Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

PDB ID	:	3VKJ
Title	:	Crystal structure of Sulfolobus shibatae isopentenyl diphosphate isomerase, octameric form
Authors	:	Nakatani, H.; Goda, S.; Unno, H.; Nagai, T.; Yoshimura, T.; Hemmi, H.
Deposited on	:	2011-11-17
Resolution	:	1.70 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 ⓘ symbol.

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

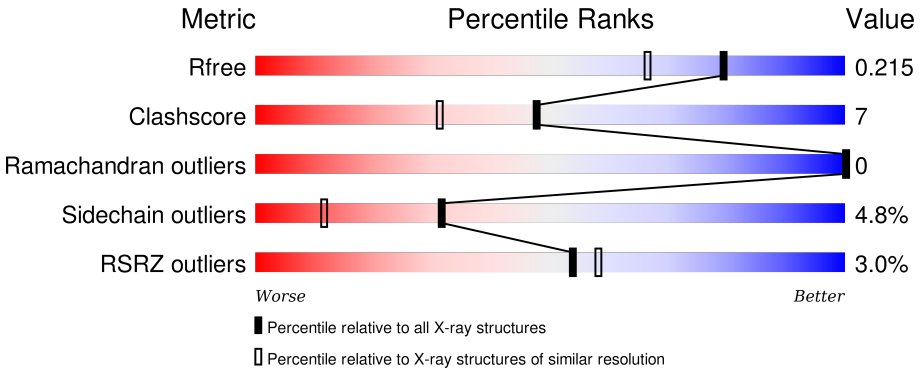
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	3% 82% 13%
1	B	368	4% 80% 14%
1	C	368	2% 76% 18%
1	D	368	2% 80% 15%

2 Entry composition

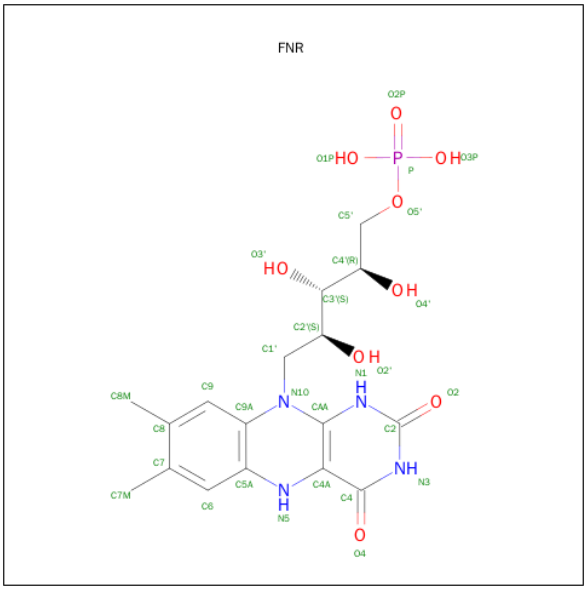
There are 3 unique types of molecules in this entry. The entry contains 12048 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	B	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	C	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	11			
1	D	363	Total	C	N	O	S	0	0	0
			2800	1795	474	520	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	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

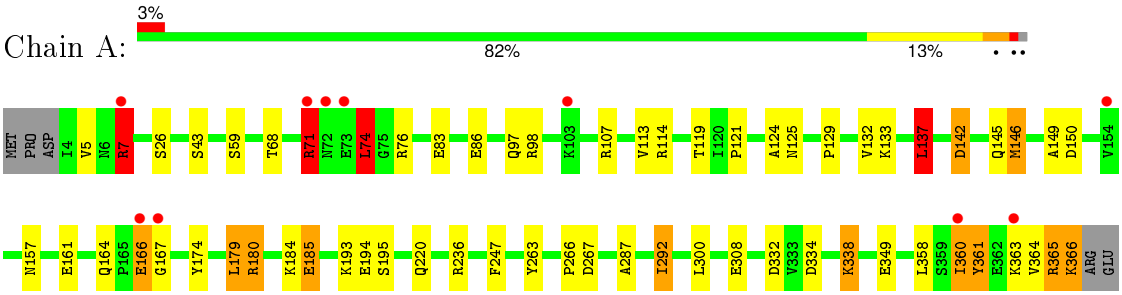
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	174	Total	O	0	0
			174	174		
3	C	207	Total	O	0	0
			207	207		
3	D	180	Total	O	0	0
			180	180		

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.

