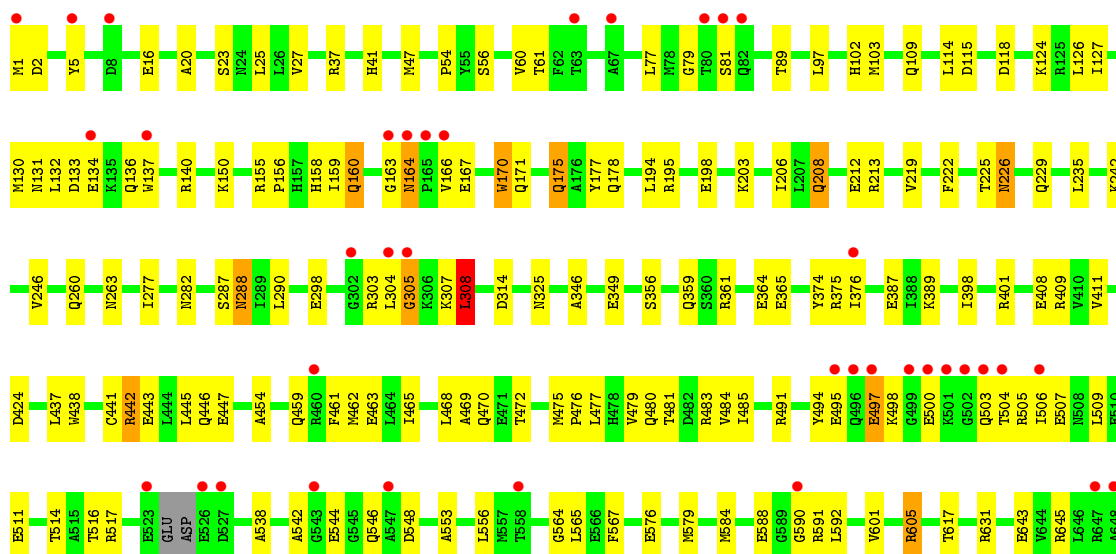
- Molecule 1: 5'-D(\*CP\*GP\*AP\*GP\*CP\*AP\*CP\*TP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*GP\*TP\*TP\*AP\*T)-3'

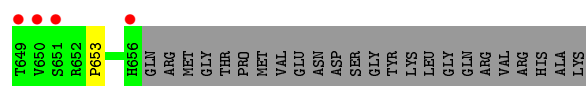


- Molecule 1: 5'-D(\*CP\*GP\*AP\*GP\*CP\*AP\*CP\*TP\*GP\*CP\*AP\*GP\*TP\*GP\*CP\*TP\*CP\*GP\*TP\*TP\*GP\*TP\*TP\*AP\*T)-3'

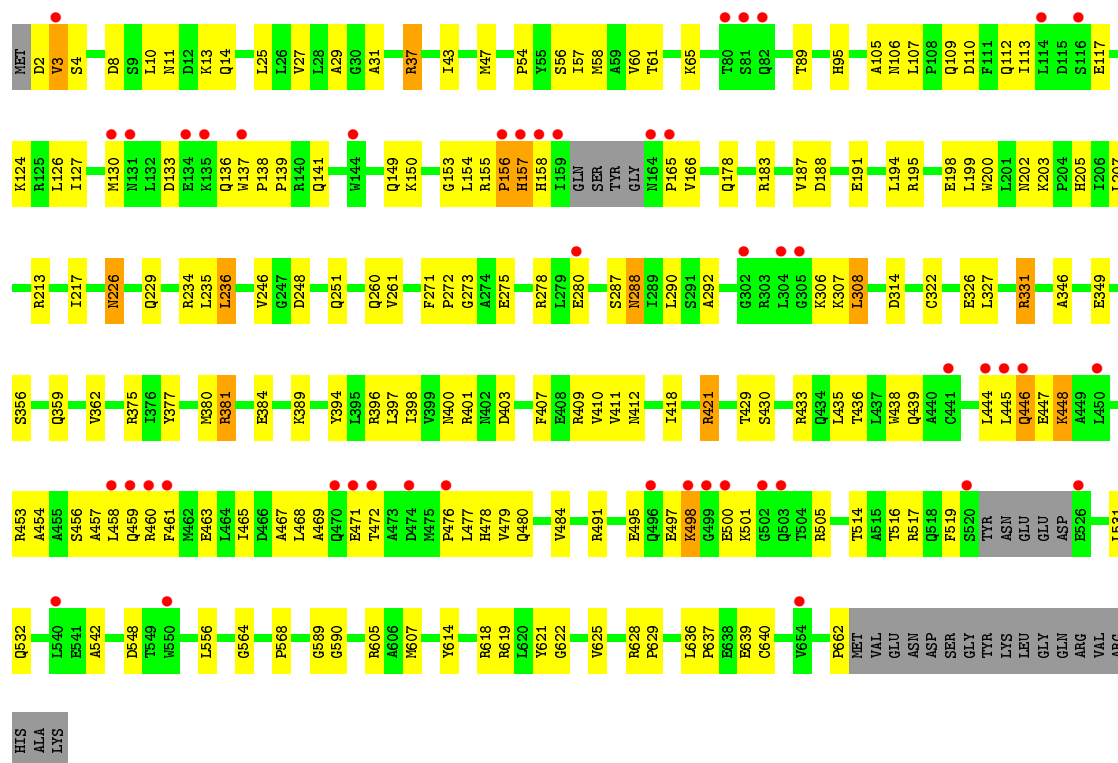


- Molecule 2: DNA helicase II





• Molecule 2: DNA helicase II



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.34Å 96.61Å 110.93Å 90.00° 94.05° 90.00°	Depositor
Resolution (Å)	29.94 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.94-2.20) 89.2 (48.01-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.240 0.204 , 0.231	Depositor DCC
$R_{free}$ test set	9797 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 102183 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, MGF, ADP

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	C	0.30	0/523	0.73	0/806
1	D	0.29	0/523	0.71	0/806
2	A	0.33	0/5251	0.57	1/7107 (0.0%)
2	B	0.34	0/5220	0.54	1/7062 (0.0%)
All	All	0.33	0/11517	0.57	2/15781 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	662	PRO	N-CA-CB	5.71	110.15	103.30
2	A	653	PRO	N-CA-CB	5.35	109.72	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	C	468	0	262	14	0
1	D	468	0	262	24	0
2	A	5155	0	4971	135	0
2	B	5127	0	4969	152	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	6	0	8	2	0
7	A	243	0	0	5	0
7	B	239	0	0	11	0
7	C	15	0	0	1	0
7	D	10	0	0	0	0
All	All	11795	0	10496	320	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 15.

