Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:30 AM GMT

PDB ID	:	3B05
Title	:	Crystal structure of Sulfolobus shibatae isopentenyl diphosphate isomerase in complex with reduced FMN and IPP at 2.2A resolution.
Authors	:	Unno, H.; Nagai, T.; Hemmi, H.
Deposited on	:	2011-06-03
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
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:

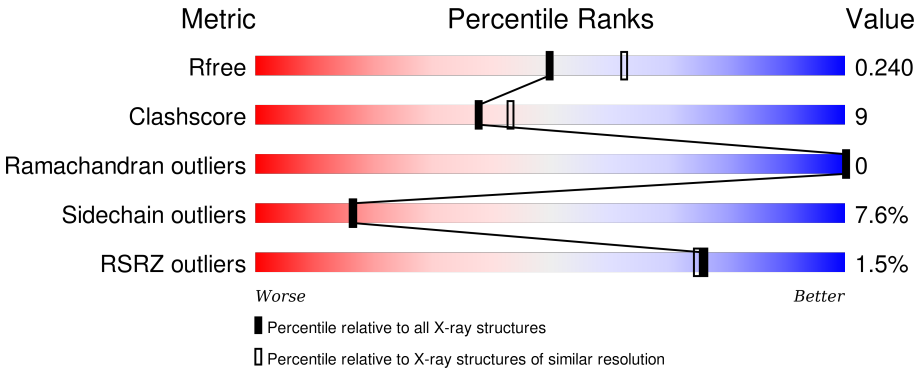
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 >=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	A	368	81% 15%
1	B	368	75% 19%
1	C	368	77% 18%
1	D	368	78% 17%

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
4	MG	B	1001	-	-	-	X

2 Entry composition

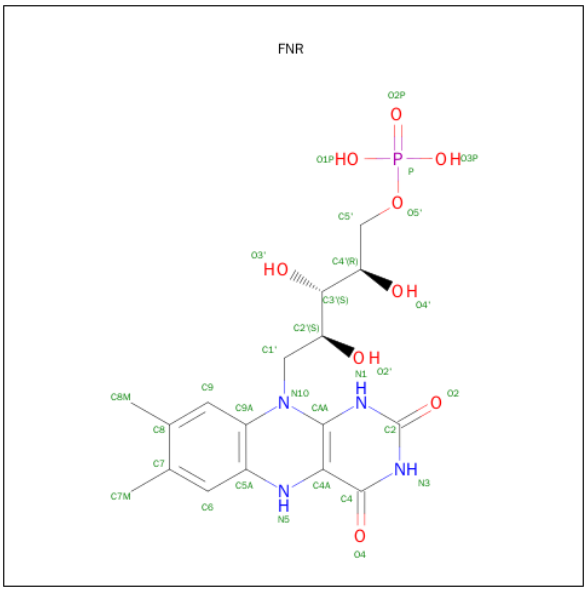
There are 5 unique types of molecules in this entry. The entry contains 11883 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isopentenyl-diphosphate delta-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2808	1799	475	523	11			
1	B	364	Total	C	N	O	S	0	0	0
			2808	1799	475	523	11			
1	C	364	Total	C	N	O	S	0	0	0
			2808	1799	475	523	11			
1	D	364	Total	C	N	O	S	0	0	0
			2808	1799	475	523	11			

- Molecule 2 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PTERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (three-letter code: FNR) (formula: $C_{17}H_{23}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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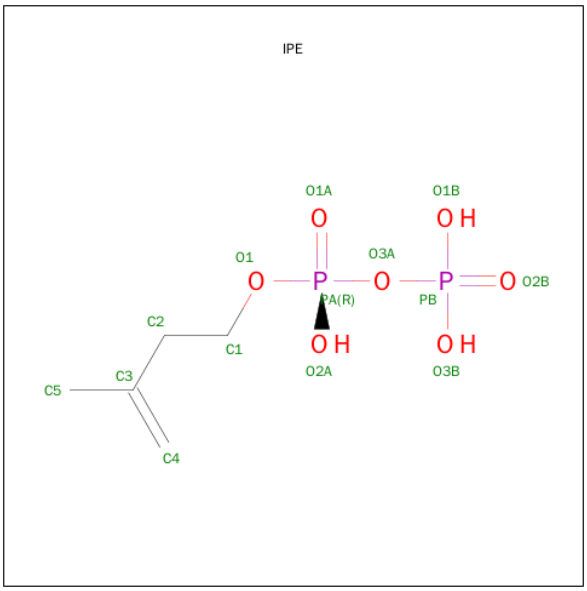
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P 31 17 4 9 1	0	0
2	C	1	Total C N O P 31 17 4 9 1	0	0
2	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 3 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 14 5 7 2	0	0
3	B	1	Total C O P 14 5 7 2	0	0
3	C	1	Total C O P 14 5 7 2	0	0
3	D	1	Total C O P 14 5 7 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

