Full wwPDB X-ray Structure Validation Report (i)

Jul 3, 2017 – 02:28 PM EDT

PDB ID	:	5NPP
Title	:	2.22A STRUCTURE OF THIOPHENE2 AND GSK945237 WITH S.AUREUS DNA GYRASE AND DNA
Authors	:	Bax, B.D.; Chan, P.F.; Stavenger, R.A.
Deposited on	:	unknown
Resolution	:	2.22 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

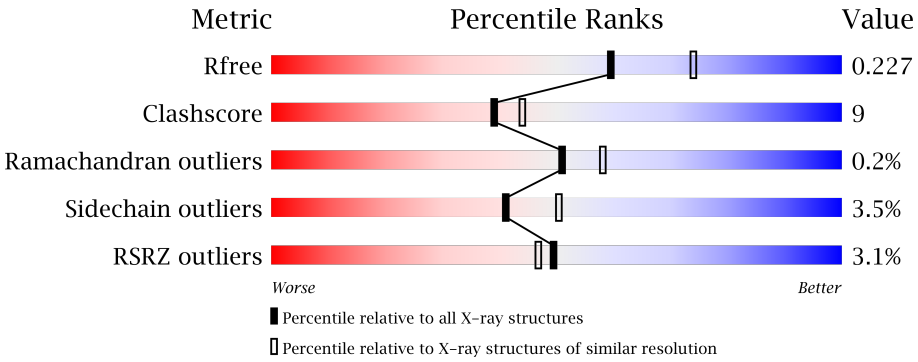
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 2.22 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	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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 >=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 <=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	B	692	3% 82% 12%
1	D	692	3% 81% 14%
2	E	8	63% 38%
2	F	8	75% 25%
3	A	12	8% 75% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	12	58% 42%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	101	-	-	-	X
6	GOL	B	1505	-	-	-	X
6	GOL	D	1505	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12913 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 DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	672	Total	C	N	O	S	0	28	0
			5536	3444	998	1067	27			
1	D	671	Total	C	N	O	S	0	14	0
			5411	3366	975	1043	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	initiating methionine	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
B	1000	ASP	-	linker	UNP P66937
B	1001	PHE	-	linker	UNP P66937
D	409	MET	-	initiating methionine	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937
D	1000	ASP	-	linker	UNP P66937
D	1001	PHE	-	linker	UNP P66937

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
2	F	8	Total	C	N	O	P	0	1	0
			181	88	38	48	7			

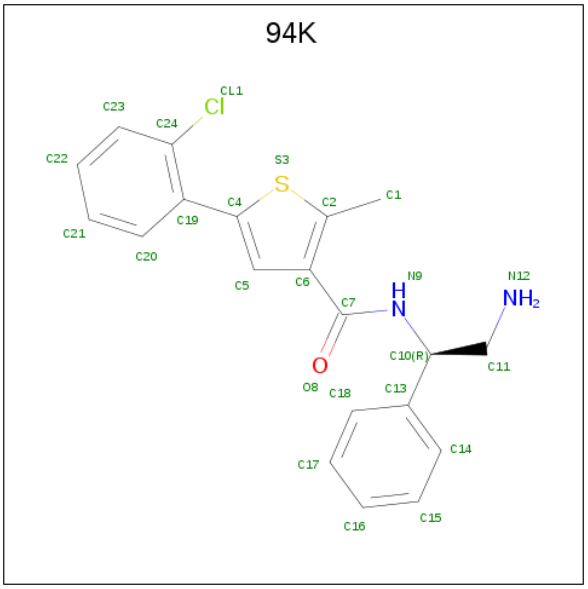
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	12	Total	C	N	O	P	0	4	0
			324	154	56	98	16			
3	C	12	Total	C	N	O	P	0	3	0
			270	124	47	84	15			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

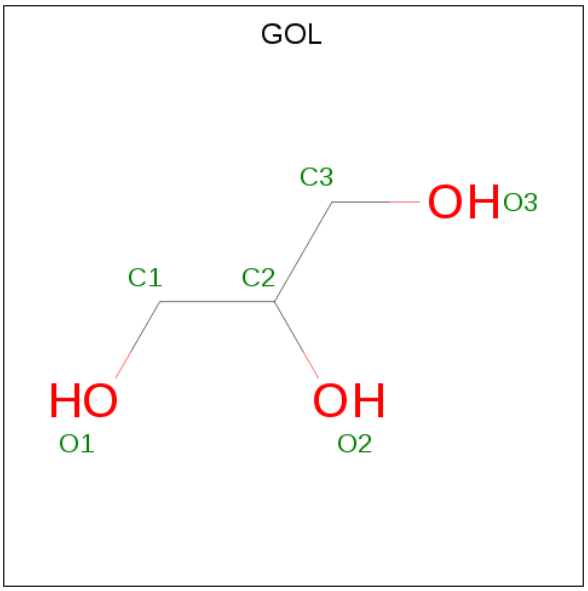
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	D	1	Total	Mn	0	0
			1	1		

- Molecule 5 is {N}-[(1 {R})-2-azanyl-1-phenyl-ethyl]-5-(2-chlorophenyl)-2-methyl-thiophene -3-carboxamide (three-letter code: 94K) (formula: $C_{20}H_{19}ClN_2OS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0	0
			25	20	1	2	1	1		
5	D	1	Total	C	Cl	N	O	S	0	0
			25	20	1	2	1	1		