All (320) 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:D:4:DG:H2''	1:D:5:DC:H5''	1.38	0.99
1:D:5:DC:H2''	1:D:6:DA:C8	2.07	0.90
1:C:18:DG:H2''	1:C:19:DT:H5'	1.52	0.89
2:A:155:ARG:H	2:A:158:HIS:HD2	1.17	0.88
2:A:401:ARG:NH1	2:A:465:ILE:HG22	1.93	0.83
2:B:375:ARG:CZ	2:B:548:ASP:HB2	2.11	0.81
2:A:23:SER:HA	2:A:242:LYS:HD2	1.62	0.80
1:C:13:DT:H2''	1:C:14:DG:C8	2.20	0.77
2:B:468:LEU:O	2:B:472:THR:HG22	1.87	0.74
2:A:475:MET:HB3	2:A:479:VAL:HG13	1.69	0.74
1:D:4:DG:C2'	1:D:5:DC:H5''	2.17	0.73
2:A:491:ARG:O	2:A:495:GLU:HG3	1.87	0.73
1:D:11:DA:H2''	1:D:12:DG:C8	2.25	0.72
1:C:18:DG:C2'	1:C:19:DT:H5'	2.19	0.72
2:A:25:LEU:HD11	2:A:277:ILE:HG13	1.72	0.72
2:A:475:MET:HB3	2:A:479:VAL:CG1	2.19	0.72
2:A:401:ARG:HH11	2:A:465:ILE:HG22	1.53	0.71
2:B:396:ARG:HD2	2:B:403:ASP:OD2	1.91	0.71
2:B:438:TRP:HZ3	2:B:465:ILE:HD12	1.56	0.70
2:A:150:LYS:NZ	2:A:178:GLN:HE22	1.89	0.70
2:B:183:ARG:HD2	2:B:435:LEU:HA	1.73	0.70
2:A:443:GLU:HA	2:A:446:GLN:HG2	1.73	0.70
1:D:6:DA:H1'	1:D:7:DC:H5''	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLN:CD	2:B:396:ARG:HD3	2.11	0.70
2:B:112:GLN:HG2	2:B:396:ARG:HH11	1.58	0.69
2:A:155:ARG:H	2:A:158:HIS:CD2	2.05	0.68
2:B:226:ASN:HD21	2:B:229:GLN:HG3	1.58	0.67
2:B:150:LYS:NZ	2:B:178:GLN:HE22	1.92	0.67
2:B:459:GLN:O	2:B:463:GLU:HG3	1.94	0.67
2:A:503:GLN:O	2:A:506:ILE:HG22	1.95	0.67
2:A:25:LEU:HD21	2:A:277:ILE:HD12	1.77	0.66
2:A:1:MET:H3	2:A:5:TYR:HE2	1.44	0.66
2:A:564:GLY:H	2:A:605:ARG:NH2	1.92	0.66
2:A:47:MET:CE	2:A:54:PRO:HG3	2.26	0.66
2:A:477:LEU:HG	2:A:516:THR:HB	1.77	0.65
2:B:436:THR:OG1	2:B:439:GLN:HG3	1.97	0.65
2:B:155:ARG:HB3	2:B:156:PRO:HD2	1.78	0.65
2:B:136:GLN:HE21	2:B:137:TRP:HE1	1.45	0.64
2:A:260:GLN:HG2	7:A:801:HOH:O	1.97	0.64
2:B:187:VAL:HG13	2:B:191:GLU:CG	2.28	0.64
2:B:290:LEU:HD11	2:B:308:LEU:HD13	1.79	0.64
2:A:511:GLU:OE2	2:A:546:GLN:HG3	1.98	0.64
2:B:477:LEU:HG	2:B:516:THR:HB	1.80	0.63
2:B:628:ARG:HB2	2:B:628:ARG:NH2	2.13	0.63
2:A:208:GLN:O	2:A:212:GLU:HG3	1.98	0.63
2:B:628:ARG:HH21	2:B:628:ARG:CB	2.12	0.62
2:A:1:MET:N	2:A:5:TYR:HE2	1.98	0.61
1:C:6:DA:H1'	1:C:7:DC:H5''	1.83	0.61
2:B:191:GLU:OE2	2:B:195:ARG:HD3	2.00	0.60
2:B:398:ILE:HG23	2:B:469:ALA:HA	1.82	0.60
2:A:472:THR:HB	2:A:480:GLN:HG3	1.83	0.60
1:D:11:DA:H2''	1:D:12:DG:H8	1.63	0.60
2:A:356:SER:H	2:A:359:GLN:NE2	2.00	0.60
1:D:6:DA:H2''	1:D:7:DC:H5'	1.83	0.60
2:A:443:GLU:O	2:A:447:GLU:HG3	2.02	0.60
2:B:187:VAL:HG13	2:B:191:GLU:HG3	1.83	0.59
2:A:156:PRO:HB2	2:A:175:GLN:HE21	1.66	0.59
2:A:643:GLU:HG2	2:A:645:ARG:CZ	2.33	0.59
2:B:445:LEU:HD13	2:B:459:GLN:HB2	1.83	0.59
2:A:565:LEU:HD22	6:A:701:GOL:H11	1.85	0.59
2:A:287:SER:HB3	2:A:314:ASP:HA	1.85	0.59
1:D:19:DT:H2''	1:D:20:DT:OP1	2.02	0.58
2:B:202:ASN:O	2:B:203:LYS:HD2	2.03	0.58
2:B:226:ASN:C	2:B:226:ASN:HD22	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:ARG:HH11	2:A:140:ARG:HG3	1.69	0.58