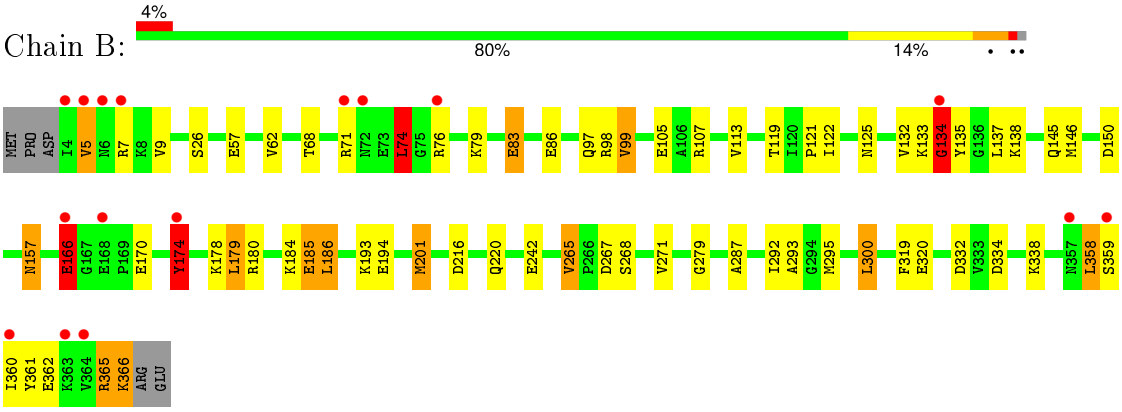
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain A:



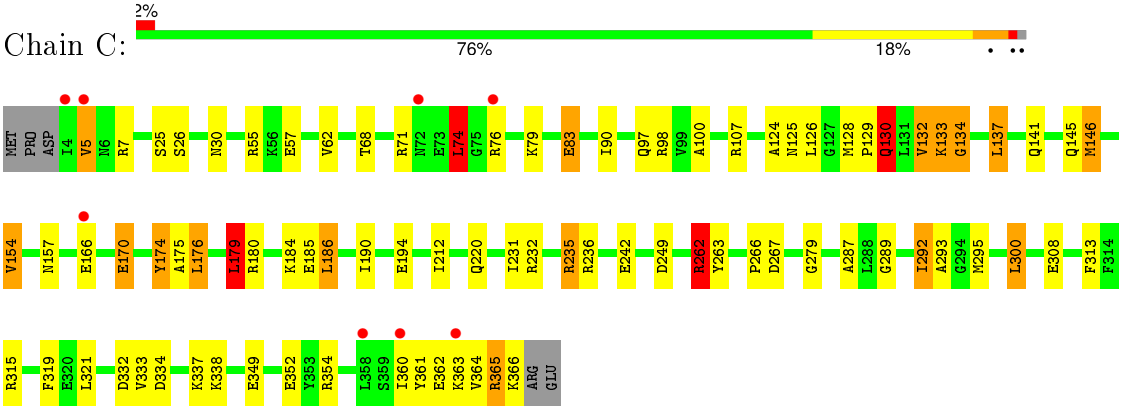
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

Chain B:



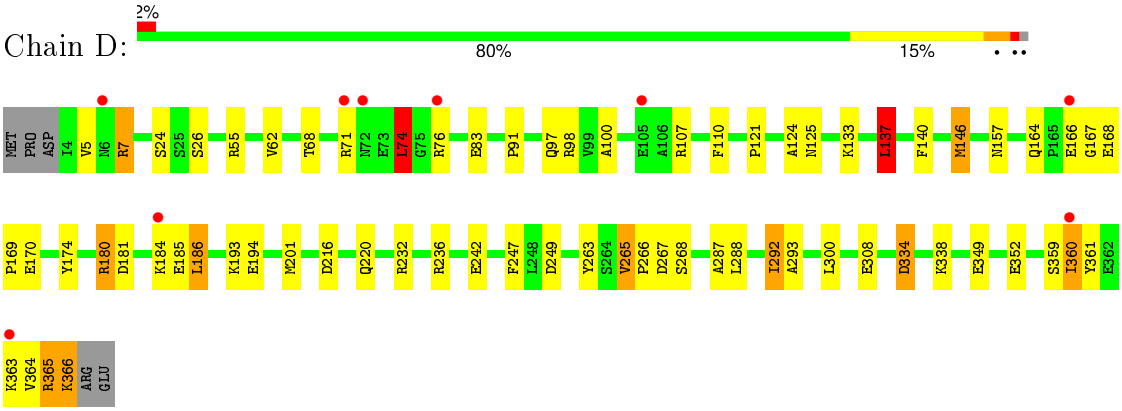
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

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	100.84Å 100.84Å 336.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.15 – 1.70 35.15 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (35.15-1.70) 94.6 (35.15-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.217 0.184 , 0.215	Depositor DCC
R_{free} test set	9047 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 179998 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12048	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: FNR