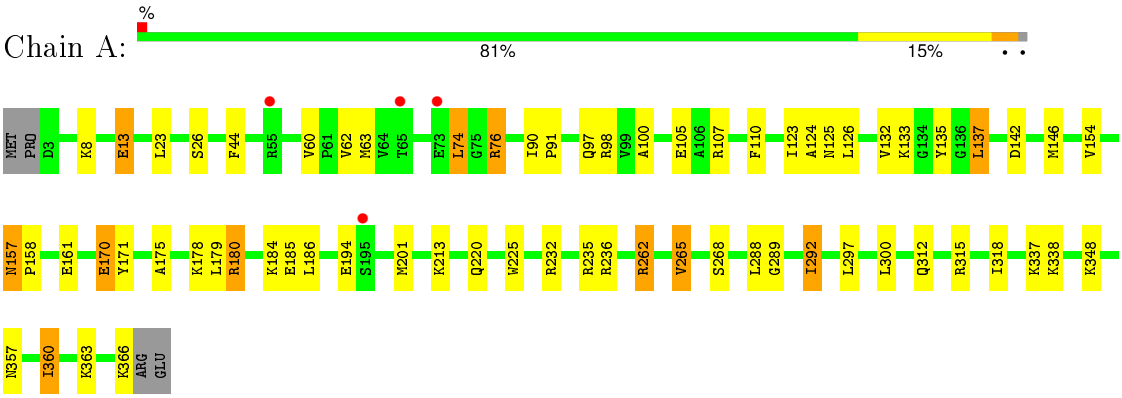
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0
5	B	116	Total O 116 116	0	0
5	C	119	Total O 119 119	0	0
5	D	116	Total O 116 116	0	0

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 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.

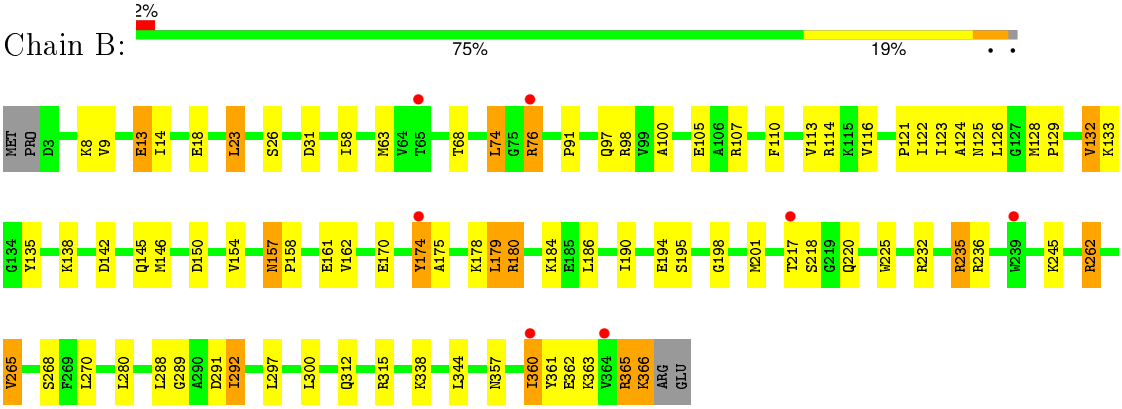
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain A:



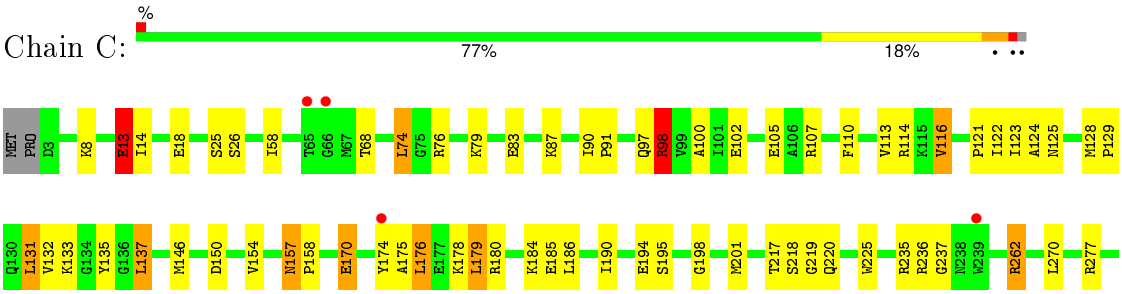
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain B:



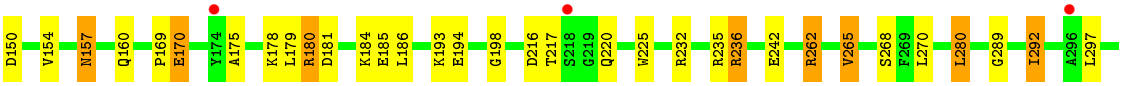
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

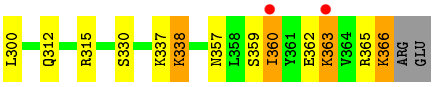
Chain C:



• Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.62Å 101.62Å 333.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.62 – 2.20 31.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (31.62-2.20) 97.8 (31.62-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.242 0.197 , 0.240	Depositor DCC
R_{free} test set	4392 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	3 of 87761 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, FNR, IPE

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	1.03	1/2855 (0.0%)	1.07	15/3846 (0.4%)
1	B	1.06	4/2855 (0.1%)	1.08	17/3846 (0.4%)
1	C	1.06	3/2855 (0.1%)	1.08	17/3846 (0.4%)
1	D	1.04	4/2855 (0.1%)	0.99	9/3846 (0.2%)
All	All	1.04	12/11420 (0.1%)	1.05	58/15384 (0.4%)