2:B:461:PHE:CZ	2:B:465:ILE:HD11	2.39	0.58
2:A:150:LYS:HZ1	2:A:178:GLN:HE22	1.52	0.57
2:B:472:THR:HG23	2:B:480:GLN:HE21	1.69	0.57
2:A:601:VAL:O	2:A:605:ARG:CD	2.53	0.57
2:A:387:GLU:CD	2:A:505:ARG:HG3	2.24	0.57
2:B:29:ALA:O	2:B:248:ASP:HB2	2.04	0.57
1:D:6:DA:H2''	1:D:7:DC:C5'	2.35	0.57
2:B:326:GLU:CG	2:B:618:ARG:HB2	2.35	0.57
2:B:226:ASN:ND2	2:B:229:GLN:H	2.03	0.57
2:A:170:TRP:CE3	2:A:170:TRP:HA	2.40	0.57
2:A:472:THR:CB	2:A:480:GLN:HG3	2.35	0.56
2:A:601:VAL:O	2:A:605:ARG:HD3	2.05	0.56
2:B:637:PRO:HG2	2:B:640:CYS:SG	2.45	0.56
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.88	0.56
2:A:567:PHE:CE2	6:A:701:GOL:H2	2.40	0.56
2:A:590:GLY:C	2:A:592:LEU:H	2.06	0.56
2:A:140:ARG:HG3	2:A:140:ARG:NH1	2.21	0.56
2:B:47:MET:CE	2:B:54:PRO:HG3	2.36	0.56
2:B:381:ARG:HA	2:B:381:ARG:NE	2.21	0.55
2:B:56:SER:HA	2:B:213:ARG:O	2.06	0.55
2:A:303:ARG:C	2:A:305:GLY:H	2.08	0.55
2:A:47:MET:HE1	2:A:54:PRO:HG3	1.87	0.55
2:A:346:ALA:HB3	2:A:349:GLU:HG3	1.88	0.55
2:B:331:ARG:HB3	2:B:331:ARG:HH11	1.72	0.55
2:B:107:LEU:HD21	2:B:195:ARG:NH1	2.22	0.54
2:B:618:ARG:HD3	7:B:829:HOH:O	2.07	0.54
2:A:288:ASN:HB2	2:A:314:ASP:O	2.07	0.54
2:B:381:ARG:H	2:B:384:GLU:HG3	1.73	0.54
2:A:476:PRO:HD2	2:A:479:VAL:HG11	1.90	0.54
2:A:538:ALA:O	2:A:542:ALA:HB2	2.07	0.54
2:B:124:LYS:HG2	2:B:139:PRO:HG2	1.90	0.54
2:A:503:GLN:O	2:A:507:GLU:HG3	2.08	0.54
2:B:429:THR:OG1	2:B:444:LEU:HD11	2.07	0.54
2:A:156:PRO:HA	2:A:171:GLN:NE2	2.24	0.53
2:A:442:ARG:HD3	2:A:462:MET:HE1	1.91	0.53
2:B:430:SER:HA	2:B:435:LEU:HD12	1.90	0.53
2:B:105:ALA:O	2:B:106:ASN:HB3	2.08	0.53
2:B:346:ALA:HB3	2:B:349:GLU:HG3	1.90	0.53
2:B:43:ILE:HG23	2:B:57:ILE:HD13	1.91	0.53
2:A:61:THR:O	2:A:89:THR:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:HG23	7:B:905:HOH:O	2.08	0.53
2:B:47:MET:HE1	2:B:54:PRO:HG3	1.90	0.53
2:A:506:ILE:HD12	2:A:509:LEU:HD12	1.91	0.53
2:A:605:ARG:N	2:A:605:ARG:HD2	2.24	0.53
2:B:497:GLU:OE1	2:B:505:ARG:HD2	2.09	0.52
2:A:163:GLY:O	2:A:164:ASN:C	2.48	0.52
2:A:170:TRP:HE3	2:A:170:TRP:HA	1.75	0.52
2:A:222:PHE:O	2:A:225:THR:HG23	2.10	0.52
2:B:421:ARG:HD2	2:B:421:ARG:N	2.24	0.52
2:A:137:TRP:CZ3	2:A:166:VAL:HA	2.45	0.52
2:A:470:GLN:HG3	7:A:919:HOH:O	2.09	0.52
2:B:153:GLY:HA2	2:B:194:LEU:HD13	1.90	0.52
2:B:11:ASN:OD1	2:B:14:GLN:HG3	2.10	0.52
2:B:326:GLU:HG3	2:B:618:ARG:HB2	1.92	0.51
1:D:10:DC:H2''	1:D:11:DA:C5'	2.39	0.51
1:D:10:DC:H2''	1:D:11:DA:H5'	1.92	0.51
2:B:356:SER:H	2:B:359:GLN:NE2	2.08	0.51
2:A:194:LEU:O	2:A:198:GLU:HG3	2.11	0.51
2:A:361:ARG:O	2:A:365:GLU:HG3	2.09	0.51
2:A:472:THR:HG22	2:A:475:MET:SD	2.51	0.51
2:B:430:SER:HB3	2:B:435:LEU:O	2.09	0.51
1:D:18:DG:H21	1:D:19:DT:H71	1.75	0.51
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.25	0.51
2:B:25:LEU:HD12	2:B:275:GLU:O	2.10	0.51
2:B:226:ASN:ND2	2:B:229:GLN:HG3	2.24	0.51
2:A:592:LEU:HD21	7:A:934:HOH:O	2.10	0.51