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

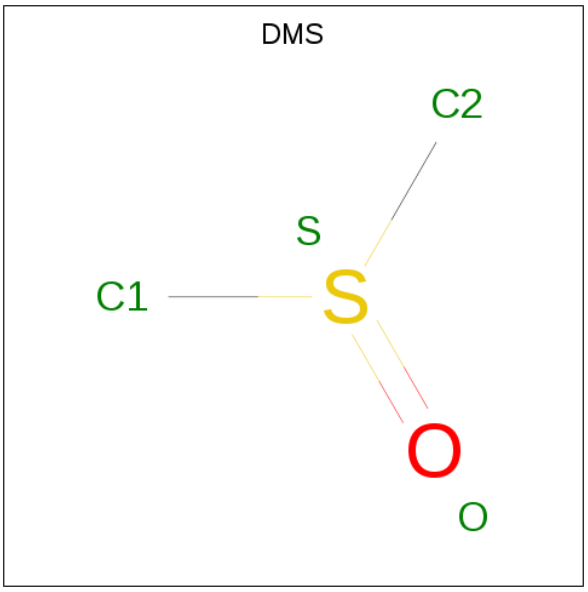


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

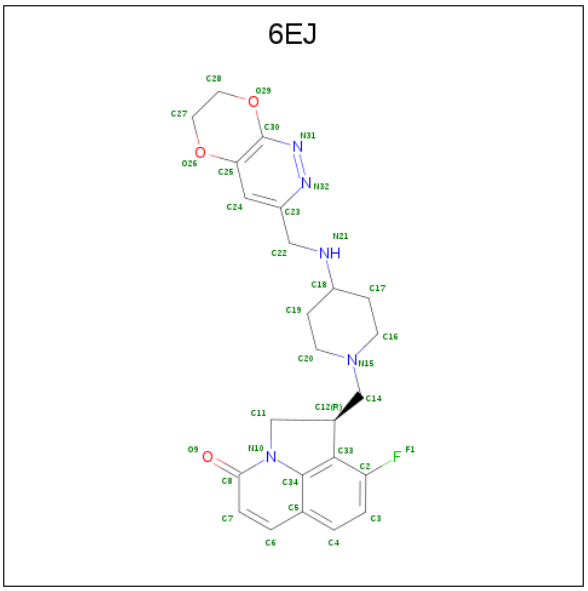
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
8	B	1	4	2	1	1	0	0

- Molecule 9 is (1R)-1-[(4-{[(6,7-dihydro[1,4]dioxino[2,3-c]pyridazin-3-yl)methyl]amino}piperidin-1-yl)methyl]-9-fluoro-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one (three-letter code: 6EJ) (formula: $C_{24}H_{26}FN_5O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
9	C	1	66	48	2	10	6	0	1

- Molecule 10 is water.

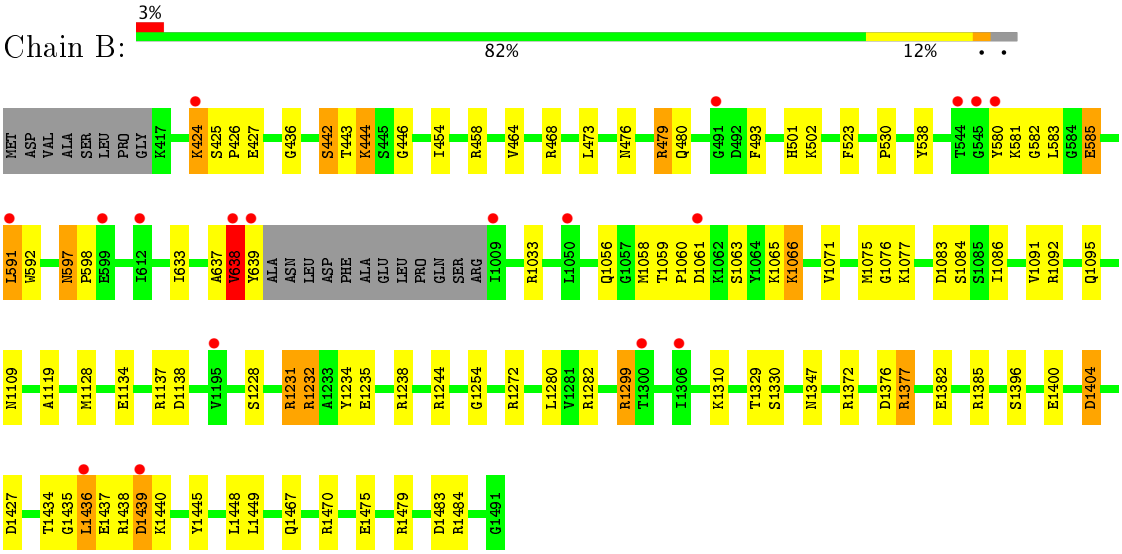
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	394	Total O 399 399	0	5
10	D	366	Total O 368 368	0	2
10	E	13	Total O 13 13	0	0
10	A	27	Total O 28 28	0	1
10	F	18	Total O 18 18	0	0
10	C	25	Total O 25 25	0	0

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 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.

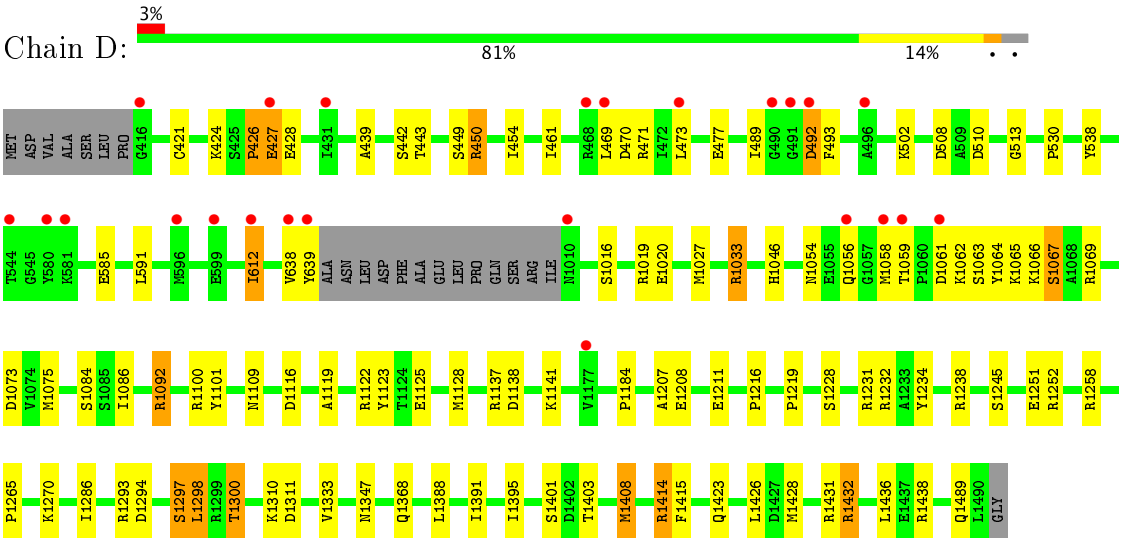
• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain B:



• Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B,DNA gyrase subunit A

Chain D:



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

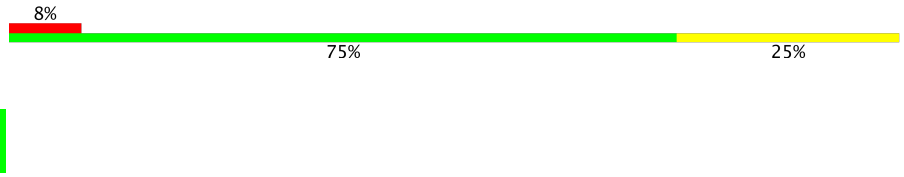
Chain E:

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

Chain F:

• Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain A:



• Molecule 3: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	92.85Å 92.85Å 409.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.22 19.89 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.89-2.22) 99.2 (19.89-2.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.182 , 0.227 0.182 , 0.227	Depositor DCC
R_{free} test set	4893 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12913	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: GOL, NA, MN, DMS, 94K, 6EJ

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	B	0.79	0/5609	0.89	8/7554 (0.1%)
1	D	0.79	0/5483	0.87	11/7389 (0.1%)
2	E	0.74	0/183	0.92	1/281 (0.4%)
2	F	1.03	1/204 (0.5%)	2.38	8/314 (2.5%)
3	A	0.74	0/361	0.83	1/554 (0.2%)
3	C	0.83	0/299	1.08	2/457 (0.4%)
All	All	0.79	1/12139 (0.0%)	0.93	31/16549 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	-7	DG	P-OP2	-9.00	1.33	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	-7	DG	O5'-P-OP1	-30.12	74.56	110.70
2	F	-7	DG	OP1-P-OP2	11.17	136.36	119.60
2	F	-7	DG	O5'-P-OP2	10.36	123.14	110.70
2	F	-8[A]	DA	C4'-C3'-O3'	8.96	132.10	109.70
2	F	-8[B]	DA	C4'-C3'-O3'	8.96	132.10	109.70
3	C	4	DC	C1'-O4'-C4'	-8.47	101.62	110.10
2	F	-8[A]	DA	C2'-C3'-O3'	-7.54	87.72	112.60
2	F	-8[B]	DA	C2'-C3'-O3'	-7.54	87.72	112.60
1	B	1377	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	468	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	D	1122	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	1231	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	1484	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	D	1033	ARG	NE-CZ-NH2	-6.32	117.14	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1372	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	1432	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	E	-4	DG	O5'-P-OP1	-5.99	100.31	105.70
1	B	1280	LEU	CA-CB-CG	5.97	129.04	115.30
1	D	1122	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	426	PRO	C-N-CA	-5.68	107.50	121.70
3	C	6	DT	O5'-P-OP2	-5.61	100.65	105.70
1	B	468	ARG	NE-CZ-NH2	5.51	123.06	120.30
3	A	11	DC	C1'-O4'-C4'	-5.47	104.63	110.10
1	B	1376	ASP	CB-CG-OD1	5.43	123.19	118.30
1	D	1067	SER	N-CA-CB	-5.34	102.49	110.50
1	D	1092	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	471	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	D	510	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	427[A]	GLU	N-CA-CB	-5.17	101.30	110.60
1	D	427[B]	GLU	N-CA-CB	-5.17	101.30	110.60
2	F	-7	DG	P-O5'-C5'	-5.06	112.80	120.90