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	D	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	GLU	CD-OE2	-7.53	1.17	1.25
1	C	131	LEU	CG-CD2	-6.09	1.29	1.51
1	B	161	GLU	CD-OE1	-5.94	1.19	1.25
1	B	174	TYR	CD1-CE1	5.79	1.48	1.39
1	B	362	GLU	CG-CD	5.66	1.60	1.51
1	A	13	GLU	CD-OE2	5.63	1.31	1.25
1	C	352	GLU	CB-CG	5.33	1.62	1.52
1	D	13	GLU	CB-CG	-5.32	1.42	1.52
1	D	337	LYS	CE-NZ	5.30	1.62	1.49
1	C	13	GLU	CB-CG	-5.16	1.42	1.52
1	D	242	GLU	CG-CD	5.08	1.59	1.51
1	D	13	GLU	CD-OE2	5.02	1.31	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	ARG	NE-CZ-NH2	16.81	128.70	120.30
1	B	236	ARG	NE-CZ-NH1	-15.95	112.32	120.30
1	C	98	ARG	NE-CZ-NH1	-15.58	112.51	120.30
1	A	76	ARG	NE-CZ-NH2	14.66	127.63	120.30
1	A	76	ARG	NE-CZ-NH1	-14.42	113.09	120.30
1	D	236	ARG	NE-CZ-NH1	-14.21	113.20	120.30
1	C	180	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	A	236	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	C	236	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	B	161	GLU	OE1-CD-OE2	-12.00	108.90	123.30
1	B	236	ARG	NE-CZ-NH2	11.15	125.88	120.30
1	D	262	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	A	262	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	D	236	ARG	NE-CZ-NH2	9.95	125.28	120.30
1	B	180	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	262	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	C	180	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	180	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	B	262	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	A	236	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	C	236	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	262	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	A	76	ARG	CD-NE-CZ	7.88	134.64	123.60
1	D	180	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	365	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	B	235	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	180	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	365	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	262	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	B	201	MET	CA-CB-CG	6.87	124.97	113.30
1	C	131	LEU	CD1-CG-CD2	-6.57	90.79	110.50
1	C	98	ARG	CD-NE-CZ	6.50	132.70	123.60
1	D	365	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	98	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	262	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	D	236	ARG	CG-CD-NE	-6.03	99.15	111.80
1	A	74	LEU	CB-CG-CD1	6.02	121.23	111.00
1	B	23	LEU	CB-CG-CD2	6.01	121.22	111.00
1	D	365	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	76	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	176	LEU	CB-CG-CD1	5.89	121.01	111.00
1	C	154	VAL	CG1-CB-CG2	5.84	120.25	110.90
1	B	232	ARG	NE-CZ-NH2	-5.77	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	201	MET	CA-CB-CG	5.76	123.10	113.30
1	A	201	MET	CA-CB-CG	5.74	123.06	113.30
1	D	280	LEU	CB-CG-CD2	5.68	120.65	111.00
1	C	365	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	131	LEU	CA-CB-CG	-5.55	102.53	115.30
1	A	98	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	161	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	B	9	VAL	CG1-CB-CG2	5.42	119.57	110.90
1	C	116	VAL	CG1-CB-CG2	5.38	119.50	110.90
1	A	288	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	277	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	291	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	13	GLU	CG-CD-OE1	-5.10	108.10	118.30
1	A	232	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	236	ARG	CG-CD-NE	-5.07	101.16	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	3	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2808	0	2890	45	0
1	B	2808	0	2890	59	0
1	C	2808	0	2890	56	0
1	D	2808	0	2890	51	0
2	A	31	0	22	0	0
2	B	31	0	22	1	0
2	C	31	0	22	2	0
2	D	31	0	22	0	0
3	A	14	0	9	1	0
3	B	14	0	9	2	0
3	C	14	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	9	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	116	0	0	7	0
5	B	116	0	0	6	0
5	C	119	0	0	5	0
5	D	116	0	0	4	0
All	All	11883	0	11684	213	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 9.