2:A:592:LEU:HD21	2:A:631:ARG:NH1	2.26	0.50
2:B:61:THR:O	2:B:89:THR:HA	2.11	0.50
2:A:375:ARG:CZ	2:A:548:ASP:HB3	2.41	0.50
2:A:156:PRO:HA	2:A:171:GLN:HE22	1.76	0.50
2:A:102:HIS:NE2	2:A:109:GLN:HB2	2.27	0.50
2:A:389:LYS:HB3	2:A:409:ARG:NE	2.26	0.50
2:A:514:THR:O	2:A:517:ARG:HB3	2.12	0.50
2:A:164:ASN:OD1	2:A:166:VAL:HG23	2.12	0.50
2:A:102:HIS:CE1	2:A:109:GLN:HB2	2.46	0.50
2:B:375:ARG:NE	2:B:548:ASP:HB2	2.27	0.50
2:B:133:ASP:HB3	2:B:136:GLN:HB3	1.93	0.50
2:A:576:GLU:HG3	2:A:579:MET:CG	2.42	0.50
2:A:480:GLN:O	2:A:484:VAL:HG23	2.11	0.50
2:A:114:LEU:CD1	2:A:118:ASP:HB3	2.41	0.50
2:A:500:GLU:O	2:A:504:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:442:ARG:NH1	2:A:462:MET:HE2	2.27	0.49
2:B:37:ARG:HD2	7:B:790:HOH:O	2.11	0.49
2:B:456:SER:O	2:B:460:ARG:HB2	2.12	0.49
2:A:263:ASN:HB2	7:A:721:HOH:O	2.11	0.49
2:A:376:ILE:HG12	2:A:556:LEU:HB2	1.94	0.49
2:B:394:TYR:O	2:B:398:ILE:HG13	2.13	0.49
2:B:194:LEU:O	2:B:198:GLU:HG3	2.12	0.49
2:B:133:ASP:HB3	2:B:136:GLN:CB	2.42	0.49
2:B:381:ARG:HB3	7:B:835:HOH:O	2.12	0.49
2:A:494:TYR:CE2	2:A:505:ARG:HD3	2.47	0.49
2:A:126:LEU:O	2:A:130:MET:HG3	2.13	0.49
2:A:130:MET:O	2:A:131:ASN:HB2	2.13	0.48
2:B:531:LEU:HD23	2:B:531:LEU:O	2.14	0.48
2:A:79:GLY:C	2:A:81:SER:H	2.16	0.48
2:A:401:ARG:HB3	2:A:438:TRP:CD2	2.48	0.48
2:B:31:ALA:HB2	2:B:251:GLN:NE2	2.29	0.48
2:B:435:LEU:HB2	2:B:439:GLN:OE1	2.14	0.48
2:B:498:LYS:C	2:B:500:GLU:H	2.16	0.48
1:D:9:DG:H3'	2:B:421:ARG:HB2	1.95	0.48
1:D:5:DC:P	2:A:124:LYS:HE2	2.54	0.48
1:C:2:DG:H2''	1:C:3:DA:OP2	2.14	0.48
2:B:149:GLN:HG3	2:B:154:LEU:HB2	1.95	0.48
2:B:394:TYR:CE1	2:B:410:VAL:HB	2.49	0.47
2:B:331:ARG:HH11	2:B:331:ARG:CB	2.27	0.47
2:B:568:PRO:HA	2:B:607:MET:HB2	1.96	0.47
2:A:408:GLU:HG2	2:A:437:LEU:CD1	2.44	0.47
2:A:364:GLU:HG3	2:A:374:TYR:CZ	2.49	0.47
2:B:447:GLU:O	2:B:448:LYS:C	2.52	0.47
2:B:628:ARG:NH2	2:B:628:ARG:CB	2.73	0.47
2:B:199:LEU:O	2:B:203:LYS:HB2	2.14	0.47
2:A:588:GLU:CB	2:A:591:ARG:HD2	2.44	0.47
2:B:476:PRO:HB2	2:B:479:VAL:HG23	1.96	0.47
1:D:18:DG:H21	1:D:19:DT:C7	2.27	0.47
1:D:23:DT:H2'	7:B:766:HOH:O	2.12	0.47
2:A:601:VAL:O	2:A:605:ARG:HD2	2.15	0.47
1:C:6:DA:H2''	1:C:7:DC:H5'	1.95	0.47
2:A:442:ARG:HH11	2:A:462:MET:HE2	1.78	0.47
2:B:380:MET:SD	2:B:384:GLU:HB2	2.54	0.47
2:B:165:PRO:HG2	2:B:166:VAL:H	1.79	0.47
2:A:476:PRO:O	2:A:479:VAL:HG12	2.15	0.47
2:B:618:ARG:O	2:B:625:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:ARG:CG	2:B:454:ALA:N	2.78	0.47
2:A:56:SER:HA	2:A:213:ARG:O	2.15	0.47
2:A:481:THR:O	2:A:485:ILE:HG13	2.14	0.47
2:A:1:MET:N	2:A:5:TYR:CE2	2.79	0.47
2:A:564:GLY:H	2:A:605:ARG:HH21	1.59	0.47
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.97	0.47
2:A:150:LYS:NZ	2:A:178:GLN:NE2	2.60	0.47
2:A:60:VAL:HG22	2:A:61:THR:N	2.30	0.47
2:A:290:LEU:HD11	2:A:308:LEU:HD13	1.96	0.47
2:A:27:VAL:HB	2:A:246:VAL:HG12	1.97	0.46
2:B:13:LYS:HG2	2:B:278:ARG:O	2.14	0.46