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	1.53	27/2847 (0.9%)	1.45	39/3835 (1.0%)
1	B	1.58	27/2847 (0.9%)	1.38	39/3835 (1.0%)
1	C	1.57	34/2847 (1.2%)	1.73	46/3835 (1.2%)
1	D	1.54	24/2847 (0.8%)	1.40	35/3835 (0.9%)
All	All	1.56	112/11388 (1.0%)	1.50	159/15340 (1.0%)

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	B	0	2

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	TYR	CD2-CE2	-16.21	1.15	1.39
1	C	134	GLY	N-CA	15.29	1.69	1.46
1	B	170	GLU	CD-OE1	-13.06	1.11	1.25
1	D	5	VAL	CB-CG2	-12.33	1.26	1.52
1	A	83	GLU	CB-CG	-12.00	1.29	1.52
1	B	83	GLU	CB-CG	-11.01	1.31	1.52
1	D	166	GLU	CB-CG	-10.06	1.33	1.52
1	A	164	GLN	CB-CG	-9.86	1.25	1.52
1	B	174	TYR	CE2-CZ	-9.85	1.25	1.38
1	B	174	TYR	CB-CG	-9.78	1.36	1.51
1	C	174	TYR	CD2-CE2	-9.70	1.24	1.39
1	A	166	GLU	CB-CG	-9.58	1.33	1.52
1	D	265	VAL	CB-CG2	-9.26	1.33	1.52
1	C	174	TYR	CE2-CZ	-9.25	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	174	TYR	CD1-CE1	-9.24	1.25	1.39
1	A	161	GLU	CD-OE2	-9.14	1.15	1.25
1	D	360	ILE	CB-CG2	-9.06	1.24	1.52
1	B	170	GLU	CD-OE2	-9.01	1.15	1.25
1	C	132	VAL	CB-CG2	-8.99	1.33	1.52
1	D	5	VAL	CB-CG1	-8.72	1.34	1.52
1	A	174	TYR	CD1-CE1	-8.20	1.27	1.39
1	C	235	ARG	CD-NE	-8.19	1.32	1.46
1	C	5	VAL	CB-CG2	-8.15	1.35	1.52
1	C	174	TYR	CB-CG	-8.04	1.39	1.51
1	B	99	VAL	CB-CG1	-7.47	1.37	1.52
1	C	262	ARG	CD-NE	-7.38	1.33	1.46
1	A	166	GLU	CG-CD	-7.36	1.41	1.51
1	C	5	VAL	CB-CG1	-7.29	1.37	1.52
1	B	5	VAL	CB-CG2	-7.26	1.37	1.52
1	C	170	GLU	CD-OE1	-7.24	1.17	1.25
1	D	164	GLN	CB-CG	-7.21	1.33	1.52
1	D	361	TYR	CD1-CE1	7.07	1.50	1.39
1	A	5	VAL	CB-CG1	-7.03	1.38	1.52
1	A	236	ARG	CZ-NH2	-6.91	1.24	1.33
1	B	174	TYR	CG-CD2	-6.91	1.30	1.39
1	C	7	ARG	CZ-NH1	-6.76	1.24	1.33
1	A	142	ASP	CB-CG	-6.71	1.37	1.51
1	D	174	TYR	CG-CD2	-6.68	1.30	1.39
1	D	24	SER	CB-OG	6.65	1.50	1.42
1	C	235	ARG	CZ-NH2	-6.62	1.24	1.33
1	A	149	ALA	CA-CB	6.61	1.66	1.52
1	C	145	GLN	CB-CG	-6.53	1.34	1.52
1	C	174	TYR	CG-CD2	-6.48	1.30	1.39
1	A	7	ARG	CB-CG	-6.44	1.35	1.52
1	B	135	TYR	CD1-CE1	-6.35	1.29	1.39
1	D	7	ARG	CZ-NH2	-6.31	1.24	1.33
1	C	166	GLU	CD-OE1	-6.29	1.18	1.25
1	B	185	GLU	CB-CG	-6.27	1.40	1.52
1	D	7	ARG	CB-CG	-6.26	1.35	1.52
1	B	5	VAL	CB-CG1	-6.25	1.39	1.52
1	C	242	GLU	CG-CD	6.21	1.61	1.51
1	D	167	GLY	CA-C	-6.21	1.42	1.51
1	A	167	GLY	CA-C	-6.20	1.42	1.51
1	C	55	ARG	CZ-NH1	-6.20	1.25	1.33
1	C	83	GLU	CB-CG	-6.20	1.40	1.52