All (213) 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:142:ASP:HB3	5:D:473:HOH:O	1.41	1.20
1:A:142:ASP:HB3	5:A:453:HOH:O	1.42	1.15
1:B:184:LYS:HE2	1:B:184:LYS:HA	1.22	1.13
1:C:184:LYS:HE2	1:C:184:LYS:HA	1.24	1.10
1:A:184:LYS:HE2	1:A:184:LYS:HA	1.34	1.10
1:D:184:LYS:HE2	1:D:184:LYS:HA	1.29	1.07
1:B:138:LYS:HE3	5:B:456:HOH:O	1.69	0.93
1:B:184:LYS:HE2	1:B:184:LYS:CA	2.02	0.89
1:C:184:LYS:CA	1:C:184:LYS:HE2	2.08	0.83
1:D:180:ARG:HD2	5:D:430:HOH:O	1.81	0.81
1:A:265:VAL:HG22	1:A:268:SER:HB3	1.61	0.81
1:D:265:VAL:HG22	1:D:268:SER:HB3	1.63	0.80
1:B:138:LYS:CE	5:B:456:HOH:O	2.29	0.79
1:B:265:VAL:HG22	1:B:268:SER:HB3	1.63	0.79
1:B:132:VAL:HG23	1:B:175:ALA:HB2	1.66	0.77
1:C:137:LEU:HD11	1:C:185:GLU:HG2	1.68	0.76
1:D:184:LYS:HE2	1:D:184:LYS:CA	2.14	0.75
1:D:107:ARG:HA	1:D:146:MET:HE3	1.68	0.75
1:B:312:GLN:NE2	1:B:315:ARG:HH11	1.85	0.74
1:D:312:GLN:NE2	1:D:315:ARG:HH11	1.85	0.73
1:B:107:ARG:HA	1:B:146:MET:HE3	1.71	0.72
1:B:180:ARG:HD2	5:B:464:HOH:O	1.89	0.71
1:C:87:LYS:HE2	5:C:435:HOH:O	1.90	0.71
1:A:184:LYS:HE2	1:A:184:LYS:CA	2.17	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ARG:HA	1:C:146:MET:HE3	1.73	0.70
1:A:107:ARG:HA	1:A:146:MET:HE3	1.73	0.70
1:D:184:LYS:CE	1:D:184:LYS:HA	2.16	0.70
1:C:184:LYS:HA	1:C:184:LYS:CE	2.14	0.69
1:B:245:LYS:HE3	5:B:476:HOH:O	1.93	0.69
1:C:110:PHE:CD1	1:C:146:MET:HE1	2.28	0.68
1:C:312:GLN:NE2	1:C:315:ARG:HH11	1.91	0.68
1:C:135:TYR:O	1:C:178:LYS:HE2	1.93	0.67
1:D:97:GLN:HE21	1:D:125:ASN:H	1.40	0.67
1:C:97:GLN:HE21	1:C:125:ASN:H	1.43	0.67
1:C:132:VAL:HG12	1:C:175:ALA:HB2	1.77	0.67
1:A:142:ASP:CB	5:A:453:HOH:O	2.16	0.66
1:A:97:GLN:HE21	1:A:125:ASN:H	1.44	0.66
1:C:132:VAL:HG21	1:C:170:GLU:HB2	1.76	0.65
1:A:110:PHE:CD1	1:A:146:MET:HE1	2.32	0.65
1:D:312:GLN:HE21	1:D:315:ARG:NH1	1.95	0.64
1:B:97:GLN:HE21	1:B:125:ASN:H	1.46	0.63
1:A:312:GLN:NE2	1:A:315:ARG:HH11	1.96	0.63
1:C:174:TYR:HB3	5:C:465:HOH:O	1.98	0.63
1:D:312:GLN:HE21	1:D:315:ARG:HH11	1.47	0.63
1:D:107:ARG:HA	1:D:146:MET:CE	2.29	0.62
1:C:135:TYR:O	1:C:178:LYS:CE	2.48	0.62
1:A:110:PHE:HB2	1:A:146:MET:HE2	1.80	0.62
1:C:312:GLN:HE21	1:C:315:ARG:HH11	1.47	0.62
1:A:26:SER:H	1:A:220:GLN:HE21	1.48	0.61
1:B:132:VAL:HG11	1:B:170:GLU:HB2	1.83	0.61
1:D:160:GLN:HE22	3:D:701:IPE:H21	1.65	0.61
1:A:132:VAL:HG21	1:A:170:GLU:HB2	1.82	0.61
1:B:26:SER:H	1:B:220:GLN:HE21	1.48	0.60
1:B:184:LYS:CE	1:B:184:LYS:HA	2.15	0.59
1:A:366:LYS:O	5:A:463:HOH:O	2.17	0.59
1:D:338:LYS:HB3	1:D:366:LYS:C	2.22	0.59
1:D:100:ALA:HB1	1:D:146:MET:HE3	1.85	0.59
1:D:110:PHE:CD1	1:D:146:MET:HE1	2.38	0.59
1:A:137:LEU:HD11	1:A:185:GLU:HG2	1.84	0.59
1:B:312:GLN:HE21	1:B:315:ARG:NH1	2.01	0.58
1:C:357:ASN:OD1	1:C:360:ILE:HG23	2.02	0.58
1:B:312:GLN:HE21	1:B:315:ARG:HH11	1.50	0.58
1:C:97:GLN:HE22	1:C:124:ALA:HB1	1.68	0.58
1:C:58:ILE:HG21	1:C:91:PRO:HG3	1.84	0.58
1:A:100:ALA:HB1	1:A:146:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:CD1	1:B:146:MET:HE1	2.39	0.57
1:D:132:VAL:HG21	1:D:170:GLU:HB2	1.85	0.57
1:A:132:VAL:HG21	1:A:170:GLU:CB	2.35	0.57
1:D:137:LEU:HD11	1:D:185:GLU:HG2	1.87	0.57
1:D:357:ASN:OD1	1:D:360:ILE:HG23	2.05	0.57
1:C:110:PHE:HB2	1:C:146:MET:HE2	1.86	0.57
1:A:180:ARG:HD2	5:A:468:HOH:O	2.05	0.57
1:B:100:ALA:HB1	1:B:146:MET:HE3	1.85	0.56
1:C:98:ARG:HD2	1:C:102:GLU:OE2	2.06	0.56
1:C:312:GLN:HE21	1:C:315:ARG:NH1	2.03	0.56
1:B:110:PHE:HB2	1:B:146:MET:HE2	1.87	0.56
1:D:157:ASN:HD22	1:D:157:ASN:N	2.04	0.55
1:C:184:LYS:HG3	5:C:456:HOH:O	2.06	0.55
1:B:132:VAL:HG11	1:B:170:GLU:CB	2.37	0.55
1:D:132:VAL:HG21	1:D:170:GLU:CB	2.36	0.55
1:A:357:ASN:OD1	1:A:360:ILE:HG23	2.06	0.55
1:C:100:ALA:HB1	1:C:146:MET:HE3	1.89	0.55
1:A:337:LYS:HD3	5:A:466:HOH:O	2.06	0.55
1:D:63:MET:HB3	1:D:292:ILE:HD11	1.87	0.55
1:C:365:ARG:O	1:C:366:LYS:HB2	2.07	0.54
1:B:13:GLU:OE1	1:B:235:ARG:NH2	2.36	0.54
1:C:132:VAL:CG1	1:C:175:ALA:HB2	2.38	0.54
1:D:100:ALA:CB	1:D:146:MET:HE3	2.38	0.54
1:B:357:ASN:OD1	1:B:360:ILE:HG23	2.07	0.54
1:D:157:ASN:HD22	1:D:157:ASN:H	1.56	0.53
1:A:157:ASN:N	1:A:158:PRO:CD	2.71	0.53
1:B:63:MET:HB3	1:B:292:ILE:HD11	1.90	0.53
1:B:157:ASN:HD22	1:B:157:ASN:N	2.06	0.53
1:B:198:GLY:HA2	1:B:217:THR:O	2.09	0.53
1:A:97:GLN:HE22	1:A:124:ALA:HB1	1.72	0.53
1:B:157:ASN:HD22	1:B:157:ASN:H	1.57	0.53
1:A:100:ALA:CB	1:A:146:MET:HE3	2.39	0.53
1:B:184:LYS:CE	1:B:184:LYS:CA	2.83	0.52
1:B:133:LYS:HD2	1:B:170:GLU:HG3	1.91	0.52
1:B:107:ARG:HA	1:B:146:MET:CE	2.38	0.52
1:D:235:ARG:HD2	5:D:483:HOH:O	2.09	0.52
1:B:135:TYR:O	1:B:178:LYS:HE2	2.08	0.52
1:A:135:TYR:O	1:A:178:LYS:HE2	2.11	0.51
1:B:365:ARG:O	1:B:366:LYS:HB2	2.09	0.51
1:C:133:LYS:HD2	1:C:170:GLU:HG3	1.92	0.51
2:C:669:FNR:H9	2:C:669:FNR:H6	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ARG:HA	1:C:146:MET:CE	2.40	0.50
1:C:184:LYS:CA	1:C:184:LYS:CE	2.84	0.50
1:A:312:GLN:HE21	1:A:315:ARG:NH1	2.09	0.50
1:B:288:LEU:O	1:B:361:TYR:OH	2.26	0.50
1:D:135:TYR:O	1:D:178:LYS:HE2	2.12	0.49