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	B	5536	0	5509	100	0
1	D	5411	0	5394	92	0
2	E	163	0	91	3	0
2	F	181	0	103	5	0
3	A	324	0	181	6	0
3	C	270	0	145	4	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	25	0	0	1	0
5	D	25	0	0	1	0
6	A	6	0	8	3	0
6	B	18	0	24	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	6	0	8	3	0
6	D	24	0	32	1	0
7	B	1	0	0	0	0
8	B	4	0	6	0	0
9	C	66	0	0	0	0
10	A	28	0	0	1	0
10	B	399	0	0	15	2
10	C	25	0	0	4	0
10	D	368	0	0	12	2
10	E	13	0	0	1	0
10	F	18	0	0	1	0
All	All	12913	0	11501	201	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (201) 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:443:THR:CG2	1:B:454:ILE:HD12	1.86	1.06
2:E:-1:DG:H2"	3:A:1[A]:DG:H5'	1.41	1.02
1:D:443[B]:THR:HG22	1:D:591:LEU:HD21	1.36	1.02
1:D:1138:ASP:OD1	1:D:1141:LYS:NZ	1.93	1.01
1:B:443:THR:HG22	1:B:454:ILE:HD12	1.44	0.97
1:B:443:THR:HG22	1:B:454:ILE:CD1	1.94	0.97
1:B:581[A]:LYS:HG2	1:B:581[A]:LYS:O	1.65	0.97
1:B:639[B]:TYR:OH	10:B:1601:HOH:O	1.85	0.91
6:C:102:GOL:H11	10:C:206:HOH:O	1.72	0.90
3:C:5[A]:DC:OP2	10:C:201:HOH:O	1.92	0.88
3:A:1[B]:DG:N7	6:A:101:GOL:H2	1.93	0.84
1:B:1435[A]:GLY:HA2	10:B:1839:HOH:O	1.78	0.84
3:C:1:DG:N7	6:C:102:GOL:H12	1.93	0.83
1:B:638[B]:VAL:O	1:B:639[B]:TYR:HB3	1.78	0.82
1:D:443[A]:THR:HG22	1:D:454:ILE:HD12	1.61	0.82
1:B:1475[A]:GLU:OE1	1:B:1479[A]:ARG:NH2	2.11	0.82
1:D:439:ALA:O	1:D:443[B]:THR:HG23	1.79	0.82
1:B:443:THR:HG21	1:B:454:ILE:HD12	1.63	0.79
1:B:502:LYS:HG2	1:B:538:TYR:CE1	2.18	0.79
1:D:1297:SER:OG	1:D:1300:THR:HG23	1.83	0.77
1:D:443[A]:THR:CG2	1:D:454:ILE:HD12	2.17	0.74
1:D:1138:ASP:OD2	10:D:1601:HOH:O	2.05	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1385[A]:ARG:HD3	10:B:1705:HOH:O	1.87	0.72
1:D:1058[A]:MET:SD	1:D:1065:LYS:CB	2.77	0.72
3:A:1[B]:DG:O5'	3:A:1[B]:DG:C8	2.42	0.72
1:B:501:HIS:ND1	10:B:1604:HOH:O	2.24	0.71
1:B:1299:ARG:N	1:B:1299:ARG:HD3	2.06	0.71
1:B:1434:THR:O	1:B:1438[B]:ARG:HB2	1.90	0.71
1:D:1234:TYR:O	1:D:1347:ASN:HB2	1.91	0.70
1:D:427[A]:GLU:H	1:D:427[A]:GLU:CD	1.96	0.68
1:B:1059:THR:OG1	1:B:1061:ASP:OD1	2.06	0.67
1:B:639[B]:TYR:O	1:B:639[B]:TYR:CD1	2.47	0.67
1:D:493:PHE:CE2	1:D:530:PRO:HB2	2.30	0.67
1:D:1064:TYR:HB3	1:D:1125:GLU:HB3	1.76	0.66
1:B:1134:GLU:OE1	1:B:1479[A]:ARG:NH1	2.28	0.66
2:F:-8[A]:DA:N3	2:F:-8[A]:DA:H2'	2.09	0.66
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.60	0.66
1:B:1059:THR:HA	1:B:1128:MET:HE3	1.76	0.66
1:B:1238:ARG:HD3	10:B:1862:HOH:O	1.96	0.65
1:D:502:LYS:HG3	1:D:538:TYR:CE1	2.32	0.65
1:B:424[A]:LYS:C	1:B:424[A]:LYS:HD3	2.17	0.64
1:D:1063:SER:O	10:D:1602:HOH:O	2.15	0.64
1:D:450:ARG:NH2	1:D:450:ARG:HG2	2.12	0.64
1:D:443[A]:THR:HG22	1:D:454:ILE:CD1	2.26	0.64
1:B:597:ASN:HD22	1:B:598:PRO:CD	2.11	0.64
1:D:1066[B]:LYS:HD2	1:D:1066[B]:LYS:H	1.62	0.64
1:D:450:ARG:HH21	1:D:450:ARG:HG2	1.63	0.64
1:B:1056[B]:GLN:HA	1:B:1056[B]:GLN:OE1	1.98	0.63
1:B:1058[A]:MET:SD	1:B:1065:LYS:CB	2.87	0.63
1:B:1385[A]:ARG:NH1	10:B:1603:HOH:O	2.20	0.63
3:A:1[B]:DG:O5'	3:A:1[B]:DG:H8	1.81	0.63
1:D:585:GLU:O	1:D:585:GLU:HG2	2.00	0.62
1:D:492:ASP:OD1	1:D:492:ASP:N	2.32	0.62
1:B:1075[B]:MET:HE1	1:B:1083:ASP:HB3	1.82	0.62
1:D:1414:ARG:HB2	1:D:1414:ARG:HH11	1.65	0.61
1:B:443:THR:CG2	1:B:454:ILE:CD1	2.62	0.61
1:D:443[B]:THR:HG22	1:D:591:LEU:CD2	2.22	0.61
1:B:1475[A]:GLU:CD	1:B:1479[A]:ARG:NH2	2.54	0.61