2:B:397:LEU:O	2:B:401:ARG:HD2	2.16	0.46
7:C:596:HOH:O	2:B:619:ARG:HD3	2.14	0.46
2:B:619:ARG:NH1	2:B:622:GLY:O	2.48	0.46
2:B:155:ARG:O	2:B:157:HIS:N	2.48	0.46
2:B:480:GLN:O	2:B:484:VAL:HG23	2.15	0.46
2:B:429:THR:O	2:B:433:ARG:HG2	2.15	0.46
2:A:97:LEU:HD13	7:A:789:HOH:O	2.15	0.46
2:B:497:GLU:O	2:B:498:LYS:C	2.54	0.46
2:B:290:LEU:HD11	2:B:308:LEU:CD1	2.45	0.46
2:B:110:ASP:OD1	2:B:532:GLN:HG2	2.16	0.46
2:A:282:ASN:HB2	2:A:308:LEU:HD22	1.97	0.46
2:A:308:LEU:HA	2:A:308:LEU:HD23	1.82	0.46
2:B:126:LEU:HG	2:B:130:MET:CE	2.46	0.46
2:A:126:LEU:CD1	2:A:177:TYR:HA	2.46	0.45
2:B:411:VAL:HG13	2:B:412:ASN:N	2.31	0.45
2:B:331:ARG:NH1	2:B:331:ARG:HB3	2.31	0.45
2:B:2:ASP:O	2:B:3:VAL:C	2.54	0.45
2:B:150:LYS:HZ1	2:B:178:GLN:HE22	1.63	0.45
2:B:292:ALA:HB1	2:B:636:LEU:HD22	1.99	0.45
2:B:564:GLY:H	2:B:605:ARG:NH2	2.15	0.45
2:A:494:TYR:O	2:A:497:GLU:HB2	2.17	0.45
1:C:11:DA:H2"	1:C:12:DG:C8	2.51	0.45
2:B:112:GLN:OE1	2:B:396:ARG:HD3	2.17	0.45
2:B:384:GLU:OE2	2:B:542:ALA:HB1	2.16	0.45
1:D:5:DC:H2"	1:D:6:DA:N7	2.29	0.45
2:B:234:ARG:HD3	7:B:903:HOH:O	2.17	0.45
2:A:475:MET:CE	2:A:479:VAL:HG22	2.47	0.44
2:A:16:GLU:O	2:A:20:ALA:HB2	2.17	0.44
2:A:459:GLN:HG3	2:A:463:GLU:OE2	2.17	0.44
2:A:114:LEU:HD12	2:A:118:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:PRO:O	2:B:141:GLN:HB2	2.17	0.44
1:D:21:DG:H2'	1:D:21:DG:H8	1.71	0.44
2:A:226:ASN:ND2	2:A:229:GLN:H	2.15	0.44
2:A:542:ALA:C	2:A:544:GLU:H	2.21	0.44
2:A:411:VAL:HA	2:A:461:PHE:CZ	2.52	0.44
1:C:18:DG:H1'	1:C:19:DT:H5'	1.99	0.44
2:A:226:ASN:C	2:A:226:ASN:HD22	2.21	0.44
2:B:327:LEU:HD23	2:B:362:VAL:HG13	1.98	0.44
2:B:271:PHE:HA	2:B:272:PRO:HD3	1.83	0.44
1:D:15:DC:H2''	1:D:16:DT:H72	1.99	0.44
2:A:401:ARG:HH22	2:A:469:ALA:CB	2.29	0.44
2:A:41:HIS:CD2	2:A:77:LEU:HD22	2.53	0.44
1:C:6:DA:H2''	1:C:7:DC:C5'	2.48	0.43
2:A:374:TYR:HA	2:A:553:ALA:HB1	2.00	0.43
2:A:133:ASP:HB3	2:A:136:GLN:CB	2.48	0.43
1:C:12:DG:H2''	1:C:13:DT:OP2	2.19	0.43
1:D:18:DG:C4	2:B:621:TYR:HD2	2.36	0.43
2:B:60:VAL:HG22	2:B:61:THR:N	2.33	0.43
2:B:418:ILE:HD11	2:B:458:LEU:HA	2.00	0.43
2:B:457:ALA:O	2:B:460:ARG:HB3	2.17	0.43
2:B:446:GLN:HE21	2:B:447:GLU:N	2.17	0.43
2:B:110:ASP:CG	2:B:532:GLN:HE21	2.21	0.43
2:B:260:GLN:HG2	7:B:808:HOH:O	2.17	0.43
2:A:398:ILE:HD11	2:A:468:LEU:HB3	2.00	0.43
2:A:156:PRO:CB	2:A:175:GLN:HE21	2.28	0.43
2:B:322:CYS:HB2	2:B:614:TYR:CZ	2.53	0.43
2:A:155:ARG:N	2:A:158:HIS:HD2	1.99	0.43
2:B:155:ARG:CB	2:B:156:PRO:HD2	2.48	0.43
2:B:10:LEU:HB3	2:B:14:GLN:HB2	2.01	0.43
2:B:280:GLU:HG3	7:B:837:HOH:O	2.18	0.43
2:B:95:HIS:CD2	2:B:113:ILE:HD11	2.54	0.43
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.32	0.42
2:B:202:ASN:C	2:B:203:LYS:HD2	2.38	0.42
2:A:542:ALA:C	2:A:544:GLU:N	2.73	0.42
2:A:79:GLY:C	2:A:81:SER:N	2.72	0.42
2:B:614:TYR:CE2	2:B:629:PRO:HG3	2.53	0.42
2:B:467:ALA:O	2:B:471:GLU:HG3	2.19	0.42
2:A:127:ILE:HG23	2:A:132:LEU:HB2	2.02	0.42