1:A:184:LYS:HA	1:A:184:LYS:CE	2.22	0.49
1:C:195:SER:HB2	3:C:701:IPE:H42	1.94	0.49
1:C:14:ILE:HG23	1:C:18:GLU:HG3	1.94	0.49
1:D:362:GLU:HA	1:D:362:GLU:OE2	2.12	0.49
1:A:312:GLN:NE2	1:A:315:ARG:NH1	2.61	0.48
1:D:58:ILE:HG21	1:D:91:PRO:HG3	1.94	0.48
1:C:132:VAL:HG23	1:C:133:LYS:HG3	1.95	0.48
1:B:97:GLN:HE22	1:B:124:ALA:HB1	1.78	0.48
1:A:265:VAL:CG2	1:A:268:SER:HB3	2.40	0.48
1:D:110:PHE:HB2	1:D:146:MET:HE2	1.96	0.48
1:B:121:PRO:HA	1:B:150:ASP:OD2	2.14	0.48
1:C:26:SER:H	1:C:220:GLN:HE21	1.61	0.48
1:C:110:PHE:CD1	1:C:146:MET:CE	2.96	0.48
1:B:58:ILE:HG21	1:B:91:PRO:HG3	1.95	0.48
1:C:113:VAL:CG1	1:C:122:ILE:HD12	2.44	0.47
1:C:132:VAL:HG21	1:C:170:GLU:CB	2.42	0.47
1:D:262:ARG:HD2	1:D:289:GLY:O	2.14	0.47
1:B:68:THR:OG1	1:B:74:LEU:HG	2.14	0.47
1:A:135:TYR:O	1:A:178:LYS:CE	2.62	0.47
1:D:25:SER:HB2	1:D:220:GLN:HE21	1.80	0.47
1:C:262:ARG:HD2	1:C:289:GLY:O	2.15	0.47
1:B:26:SER:H	1:B:220:GLN:NE2	2.13	0.47
1:D:181:ASP:O	1:D:184:LYS:HB2	2.15	0.46
1:D:121:PRO:HA	1:D:150:ASP:OD2	2.15	0.46
1:C:121:PRO:HA	1:C:150:ASP:OD2	2.15	0.46
1:D:359:SER:O	1:D:363:LYS:HG3	2.14	0.46
1:C:97:GLN:NE2	1:C:125:ASN:H	2.11	0.46
1:C:123:ILE:N	1:C:123:ILE:HD12	2.31	0.46
1:B:138:LYS:HE2	5:B:456:HOH:O	2.09	0.46
1:C:100:ALA:CB	1:C:146:MET:HE3	2.44	0.46
1:A:107:ARG:HA	1:A:146:MET:CE	2.43	0.46
1:C:114:ARG:HA	1:C:114:ARG:HD3	1.80	0.46
1:A:348:LYS:HD2	5:A:470:HOH:O	2.13	0.46
1:A:225:TRP:CE2	3:A:701:IPE:H41	2.52	0.45
1:B:135:TYR:O	1:B:178:LYS:CE	2.65	0.45
1:D:26:SER:H	1:D:220:GLN:HE21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:HB3	5:B:451:HOH:O	2.17	0.45
1:A:110:PHE:CD1	1:A:146:MET:CE	2.99	0.45
1:C:157:ASN:N	1:C:158:PRO:CD	2.79	0.45
1:A:123:ILE:HD12	1:A:123:ILE:N	2.32	0.45
1:C:349:GLU:OE2	5:C:410:HOH:O	2.21	0.45
1:D:68:THR:OG1	1:D:74:LEU:HG	2.16	0.45
1:B:158:PRO:O	1:B:162:VAL:HG23	2.17	0.45
1:D:198:GLY:HA2	1:D:217:THR:O	2.17	0.44
1:A:132:VAL:CG1	1:A:175:ALA:HB2	2.47	0.44
1:D:135:TYR:O	1:D:178:LYS:CE	2.65	0.44
1:C:179:LEU:HD22	1:C:190:ILE:HD13	2.00	0.44
1:B:312:GLN:HA	1:B:312:GLN:NE2	2.33	0.44
1:D:97:GLN:NE2	1:D:125:ASN:H	2.13	0.44
1:B:114:ARG:HA	1:B:114:ARG:HD3	1.74	0.44
1:D:184:LYS:CE	1:D:184:LYS:CA	2.85	0.44
1:D:113:VAL:CG1	1:D:122:ILE:HD12	2.47	0.44
1:B:123:ILE:N	1:B:123:ILE:HD12	2.34	0.43
1:B:217:THR:O	1:B:218:SER:C	2.56	0.43
1:C:25:SER:HB2	1:C:220:GLN:HE21	1.83	0.43
1:B:195:SER:HB2	3:B:701:IPE:H42	2.01	0.43
1:B:97:GLN:NE2	1:B:125:ASN:H	2.15	0.43
1:C:68:THR:OG1	1:C:74:LEU:HG	2.18	0.43
1:B:128:MET:N	1:B:129:PRO:CD	2.81	0.43
1:B:14:ILE:HG23	1:B:18:GLU:HG3	2.01	0.43
1:A:235:ARG:HD2	5:A:469:HOH:O	2.18	0.43
1:C:79:LYS:O	1:C:83:GLU:HG2	2.19	0.43
1:A:60:VAL:HG21	1:A:318:ILE:HG12	2.00	0.43
1:B:31:ASP:HB3	1:B:344:LEU:O	2.18	0.43
1:C:13:GLU:OE1	1:C:235:ARG:NH2	2.45	0.43
2:C:669:FNR:N5	3:C:701:IPE:H22	2.34	0.42
1:A:62:VAL:O	1:A:91:PRO:HD2	2.19	0.42
1:B:262:ARG:HD2	1:B:289:GLY:O	2.20	0.42
1:D:330:SER:OG	5:D:456:HOH:O	2.22	0.42
1:D:132:VAL:CG1	1:D:175:ALA:HB2	2.50	0.42
1:D:225:TRP:CE2	3:D:701:IPE:H41	2.55	0.42
1:A:262:ARG:HD2	1:A:289:GLY:O	2.19	0.42
1:A:126:LEU:O	1:A:154:VAL:HA	2.20	0.42
1:A:44:PHE:HB2	1:D:169:PRO:HG2	2.02	0.42
1:B:113:VAL:CG1	1:B:122:ILE:HD12	2.48	0.42
1:B:142:ASP:HA	1:B:145:GLN:HG3	2.01	0.42
1:B:100:ALA:CB	1:B:146:MET:CE	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:CD1	1:B:146:MET:CE	3.01	0.41
1:B:179:LEU:HD22	1:B:190:ILE:HD13	2.01	0.41
1:C:237:GLY:HA2	5:C:460:HOH:O	2.20	0.41
1:A:97:GLN:NE2	1:A:124:ALA:HB1	2.34	0.41
1:A:157:ASN:ND2	1:A:171:TYR:OH	2.51	0.41
1:B:225:TRP:CE2	3:B:701:IPE:H41	2.55	0.41
1:D:69:GLY:HA3	1:D:110:PHE:CZ	2.56	0.41
1:B:100:ALA:CB	1:B:146:MET:HE3	2.50	0.41
1:C:128:MET:HB3	1:C:129:PRO:HD3	2.03	0.41
1:C:137:LEU:CD1	1:C:185:GLU:HG2	2.46	0.41
1:A:100:ALA:CB	1:A:146:MET:CE	2.98	0.41
1:C:292:ILE:HD13	1:C:292:ILE:HG21	1.88	0.41
1:A:63:MET:HB3	1:A:292:ILE:HD11	2.03	0.41
1:D:126:LEU:O	1:D:154:VAL:HA	2.21	0.41
1:D:232:ARG:O	1:D:236:ARG:HG2	2.21	0.41
1:C:128:MET:N	1:C:129:PRO:CD	2.84	0.41
1:C:198:GLY:CA	1:C:219:GLY:HA2	2.51	0.41
1:C:225:TRP:CE2	3:C:701:IPE:H41	2.56	0.40
2:B:669:FNR:H6	2:B:669:FNR:H9	2.02	0.40
1:D:97:GLN:HE22	1:D:124:ALA:HB1	1.86	0.40
1:C:217:THR:O	1:C:218:SER:C	2.59	0.40
1:A:133:LYS:HD2	1:A:170:GLU:HG3	2.03	0.40
1:D:100:ALA:CB	1:D:146:MET:CE	3.00	0.40
1:B:126:LEU:O	1:B:154:VAL:HA	2.22	0.40
1:D:193:LYS:CB	1:D:216:ASP:HB3	2.52	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	362/368 (98%)	350 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	362/368 (98%)	347 (96%)	15 (4%)	0	100	100
1	C	362/368 (98%)	352 (97%)	10 (3%)	0	100	100
1	D	362/368 (98%)	350 (97%)	12 (3%)	0	100	100
All	All	1448/1472 (98%)	1399 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/302 (99%)	277 (93%)	21 (7%)	19	19
1	B	298/302 (99%)	276 (93%)	22 (7%)	17	17
1	C	298/302 (99%)	276 (93%)	22 (7%)	17	17
1	D	298/302 (99%)	273 (92%)	25 (8%)	14	13
All	All	1192/1208 (99%)	1102 (92%)	90 (8%)	16	16