1:B:1436[A]:LEU:O	1:B:1440[A]:LYS:CB	2.49	0.61
1:B:1063:SER:HB2	10:B:1842:HOH:O	2.01	0.60
1:D:1066[B]:LYS:N	1:D:1066[B]:LYS:HD2	2.16	0.60
1:B:1475[A]:GLU:CD	1:B:1479[A]:ARG:HH22	2.04	0.60
2:E:-1:DG:C2'	3:A:1[A]:DG:H5'	2.25	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580[A]:TYR:O	1:B:585:GLU:HG3	2.02	0.60
1:D:427[A]:GLU:N	1:D:427[A]:GLU:CD	2.54	0.60
1:B:1232[B]:ARG:HD3	10:B:1888:HOH:O	2.02	0.59
1:B:1475[A]:GLU:OE2	1:B:1479[A]:ARG:NH2	2.36	0.59
1:D:450:ARG:HH21	1:D:450:ARG:CG	2.15	0.59
1:B:1066:LYS:HB2	10:B:1870:HOH:O	2.03	0.58
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.38	0.58
1:B:1232[A]:ARG:NH2	10:B:1608:HOH:O	2.37	0.57
1:B:424[A]:LYS:HD3	1:B:425:SER:N	2.19	0.57
1:B:476:ASN:O	1:B:480:GLN:HG3	2.04	0.57
1:B:1076:GLY:HA2	1:D:1066[B]:LYS:HG3	1.86	0.56
1:B:1467:GLN:OE1	1:B:1470:ARG:NH1	2.38	0.56
2:F:-8[A]:DA:H4'	2:F:-7:DG:OP1	2.04	0.56
1:B:1436[A]:LEU:O	1:B:1440[A]:LYS:HB3	2.06	0.56
1:D:1368:GLN:NE2	10:D:1611:HOH:O	2.40	0.55
1:B:597:ASN:HD22	1:B:598:PRO:N	2.03	0.55
1:B:1445:TYR:CE2	1:B:1449:LEU:HD11	2.42	0.55
1:D:1066[B]:LYS:CD	1:D:1066[B]:LYS:H	2.19	0.54
1:D:1100:ARG:HG3	1:D:1101:TYR:CE2	2.42	0.54
1:D:1138:ASP:HB2	10:D:1601:HOH:O	2.06	0.54
1:D:1232[B]:ARG:HG3	1:D:1238:ARG:O	2.07	0.54
1:D:1046:HIS:ND1	10:D:1608:HOH:O	2.33	0.54
1:B:1084:SER:OG	6:A:101:GOL:H12	2.08	0.54
1:B:1058[A]:MET:CE	1:B:1058[A]:MET:HA	2.38	0.54
1:D:1408:MET:HG2	1:D:1426:LEU:HD12	1.90	0.53
1:B:442:SER:HB2	1:B:591:LEU:HD23	1.90	0.53
1:D:502:LYS:HD3	10:D:1695:HOH:O	2.08	0.53
2:F:-8[B]:DA:N3	2:F:-8[B]:DA:H2'	2.23	0.53
1:B:1075[B]:MET:HE1	1:B:1083:ASP:CB	2.38	0.53
1:B:585:GLU:HG2	1:D:1123:TYR:O	2.09	0.53
1:B:1436[B]:LEU:HG	1:D:1403:THR:HG22	1.90	0.53
1:D:1388:LEU:HD13	1:D:1438:ARG:HG2	1.90	0.53
1:B:581[A]:LYS:CG	1:B:581[A]:LYS:O	2.47	0.53
1:B:424[B]:LYS:O	1:B:426:PRO:HD3	2.08	0.52
2:F:-8[B]:DA:H4'	2:F:-7:DG:OP1	2.09	0.52
1:B:1075[A]:MET:HG2	1:B:1086:ILE:CD1	2.40	0.52
1:B:1385[A]:ARG:NH2	10:B:1603:HOH:O	2.32	0.52
3:C:2:DT:OP2	10:C:202:HOH:O	2.19	0.52
1:B:1075[A]:MET:HG2	1:B:1086:ILE:HD12	1.92	0.52
1:B:446:GLY:HA2	1:D:1298:LEU:HD22	1.92	0.52
1:D:428:GLU:OE1	1:D:450:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG22	1:B:454:ILE:HD11	1.87	0.51
1:D:1066[A]:LYS:HG3	1:D:1067:SER:N	2.23	0.51
1:D:1391:ILE:O	1:D:1395:ILE:HG12	2.09	0.51
1:B:1071:VAL:O	1:B:1075[A]:MET:HG3	2.11	0.51
1:B:1109:ASN:HB3	1:B:1119:ALA:HB2	1.93	0.51
1:D:1245[A]:SER:OG	1:D:1265:PRO:HD3	2.11	0.51
1:B:1234:TYR:O	1:B:1347:ASN:HB2	2.10	0.51
1:D:1066[B]:LYS:HB2	10:D:1704[B]:HOH:O	2.10	0.51
1:D:1137:ARG:HD2	10:D:1787:HOH:O	2.11	0.51
1:D:1310:LYS:O	1:D:1311:ASP:HB2	2.11	0.51
1:D:638:VAL:HG22	1:D:639:TYR:N	2.26	0.51
1:B:1092:ARG:HD2	10:E:108:HOH:O	2.11	0.50
1:D:426:PRO:O	1:D:427[B]:GLU:C	2.41	0.50
3:A:3:DA:H1'	10:A:201:HOH:O	2.12	0.50
1:D:1061:ASP:OD1	1:D:1062:LYS:N	2.45	0.50
1:D:1238:ARG:HA	1:D:1333:VAL:O	2.11	0.50
1:D:1270:LYS:NZ	1:D:1294:ASP:OD2	2.39	0.50
1:D:1251:GLU:HB3	6:D:1504:GOL:H2	1.94	0.50
1:D:1414:ARG:HG2	1:D:1415:PHE:CE2	2.46	0.49
1:D:1019:ARG:NH1	10:D:1622:HOH:O	2.44	0.49
1:D:502:LYS:HG3	1:D:538:TYR:CD1	2.46	0.49
1:B:1231:ARG:O	1:B:1235:GLU:HG3	2.12	0.49
1:D:1207:ALA:HB2	1:D:1231:ARG:HH22	1.76	0.49
1:B:1077:LYS:HE3	1:D:1069:ARG:NH1	2.27	0.49
1:B:1299:ARG:H	1:B:1299:ARG:HD3	1.77	0.49
1:B:1329:THR:HG22	1:B:1330:SER:N	2.27	0.48