2:B:65:LYS:HE2	2:B:377:TYR:CG	2.54	0.42
1:C:20:DT:OP1	2:A:584:MET:HG2	2.20	0.42
2:B:628:ARG:HH21	2:B:628:ARG:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ILE:HD12	2:B:139:PRO:HG3	2.02	0.42
2:B:2:ASP:O	2:B:4:SER:N	2.53	0.42
1:D:6:DA:C1'	1:D:7:DC:H5''	2.46	0.42
2:A:159:ILE:HG13	2:A:171:GLN:NE2	2.34	0.42
2:A:590:GLY:C	2:A:592:LEU:N	2.72	0.42
1:C:4:DG:H2''	1:C:5:DC:H5'	2.02	0.42
2:B:590:GLY:HA2	7:B:857:HOH:O	2.20	0.42
2:B:226:ASN:HB2	7:B:739:HOH:O	2.20	0.42
1:D:19:DT:OP1	1:D:19:DT:O4'	2.37	0.42
2:A:115:ASP:CG	2:A:389:LYS:HZ1	2.22	0.42
2:B:639:GLU:CD	2:B:639:GLU:H	2.23	0.42
2:B:155:ARG:C	2:B:157:HIS:H	2.23	0.42
2:A:485:ILE:HG22	2:A:491:ARG:HB2	2.02	0.42
2:B:478:HIS:HB3	2:B:517:ARG:HA	2.02	0.42
2:B:556:LEU:N	2:B:556:LEU:HD12	2.35	0.42
2:B:288:ASN:HA	2:B:288:ASN:HD22	1.70	0.42
2:B:188:ASP:OD1	2:B:191:GLU:N	2.47	0.41
2:A:442:ARG:HH11	2:A:462:MET:CE	2.32	0.41
2:A:303:ARG:O	2:A:305:GLY:N	2.52	0.41
2:A:137:TRP:CH2	2:A:166:VAL:HA	2.55	0.41
2:B:273:GLY:O	2:B:275:GLU:HG2	2.20	0.41
2:A:325:ASN:HA	2:A:617:THR:O	2.20	0.41
2:B:126:LEU:HG	2:B:130:MET:HE1	2.03	0.41
2:B:491:ARG:O	2:B:495:GLU:HG3	2.20	0.41
2:B:4:SER:O	2:B:8:ASP:OD1	2.39	0.41
2:B:200:TRP:CH2	2:B:236:LEU:HG	2.55	0.41
2:A:164:ASN:HB3	2:A:167:GLU:HB3	2.02	0.41
2:A:303:ARG:C	2:A:305:GLY:N	2.73	0.41
2:B:418:ILE:CD1	2:B:458:LEU:HA	2.50	0.41
2:A:441:CYS:O	2:A:445:LEU:HG	2.21	0.41
2:A:643:GLU:OE1	2:A:645:ARG:NH2	2.54	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:A:364:GLU:HG3	2:A:374:TYR:OH	2.20	0.41
1:D:15:DC:C2'	1:D:16:DT:H72	2.51	0.41
1:C:15:DC:H2''	1:C:16:DT:OP2	2.21	0.41
2:B:287:SER:HB3	2:B:314:ASP:HA	2.03	0.41
2:A:203:LYS:CB	2:A:206:ILE:HD12	2.51	0.41
2:B:117:GLU:OE1	2:B:389:LYS:HE3	2.20	0.41
2:B:109:GLN:HG3	2:B:110:ASP:N	2.36	0.41
1:C:18:DG:C1'	1:C:19:DT:H5'	2.51	0.40
2:B:514:THR:O	2:B:517:ARG:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:GLN:HB2	2:A:160:GLN:HE21	1.68	0.40
2:B:191:GLU:O	2:B:195:ARG:HB2	2.22	0.40
2:B:203:LYS:HG3	2:B:205:HIS:CE1	2.56	0.40
1:D:10:DC:OP2	2:B:421:ARG:HB2	2.21	0.40
2:A:576:GLU:HG3	2:A:579:MET:HG3	2.03	0.40
2:B:478:HIS:CE1	2:B:479:VAL:HG23	2.56	0.40
2:B:37:ARG:CD	7:B:790:HOH:O	2.69	0.40
2:B:453:ARG:CG	2:B:454:ALA:H	2.34	0.40
2:B:397:LEU:HD11	2:B:407:PHE:HA	2.04	0.40
2:B:58:MET:HE2	2:B:217:ILE:HG23	2.04	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	
2	A	650/680 (96%)	610 (94%)	31 (5%)	9 (1%)	14	10
2	B	646/680 (95%)	608 (94%)	26 (4%)	12 (2%)	10	6
All	All	1296/1360 (95%)	1218 (94%)	57 (4%)	21 (2%)	12	8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	VAL
2	B	158	HIS
2	B	448	LYS
2	B	501	LYS
2	B	589	GLY
2	A	304	LEU
2	A	307	LYS
2	B	307	LYS

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Mol	Chain	Res	Type
2	B	519	PHE
2	A	305	GLY
2	B	156	PRO
2	B	306	LYS
2	B	498	LYS
2	A	454	ALA
2	A	498	LYS
2	B	400	ASN
2	A	2	ASP