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	13	GLU
1	A	23	LEU
1	A	74	LEU
1	A	76	ARG
1	A	90	ILE
1	A	105	GLU
1	A	137	LEU
1	A	157	ASN
1	A	170	GLU
1	A	179	LEU
1	A	186	LEU
1	A	194	GLU

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Mol	Chain	Res	Type
1	A	213	LYS
1	A	265	VAL
1	A	292	ILE
1	A	297	LEU
1	A	300	LEU
1	A	338	LYS
1	A	360	ILE
1	A	363	LYS
1	B	8	LYS
1	B	13	GLU
1	B	23	LEU
1	B	74	LEU
1	B	76	ARG
1	B	105	GLU
1	B	116	VAL
1	B	132	VAL
1	B	157	ASN
1	B	179	LEU
1	B	186	LEU
1	B	194	GLU
1	B	265	VAL
1	B	270	LEU
1	B	280	LEU
1	B	292	ILE
1	B	297	LEU
1	B	300	LEU
1	B	338	LYS
1	B	360	ILE
1	B	363	LYS
1	B	366	LYS
1	C	8	LYS
1	C	13	GLU
1	C	74	LEU
1	C	76	ARG
1	C	90	ILE
1	C	98	ARG
1	C	105	GLU
1	C	116	VAL
1	C	131	LEU
1	C	137	LEU
1	C	157	ASN
1	C	170	GLU