1:B:1436[A]:LEU:O	1:B:1440[A]:LYS:HB2	2.12	0.48
1:D:469:LEU:O	1:D:473:LEU:HG	2.14	0.48
1:B:1382:GLU:O	1:B:1385[A]:ARG:HG2	2.14	0.48
1:D:1059:THR:OG1	1:D:1061:ASP:OD1	2.23	0.48
1:B:1272:ARG:CZ	2:E:-6:DC:H5"	2.44	0.47
1:D:1016:SER:O	1:D:1020:GLU:HG3	2.14	0.47
1:B:1438[B]:ARG:HD2	10:B:1839:HOH:O	2.13	0.47
1:D:426:PRO:O	1:D:427[A]:GLU:C	2.47	0.47
1:B:583:LEU:HD22	1:B:591:LEU:HD11	1.96	0.47
1:B:1059:THR:HB	1:B:1060:PRO:CD	2.45	0.47
1:B:1385[A]:ARG:HB2	1:B:1438[A]:ARG:NH2	2.31	0.46
1:B:1438[A]:ARG:HD2	1:B:1438[A]:ARG:HA	1.53	0.46
1:B:1427:ASP:OD1	1:D:1431:ARG:NH2	2.27	0.46
1:D:421:CYS:HA	1:D:449:SER:O	2.16	0.46
1:B:582[A]:GLY:O	1:B:585:GLU:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:ARG:CD	1:B:1299:ARG:N	2.78	0.46
1:D:1075:MET:HG2	1:D:1086:ILE:HD12	1.98	0.46
1:D:1054:ASN:HA	1:D:1128:MET:CE	2.45	0.45
1:D:1428:MET:HG3	1:D:1432:ARG:HG3	1.99	0.45
1:D:427[B]:GLU:O	1:D:427[B]:GLU:CG	2.64	0.45
1:B:1377:ARG:HG3	1:B:1448:LEU:HD11	1.99	0.45
1:D:1109:ASN:HB3	1:D:1119:ALA:HB2	1.98	0.45
1:B:1404:ASP:OD1	1:D:1431:ARG:NH1	2.50	0.45
1:B:1137:ARG:HD2	10:B:1927:HOH:O	2.15	0.45
1:B:1439[A]:ASP:N	1:B:1439[A]:ASP:OD1	2.46	0.45
1:D:1058[A]:MET:HA	1:D:1058[A]:MET:CE	2.47	0.45
1:B:592:TRP:O	1:B:597:ASN:HB2	2.17	0.44
1:D:1208:GLU:O	1:D:1211:GLU:HB2	2.17	0.44
1:D:424:LYS:HD3	1:D:424:LYS:HA	1.82	0.44
1:B:1137:ARG:O	1:B:1138:ASP:HB2	2.17	0.44
1:B:1329:THR:CG2	1:B:1330:SER:N	2.80	0.44
5:D:1502:94K:S3	5:D:1502:94K:CL1	3.12	0.44
1:B:1109:ASN:HB2	1:D:442:SER:OG	2.18	0.43
1:B:1254:GLY:O	1:B:1310:LYS:HE2	2.18	0.43
1:D:1137:ARG:O	1:D:1138:ASP:HB2	2.18	0.43
1:D:1408:MET:HG2	1:D:1426:LEU:CD1	2.48	0.43
2:F:-8[A]:DA:N3	2:F:-8[A]:DA:C2'	2.80	0.43
5:B:1502:94K:CL1	5:B:1502:94K:S3	3.13	0.43
1:D:508:ASP:O	1:D:513:GLY:HA3	2.18	0.43
1:D:1084:SER:OG	6:C:102:GOL:H2	2.19	0.43
1:D:1184:PRO:HB2	1:D:1216:PRO:HB3	2.00	0.43
1:B:1091:VAL:O	1:B:1095:GLN:HG3	2.18	0.43
1:B:436:GLY:N	10:B:1626:HOH:O	2.51	0.43
1:D:1066[B]:LYS:N	1:D:1066[B]:LYS:CD	2.81	0.43
1:D:1403:THR:HB	10:D:1783:HOH:O	2.18	0.42
1:B:426:PRO:O	1:B:427[A]:GLU:C	2.54	0.42
1:B:442:SER:OG	1:D:1109:ASN:HB2	2.20	0.42
1:B:633:ILE:O	1:B:637[B]:ALA:HB2	2.20	0.42
1:B:1483:ASP:HA	6:B:1505:GOL:H12	2.02	0.42
1:D:1092:ARG:HD2	10:F:115:HOH:O	2.19	0.42
1:D:1100:ARG:HA	1:D:1219:PRO:HB3	2.01	0.42
1:D:1054:ASN:HA	1:D:1128:MET:HE1	2.01	0.42
1:B:1084:SER:OG	6:A:101:GOL:H31	2.20	0.42
1:B:473:LEU:O	1:B:479:ARG:HD2	2.20	0.42
1:D:461:ILE:HG22	10:D:1655:HOH:O	2.19	0.42
1:B:424[A]:LYS:O	1:B:426:PRO:HD3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1063:SER:HB2	10:D:1914:HOH:O	2.20	0.41
3:C:5[A]:DC:H5"	10:C:201:HOH:O	2.20	0.41
1:D:1414:ARG:HB2	1:D:1414:ARG:NH1	2.33	0.41
1:D:1056[A]:GLN:HB3	1:D:1058[A]:MET:HG2	2.02	0.41
1:B:464:VAL:HG21	1:B:523:PHE:HA	2.01	0.41
1:B:444[A]:LYS:HE2	1:D:1116:ASP:OD2	2.20	0.41
6:B:1503:GOL:H11	10:B:1861:HOH:O	2.20	0.41
1:D:1075:MET:HG2	1:D:1086:ILE:CD1	2.50	0.41
1:B:1059:THR:HB	1:B:1060:PRO:HD2	2.02	0.41
1:D:1207:ALA:HB2	1:D:1231:ARG:NH2	2.35	0.41
1:B:1437[A]:GLU:HA	1:B:1440[A]:LYS:HB3	2.03	0.41
1:D:612:ILE:HA	1:D:612:ILE:HD12	1.83	0.41
1:B:592:TRP:O	1:B:597:ASN:N	2.51	0.40
1:D:1252:ARG:HD3	1:D:1258:ARG:HB3	2.02	0.40
1:B:442:SER:HB2	1:B:591:LEU:CD2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:1921:HOH:O	10:D:1950:HOH:O[5_554]	2.14	0.06
10:B:1917:HOH:O	10:D:1938:HOH:O[1_655]	2.17	0.03