2	A	134	GLU
2	A	164	ASN
2	B	157	HIS
2	A	308	LEU

### 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	
2	A	522/574 (91%)	505 (97%)	17 (3%)	45	56
2	B	523/574 (91%)	514 (98%)	9 (2%)	68	81
All	All	1045/1148 (91%)	1019 (98%)	26 (2%)	55	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	37	ARG
2	A	103	MET
2	A	160	GLN
2	A	170	TRP
2	A	175	GLN
2	A	195	ARG
2	A	208	GLN
2	A	226	ASN
2	A	235	LEU
2	A	288	ASN

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Mol	Chain	Res	Type
2	A	298	GLU
2	A	308	LEU
2	A	424	ASP
2	A	442	ARG
2	A	483	ARG
2	A	497	GLU
2	A	605	ARG
2	B	37	ARG
2	B	226	ASN
2	B	236	LEU
2	B	288	ASN
2	B	308	LEU
2	B	331	ARG
2	B	381	ARG
2	B	421	ARG
2	B	446	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN
2	A	147	ASN
2	A	158	HIS
2	A	160	GLN
2	A	175	GLN
2	A	178	GLN
2	A	226	ASN
2	A	227	ASN
2	A	265	GLN
2	A	269	ASN
2	A	288	ASN
2	A	359	GLN
2	A	400	ASN
2	A	459	GLN
2	A	496	GLN
2	B	119	GLN
2	B	136	GLN
2	B	147	ASN
2	B	149	GLN
2	B	175	GLN
2	B	178	GLN

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Mol	Chain	Res	Type
2	B	226	ASN
2	B	227	ASN
2	B	288	ASN
2	B	359	GLN
2	B	369	GLN
2	B	446	GLN
2	B	470	GLN
2	B	480	GLN
2	B	503	GLN
2	B	508	ASN
2	B	551	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z  > 2$
4	MGF	A	699	3,5,7	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	A	700	3,4	22,29,29	2.73	8 (36%)	27,45,45	3.03	9 (33%)
6	GOL	A	701	-	5,5,5	0.28	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MGF	B	701	3,5,7	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	B	702	3,4	22,29,29	2.68	8 (36%)	27,45,45	3.01	9 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGF	A	699	3,5,7	-	0/0/0/0	0/0/0/0
5	ADP	A	700	3,4	-	0/12/32/32	0/3/3/3
6	GOL	A	701	-	-	0/4/4/4	0/0/0/0
4	MGF	B	701	3,5,7	-	0/0/0/0	0/0/0/0
5	ADP	B	702	3,4	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	ADP	PB-O2B	-2.99	1.44	1.54
5	B	702	ADP	PB-O2B	-2.89	1.44	1.54
5	A	700	ADP	C3'-C4'	-2.73	1.45	1.53
5	B	702	ADP	C3'-C4'	-2.23	1.47	1.53
5	A	700	ADP	C5-N7	-2.08	1.32	1.39
5	B	702	ADP	C6-N6	-2.03	1.28	1.34
5	A	700	ADP	PB-O3B	3.08	1.65	1.54
5	B	702	ADP	PB-O3B	3.12	1.65	1.54
5	A	700	ADP	C4-N3	4.93	1.42	1.35
5	B	702	ADP	C4-N3	5.02	1.43	1.35
5	A	700	ADP	C2-N3	5.21	1.41	1.32
5	B	702	ADP	C2-N3	5.42	1.41	1.32
5	B	702	ADP	C5-C4	5.46	1.52	1.40
5	B	702	ADP	C2-N1	5.73	1.44	1.33
5	A	700	ADP	C2-N1	5.92	1.45	1.33
5	A	700	ADP	C5-C4	5.94	1.53	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	ADP	N3-C2-N1	-11.03	120.45	128.89
5	A	700	ADP	N3-C2-N1	-10.75	120.66	128.89
5	B	702	ADP	C1'-N9-C4	-4.03	120.86	126.94
5	A	700	ADP	C1'-N9-C4	-3.91	121.03	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	ADP	C4-C5-N7	-3.54	106.23	109.48
5	A	700	ADP	C4-C5-N7	-3.50	106.26	109.48
5	A	700	ADP	O2A-PA-O1A	-2.83	97.21	112.53
5	B	702	ADP	O2A-PA-O1A	-2.60	98.45	112.53