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	179	LEU
1	C	186	LEU
1	C	194	GLU
1	C	270	LEU
1	C	292	ILE
1	C	300	LEU
1	C	338	LYS
1	C	360	ILE
1	C	365	ARG
1	D	3	ASP
1	D	8	LYS
1	D	13	GLU
1	D	51	THR
1	D	74	LEU
1	D	76	ARG
1	D	90	ILE
1	D	105	GLU
1	D	116	VAL
1	D	137	LEU
1	D	157	ASN
1	D	170	GLU
1	D	179	LEU
1	D	186	LEU
1	D	194	GLU
1	D	265	VAL
1	D	270	LEU
1	D	280	LEU
1	D	292	ILE
1	D	297	LEU
1	D	300	LEU
1	D	338	LYS
1	D	360	ILE
1	D	363	LYS
1	D	366	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	157	ASN
1	A	197	ASN

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	312	GLN
1	B	97	GLN
1	B	157	ASN
1	B	164	GLN
1	B	197	ASN
1	B	220	GLN
1	B	312	GLN
1	C	97	GLN
1	C	157	ASN
1	C	164	GLN
1	C	197	ASN
1	C	220	GLN
1	C	312	GLN
1	D	97	GLN
1	D	157	ASN
1	D	164	GLN
1	D	197	ASN
1	D	220	GLN
1	D	312	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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	FNR	A	669	-	30,33,33	1.40	5 (16%)	33,50,50	2.71	9 (27%)
3	IPE	A	701	4	10,13,13	0.65	0	14,19,19	1.33	2 (14%)
2	FNR	B	669	-	30,33,33	1.50	6 (20%)	33,50,50	2.78	8 (24%)
3	IPE	B	701	4	10,13,13	0.64	0	14,19,19	0.96	0
2	FNR	C	669	-	30,33,33	1.60	5 (16%)	33,50,50	2.09	7 (21%)
3	IPE	C	701	4	10,13,13	0.78	0	14,19,19	1.16	1 (7%)
2	FNR	D	669	-	30,33,33	1.35	4 (13%)	33,50,50	2.64	8 (24%)
3	IPE	D	701	4	10,13,13	0.68	0	14,19,19	1.26	2 (14%)