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	B	695/692 (100%)	673 (97%)	19 (3%)	3 (0%)	38	40
1	D	681/692 (98%)	668 (98%)	12 (2%)	1 (0%)	55	63
All	All	1376/1384 (99%)	1341 (98%)	31 (2%)	4 (0%)	51	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1033	ARG
1	D	1033	ARG
1	B	638[A]	VAL
1	B	638[B]	VAL

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	B	590/591 (100%)	564 (96%)	26 (4%)	33	39
1	D	579/591 (98%)	558 (96%)	21 (4%)	40	49
All	All	1169/1182 (99%)	1122 (96%)	47 (4%)	41	44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424[A]	LYS
1	B	424[B]	LYS
1	B	442	SER
1	B	444[A]	LYS
1	B	444[B]	LYS
1	B	458	ARG
1	B	479	ARG
1	B	585	GLU
1	B	591	LEU
1	B	597	ASN
1	B	638[A]	VAL
1	B	638[B]	VAL
1	B	1066	LYS
1	B	1228	SER
1	B	1232[A]	ARG
1	B	1232[B]	ARG
1	B	1244	ARG
1	B	1282	ARG
1	B	1299	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1396	SER
1	B	1400	GLU
1	B	1404	ASP
1	B	1436[A]	LEU
1	B	1436[B]	LEU
1	B	1439[A]	ASP
1	B	1439[B]	ASP
1	D	450	ARG
1	D	470	ASP
1	D	477	GLU
1	D	489	ILE
1	D	492	ASP
1	D	612	ILE
1	D	1027	MET
1	D	1073	ASP
1	D	1228	SER
1	D	1286	ILE
1	D	1293	ARG
1	D	1297	SER
1	D	1298	LEU
1	D	1300	THR
1	D	1401	SER
1	D	1408	MET
1	D	1414	ARG
1	D	1423[A]	GLN
1	D	1423[B]	GLN
1	D	1436	LEU
1	D	1489	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	501	HIS
1	B	597	ASN
1	B	1368	GLN
1	D	501	HIS
1	D	1334	ASN
1	D	1368	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 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
6	GOL	A	101	-	5,5,5	0.40	0	5,5,5	0.68	0
5	94K	B	1502	-	23,27,27	1.22	2 (8%)	24,37,37	1.37	5 (20%)
6	GOL	B	1503	-	5,5,5	0.64	0	5,5,5	0.52	0
6	GOL	B	1504	-	5,5,5	0.45	0	5,5,5	0.76	0
6	GOL	B	1505	-	5,5,5	0.41	0	5,5,5	1.08	1 (20%)
8	DMS	B	1507	-	3,3,3	0.47	0	3,3,3	0.86	0
9	6EJ	C	101[A]	-	32,38,38	1.20	5 (15%)	34,55,55	1.55	6 (17%)
9	6EJ	C	101[B]	-	32,38,38	1.12	5 (15%)	34,55,55	1.72	9 (26%)
6	GOL	C	102	-	5,5,5	0.76	0	5,5,5	0.88	0
5	94K	D	1502	-	23,27,27	0.96	1 (4%)	24,37,37	1.26	4 (16%)
6	GOL	D	1503	-	5,5,5	0.64	0	5,5,5	0.55	0
6	GOL	D	1504	-	5,5,5	0.49	0	5,5,5	0.74	0
6	GOL	D	1505	-	5,5,5	0.29	0	5,5,5	0.82	0
6	GOL	D	1506	-	5,5,5	0.47	0	5,5,5	0.70	0