5	B	702	ADP	O2B-PB-O1B	2.36	118.18	110.58
5	A	700	ADP	O2B-PB-O1B	2.50	118.64	110.58
5	B	702	ADP	C4'-O4'-C1'	2.67	112.65	109.72
5	B	702	ADP	O5'-PA-O1A	2.69	120.04	109.62
5	A	700	ADP	O5'-PA-O1A	3.03	121.37	109.62
5	A	700	ADP	C4'-O4'-C1'	3.09	113.12	109.72
5	B	702	ADP	N6-C6-N1	4.43	128.72	119.20
5	B	702	ADP	C2-N1-C6	4.48	126.78	118.77
5	A	700	ADP	N6-C6-N1	4.61	129.09	119.20
5	A	700	ADP	C2-N1-C6	4.67	127.12	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	GOL	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	23/25 (92%)	0.49	1 (4%)	39 38	35, 83, 122, 136	0
1	D	23/25 (92%)	0.59	1 (4%)	39 38	38, 82, 108, 113	0
2	A	654/680 (96%)	0.30	42 (6%)	23 22	25, 49, 85, 104	1 (0%)
2	B	652/680 (95%)	0.31	47 (7%)	18 18	26, 54, 94, 106	0
All	All	1352/1410 (95%)	0.31	91 (6%)	21 20	25, 52, 92, 136	1 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	499	GLY	7.1
2	A	590	GLY	7.0
2	B	304	LEU	6.8
2	B	159	ILE	6.6
2	A	499	GLY	5.6
2	A	526	GLU	5.3
2	A	648	ALA	5.2
2	A	649	THR	5.1
2	A	166	VAL	4.9
2	A	81	SER	4.8
2	A	304	LEU	4.6
2	B	445	LEU	4.6
2	A	496	GLN	4.6
2	B	450	LEU	4.6
2	B	654	VAL	4.5
2	B	137	TRP	4.4
2	A	305	GLY	4.4
2	A	651	SER	4.3
2	B	158	HIS	4.3
2	B	305	GLY	4.3
2	A	500	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	302	GLY	4.2
2	B	446	GLN	4.0
2	A	523	GLU	3.9
2	B	81	SER	3.8
2	B	80	THR	3.7
2	A	547	ALA	3.7
2	B	144	TRP	3.6
2	A	5	TYR	3.6
2	B	550	TRP	3.6
2	B	82	GLN	3.5
2	A	650	VAL	3.5
2	B	165	PRO	3.4
2	B	500	GLU	3.4
2	B	131	ASN	3.3
2	A	656	HIS	3.3
2	B	130	MET	3.3
2	B	460	ARG	3.2
2	A	543	GLY	3.1
2	B	503	GLN	3.1
2	A	165	PRO	3.1
2	B	459	GLN	3.1
1	D	19	DT	3.1
2	A	497	GLU	3.1
2	A	502	GLY	3.0
2	B	156	PRO	3.0
2	A	82	GLN	2.8
2	A	302	GLY	2.8
2	B	470	GLN	2.7
2	A	137	TRP	2.7
2	B	472	THR	2.7
2	A	647	ARG	2.7
2	A	1	MET	2.6
2	B	502	GLY	2.6
2	B	476	PRO	2.6
2	A	527	ASP	2.6
2	A	80	THR	2.6
2	A	495	GLU	2.5
2	B	441	CYS	2.4
2	A	504	THR	2.4
2	B	520	SER	2.4
2	A	164	ASN	2.4
2	A	63	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	558	THR	2.4
2	A	503	GLN	2.4
2	A	134	GLU	2.3
2	B	114	LEU	2.3
2	A	501	LYS	2.3
2	A	376	ILE	2.3
2	B	498	LYS	2.3
2	B	496	GLN	2.3
2	B	3	VAL	2.3
2	B	280	GLU	2.2
1	C	1	DC	2.2
2	B	526	GLU	2.2
2	B	164	ASN	2.2
2	B	474	ASP	2.2
2	A	460	ARG	2.2
2	B	135	LYS	2.2
2	A	163	GLY	2.1
2	B	458	LEU	2.1
2	B	471	GLU	2.1
2	A	506	ILE	2.1
2	A	8	ASP	2.1
2	B	134	GLU	2.1
2	B	444	LEU	2.1
2	B	540	LEU	2.1
2	A	67	ALA	2.1
2	B	157	HIS	2.1
2	B	461	PHE	2.0
2	B	116	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
6	GOL	A	701	6/6	0.67	0.28	1.87	65,68,69,69	0
5	ADP	B	702	27/27	0.98	0.12	0.19	29,34,43,44	0
4	MGF	B	701	4/4	0.98	0.11	0.15	29,31,34,36	0
5	ADP	A	700	27/27	0.98	0.13	-0.27	29,36,43,45	0
4	MGF	A	699	4/4	0.97	0.14	-0.35	33,33,35,35	0
3	MG	A	681	1/1	0.96	0.22	-	36,36,36,36	0
3	MG	B	681	1/1	0.96	0.11	-	33,33,33,33	0

## 6.5 Other polymers

There are no such residues in this entry.