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
2	FNR	A	669	-	-	0/18/18/18	0/3/3/3
3	IPE	A	701	4	-	0/13/13/13	0/0/0/0
2	FNR	B	669	-	-	0/18/18/18	0/3/3/3
3	IPE	B	701	4	-	0/13/13/13	0/0/0/0
2	FNR	C	669	-	-	0/18/18/18	0/3/3/3
3	IPE	C	701	4	-	0/13/13/13	0/0/0/0
2	FNR	D	669	-	-	0/18/18/18	0/3/3/3
3	IPE	D	701	4	-	0/13/13/13	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	669	FNR	C1'-N10	-2.52	1.45	1.48
2	D	669	FNR	C9-C8	2.06	1.43	1.37
2	A	669	FNR	C5'-C4'	2.10	1.54	1.51
2	A	669	FNR	C4-N3	2.10	1.37	1.33
2	D	669	FNR	C9A-N10	2.23	1.41	1.38
2	B	669	FNR	C5'-C4'	2.39	1.55	1.51
2	C	669	FNR	C4-N3	2.43	1.37	1.33
2	D	669	FNR	C4-C4A	2.72	1.46	1.41
2	B	669	FNR	C4A-N5	2.84	1.37	1.33
2	B	669	FNR	C4-C4A	2.89	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	669	FNR	C9A-N10	3.02	1.43	1.38
2	C	669	FNR	C4A-N5	3.22	1.38	1.33
2	B	669	FNR	C9A-N10	3.24	1.43	1.38
2	C	669	FNR	C4A-CAA	3.45	1.47	1.41
2	D	669	FNR	C4A-CAA	3.52	1.47	1.41
2	C	669	FNR	C9A-N10	3.58	1.43	1.38
2	B	669	FNR	C4A-CAA	3.58	1.47	1.41
2	A	669	FNR	C4-C4A	3.69	1.48	1.41
2	A	669	FNR	C4A-CAA	3.96	1.48	1.41
2	C	669	FNR	C4-C4A	4.11	1.49	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	669	FNR	C4-C4A-CAA	-9.81	113.67	119.94
2	D	669	FNR	C4-C4A-CAA	-8.74	114.35	119.94
2	C	669	FNR	C4-C4A-CAA	-7.92	114.87	119.94
2	A	669	FNR	C4-C4A-CAA	-6.76	115.61	119.94
2	A	669	FNR	C4A-CAA-N10	-5.99	116.99	120.52
2	B	669	FNR	C4A-CAA-N10	-5.17	117.47	120.52
2	A	669	FNR	C4A-C4-N3	-4.44	117.51	123.59
2	D	669	FNR	C4A-CAA-N10	-4.39	117.93	120.52
2	A	669	FNR	O1P-P-O5'	-3.39	96.81	106.56
3	D	701	IPE	PA-O3A-PB	-2.99	122.64	132.67
2	D	669	FNR	C4A-C4-N3	-2.90	119.63	123.59
2	C	669	FNR	C4A-C4-N3	-2.82	119.73	123.59
2	C	669	FNR	C4A-CAA-N10	-2.72	118.92	120.52
3	A	701	IPE	PA-O3A-PB	-2.62	123.87	132.67
3	D	701	IPE	O2A-PA-O3A	2.00	114.17	105.09
2	A	669	FNR	C1'-N10-C9A	2.27	121.41	118.86
2	B	669	FNR	O3P-P-O1P	2.37	116.40	107.38
3	A	701	IPE	O3B-PB-O1B	2.44	116.65	107.38
3	C	701	IPE	O3B-PB-O2B	2.44	118.43	110.58
2	D	669	FNR	C1'-N10-C9A	2.58	121.76	118.86
2	C	669	FNR	C4A-N5-C5A	2.71	119.88	116.76
2	B	669	FNR	C5A-C9A-N10	2.84	119.78	117.62
2	A	669	FNR	C5A-C9A-N10	3.21	120.06	117.62
2	D	669	FNR	C4A-N5-C5A	3.27	120.53	116.76
2	A	669	FNR	C4-C4A-N5	3.52	123.00	118.72
2	C	669	FNR	C4-C4A-N5	3.52	123.00	118.72
2	C	669	FNR	C5A-C9A-N10	3.73	120.46	117.62
2	C	669	FNR	C4-N3-C2	3.77	118.51	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	669	FNR	C1'-N10-C9A	3.91	123.25	118.86
2	B	669	FNR	C4A-N5-C5A	4.08	121.46	116.76
2	D	669	FNR	C5A-C9A-N10	4.16	120.78	117.62
2	A	669	FNR	C4A-N5-C5A	4.34	121.75	116.76
2	D	669	FNR	C4-C4A-N5	4.99	124.77	118.72
2	B	669	FNR	C4-C4A-N5	5.86	125.84	118.72
2	B	669	FNR	C4-N3-C2	5.87	120.32	115.25
2	D	669	FNR	C4-N3-C2	7.10	121.39	115.25
2	A	669	FNR	C4-N3-C2	7.91	122.08	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	IPE	1	0
2	B	669	FNR	1	0
3	B	701	IPE	2	0
2	C	669	FNR	2	0
3	C	701	IPE	3	0
3	D	701	IPE	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	364/368 (98%)	-0.25	4 (1%)	82 82	25, 34, 49, 59	0
1	B	364/368 (98%)	-0.27	7 (1%)	70 68	25, 34, 50, 59	0
1	C	364/368 (98%)	-0.31	5 (1%)	78 77	25, 34, 50, 59	0
1	D	364/368 (98%)	-0.30	6 (1%)	74 73	25, 34, 49, 59	0
All	All	1456/1472 (98%)	-0.28	22 (1%)	76 75	25, 34, 50, 59	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	364	VAL	3.4
1	D	174	TYR	3.3
1	C	65	THR	3.2
1	A	195	SER	2.9
1	B	65	THR	2.9
1	B	174	TYR	2.9
1	C	239	TRP	2.7
1	B	239	TRP	2.7
1	C	174	TYR	2.7
1	D	218	SER	2.6
1	A	65	THR	2.5
1	D	65	THR	2.4
1	B	76	ARG	2.4
1	D	360	ILE	2.3
1	D	296	ALA	2.3
1	A	55	ARG	2.2
1	C	66	GLY	2.2
1	B	364	VAL	2.1
1	D	363	LYS	2.1
1	A	73	GLU	2.1
1	B	217	THR	2.0
1	B	360	ILE	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
4	MG	B	1001	1/1	0.78	0.25	4.19	60,60,60,60	0
2	FNR	A	669	31/31	0.98	0.20	0.65	25,29,31,31	0
3	IPE	A	701	14/14	0.98	0.15	0.29	37,42,45,46	0
2	FNR	B	669	31/31	0.98	0.17	0.28	25,29,31,32	0
2	FNR	D	669	31/31	0.98	0.18	0.18	25,29,31,31	0
2	FNR	C	669	31/31	0.98	0.18	0.17	25,29,31,32	0
3	IPE	C	701	14/14	0.99	0.11	-0.32	28,35,38,41	0
3	IPE	B	701	14/14	0.98	0.12	-0.39	36,42,44,45	0
3	IPE	D	701	14/14	0.99	0.11	-0.40	30,35,38,40	0
4	MG	A	1001	1/1	0.90	0.09	-1.69	47,47,47,47	0
4	MG	D	1001	1/1	0.95	0.04	-2.33	43,43,43,43	0
4	MG	C	1001	1/1	0.88	0.06	-2.79	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.