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
6	GOL	A	101	-	-	0/4/4/4	0/0/0/0
5	94K	B	1502	-	-	0/14/18/18	0/3/3/3
6	GOL	B	1503	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1504	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1505	-	-	0/4/4/4	0/0/0/0
8	DMS	B	1507	-	-	0/0/0/0	0/0/0/0
9	6EJ	C	101[A]	-	-	0/9/34/34	0/5/6/6
9	6EJ	C	101[B]	-	-	0/9/34/34	0/5/6/6
6	GOL	C	102	-	-	0/4/4/4	0/0/0/0
5	94K	D	1502	-	-	0/14/18/18	0/3/3/3
6	GOL	D	1503	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1504	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1505	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1506	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1502	94K	C6-C7	-3.71	1.42	1.50
5	D	1502	94K	C6-C7	-2.93	1.44	1.50
5	B	1502	94K	C19-C4	-2.66	1.45	1.48
9	C	101[A]	6EJ	C8-N10	-2.54	1.34	1.38
9	C	101[A]	6EJ	C5-C34	-2.40	1.37	1.42
9	C	101[B]	6EJ	C8-N10	-2.39	1.34	1.38
9	C	101[B]	6EJ	C5-C34	-2.15	1.38	1.42
9	C	101[B]	6EJ	C4-C3	2.29	1.41	1.36
9	C	101[B]	6EJ	C11-C12	2.41	1.55	1.53
9	C	101[B]	6EJ	N31-N32	2.44	1.40	1.34
9	C	101[A]	6EJ	N31-N32	2.67	1.41	1.34
9	C	101[A]	6EJ	C11-C12	2.71	1.56	1.53
9	C	101[A]	6EJ	C4-C3	2.79	1.42	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	101[A]	6EJ	C3-C2-C33	-3.90	120.45	124.07
9	C	101[B]	6EJ	C3-C2-C33	-3.81	120.54	124.07
9	C	101[B]	6EJ	C12-C14-N15	-3.27	108.34	113.32
9	C	101[A]	6EJ	O26-C25-C30	-3.09	119.66	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	101[B]	6EJ	C22-N21-C18	-2.99	109.60	114.11
9	C	101[B]	6EJ	C17-C16-N15	-2.82	106.47	110.99
5	B	1502	94K	C6-C7-N9	-2.79	111.57	116.88
5	D	1502	94K	C10-N9-C7	-2.65	118.51	122.15
9	C	101[A]	6EJ	C19-C20-N15	-2.58	106.85	110.99
9	C	101[B]	6EJ	C16-C17-C18	-2.51	105.84	110.41
5	D	1502	94K	C21-C22-C23	-2.28	117.07	120.21
5	B	1502	94K	C15-C14-C13	-2.28	117.84	120.64
5	B	1502	94K	C10-N9-C7	-2.22	119.11	122.15
6	B	1505	GOL	C3-C2-C1	-2.03	103.45	111.52
5	D	1502	94K	C22-C21-C20	2.00	122.96	120.21
5	B	1502	94K	C18-C13-C14	2.00	120.82	118.30
5	D	1502	94K	C18-C13-C14	2.03	120.85	118.30
5	B	1502	94K	O8-C7-N9	2.15	126.38	122.46
9	C	101[A]	6EJ	O26-C25-C24	2.22	120.08	116.81
9	C	101[A]	6EJ	C27-O26-C25	2.29	117.92	113.85
9	C	101[B]	6EJ	C27-O26-C25	2.32	117.97	113.85
9	C	101[B]	6EJ	O26-C25-C24	2.44	120.40	116.81
9	C	101[B]	6EJ	C6-C7-C8	3.19	125.13	119.96
9	C	101[B]	6EJ	C5-C34-N10	3.32	125.11	122.35
9	C	101[A]	6EJ	C23-N32-N31	3.93	121.79	119.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	101	GOL	3	0
5	B	1502	94K	1	0
6	B	1503	GOL	1	0
6	B	1505	GOL	1	0
6	C	102	GOL	3	0
5	D	1502	94K	1	0
6	D	1504	GOL	1	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^{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	B	672/692 (97%)	-0.21	18 (2%) 55 53	25, 39, 61, 88	0
1	D	671/692 (96%)	-0.13	24 (3%) 43 41	24, 39, 69, 102	0
2	E	8/8 (100%)	-0.81	0 100 100	29, 32, 44, 50	0
2	F	8/8 (100%)	-0.20	0 100 100	31, 36, 66, 79	0
3	A	12/12 (100%)	-0.25	1 (8%) 12 11	33, 44, 65, 70	0
3	C	12/12 (100%)	-0.34	0 100 100	30, 46, 68, 69	0
All	All	1383/1424 (97%)	-0.18	43 (3%) 49 47	24, 39, 66, 102	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	THR	5.8
1	D	639	TYR	5.3
1	B	639[A]	TYR	5.1
1	D	544	THR	4.6
1	B	612	ILE	4.2
1	D	1061	ASP	3.9
1	D	638	VAL	3.9
1	B	424[A]	LYS	3.7
1	D	581	LYS	3.7
1	B	1009	ILE	3.7
1	D	491	GLY	3.6
1	B	599[A]	GLU	3.4
1	B	491	GLY	3.3
1	B	545	GLY	3.1
1	D	469	LEU	3.0
1	D	1059	THR	2.8
1	D	431	ILE	2.7
1	D	1058[A]	MET	2.7
1	D	427[A]	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	612	ILE	2.6
1	B	1436[A]	LEU	2.6
1	D	468	ARG	2.6
1	B	1061	ASP	2.6
1	D	599	GLU	2.6
3	A	4[A]	DC	2.6
1	B	1050	LEU	2.6
1	D	473	LEU	2.5
1	B	638[A]	VAL	2.5
1	D	1010	ASN	2.5
1	D	1177	VAL	2.4
1	B	1306	ILE	2.3
1	D	1056[A]	GLN	2.3
1	B	580[A]	TYR	2.3
1	B	1195	VAL	2.2
1	D	492	ASP	2.2
1	D	416	GLY	2.2
1	B	1439[A]	ASP	2.1
1	D	580	TYR	2.1
1	D	596	MET	2.1
1	B	591	LEU	2.0
1	D	496	ALA	2.0
1	D	490	GLY	2.0
1	B	1300	THR	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^{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	LLDF	B-factors(Å^2)	Q<0.9
6	GOL	B	1505	6/6	0.82	0.29	5.88	52,56,68,73	0
6	GOL	A	101	6/6	0.67	0.31	3.39	65,66,71,86	0
6	GOL	D	1505	6/6	0.87	0.16	2.08	56,61,68,82	0
6	GOL	D	1504	6/6	0.86	0.17	1.78	59,62,70,71	0
6	GOL	B	1503	6/6	0.78	0.18	1.45	52,58,62,65	0
6	GOL	D	1503	6/6	0.92	0.15	1.27	32,52,59,65	0
9	6EJ	C	101[A]	33/33	0.92	0.17	1.26	38,45,50,50	33
9	6EJ	C	101[B]	33/33	0.92	0.17	1.18	35,41,51,59	33
6	GOL	B	1504	6/6	0.91	0.15	0.99	38,51,58,58	0
8	DMS	B	1507	4/4	0.92	0.12	0.62	58,63,78,88	0
6	GOL	C	102	6/6	0.83	0.18	0.35	45,57,66,68	0
5	94K	D	1502	25/25	0.94	0.11	-0.54	29,40,49,58	0
5	94K	B	1502	25/25	0.94	0.11	-0.67	28,37,47,47	0
4	MN	D	1501	1/1	1.00	0.03	-1.18	48,48,48,48	0
7	NA	B	1506	1/1	0.89	0.07	-1.35	40,40,40,40	0
4	MN	B	1501	1/1	0.99	0.07	-1.49	41,41,41,41	0
6	GOL	D	1506	6/6	0.77	0.22	-	54,65,73,78	0

6.5 Other polymers (i)

There are no such residues in this entry.