1	D	352	GLU	CD-OE2	6.17	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLU	CG-CD	6.12	1.61	1.51
1	A	236	ARG	CZ-NH1	-6.09	1.25	1.33
1	D	170	GLU	CG-CD	-6.08	1.42	1.51
1	A	161	GLU	CD-OE1	-6.02	1.19	1.25
1	D	83	GLU	CB-CG	-6.02	1.40	1.52
1	B	135	TYR	CD2-CE2	-5.97	1.30	1.39
1	A	247	PHE	CE1-CZ	5.94	1.48	1.37
1	B	166	GLU	CG-CD	-5.91	1.43	1.51
1	C	279	GLY	N-CA	5.84	1.54	1.46
1	D	242	GLU	CG-CD	5.81	1.60	1.51
1	A	174	TYR	CE2-CZ	-5.81	1.30	1.38
1	A	174	TYR	CG-CD2	-5.81	1.31	1.39
1	A	43	SER	CB-OG	-5.79	1.34	1.42
1	B	83	GLU	CG-CD	5.77	1.60	1.51
1	B	7	ARG	CB-CG	-5.77	1.36	1.52
1	A	361	TYR	CD2-CE2	-5.74	1.30	1.39
1	B	292	ILE	CB-CG2	-5.69	1.35	1.52
1	C	352	GLU	CG-CD	5.67	1.60	1.51
1	B	57	GLU	CD-OE2	-5.67	1.19	1.25
1	B	180	ARG	CD-NE	-5.64	1.36	1.46
1	D	334	ASP	CB-CG	-5.62	1.40	1.51
1	D	201	MET	CB-CG	-5.59	1.33	1.51
1	C	154	VAL	CB-CG1	5.58	1.64	1.52
1	B	201	MET	CB-CG	-5.55	1.33	1.51
1	C	292	ILE	CB-CG1	-5.51	1.38	1.54
1	C	263	TYR	CD2-CE2	5.50	1.47	1.39
1	B	7	ARG	CZ-NH1	-5.47	1.25	1.33
1	D	263	TYR	CD2-CE2	5.46	1.47	1.39
1	C	185	GLU	CB-CG	-5.45	1.41	1.52
1	A	59	SER	CB-OG	5.44	1.49	1.42
1	C	174	TYR	CG-CD1	-5.43	1.32	1.39
1	D	140	PHE	CD1-CE1	5.43	1.50	1.39
1	D	157	ASN	CG-OD1	-5.41	1.12	1.24
1	D	247	PHE	CE1-CZ	5.40	1.47	1.37
1	C	349	GLU	CD-OE1	-5.39	1.19	1.25
1	A	174	TYR	CZ-OH	5.38	1.47	1.37
1	A	195	SER	CB-OG	-5.38	1.35	1.42
1	B	242	GLU	CG-CD	5.37	1.60	1.51
1	C	292	ILE	CB-CG2	5.37	1.69	1.52
1	A	292	ILE	CB-CG1	-5.37	1.39	1.54
1	B	157	ASN	CG-ND2	-5.33	1.19	1.32
1	A	349	GLU	CD-OE1	-5.33	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	130	GLN	N-CA	5.26	1.56	1.46
1	A	338	LYS	CE-NZ	5.26	1.62	1.49
1	B	166	GLU	CB-CG	-5.16	1.42	1.52
1	C	7	ARG	CB-CG	-5.14	1.38	1.52
1	D	349	GLU	CD-OE1	-5.14	1.20	1.25
1	C	174	TYR	CE1-CZ	-5.11	1.31	1.38
1	B	132	VAL	CB-CG1	-5.10	1.42	1.52
1	B	174	TYR	CD1-CE1	-5.09	1.31	1.39
1	B	271	VAL	CB-CG1	5.09	1.63	1.52
1	C	57	GLU	CD-OE2	-5.08	1.20	1.25
1	C	166	GLU	CB-CG	-5.04	1.42	1.52
1	C	319	PHE	CD1-CE1	5.04	1.49	1.39
1	C	362	GLU	CD-OE1	5.02	1.31	1.25
1	A	113	VAL	CB-CG1	-5.01	1.42	1.52

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	262	ARG	NE-CZ-NH2	34.96	137.78	120.30
1	C	235	ARG	NE-CZ-NH1	31.03	135.81	120.30
1	C	262	ARG	NE-CZ-NH1	-21.34	109.63	120.30
1	C	235	ARG	NE-CZ-NH2	-21.21	109.70	120.30
1	D	360	ILE	CG1-CB-CG2	-21.04	65.11	111.40
1	A	76	ARG	NE-CZ-NH1	-19.18	110.71	120.30
1	A	180	ARG	NE-CZ-NH1	16.87	128.73	120.30
1	A	142	ASP	CB-CG-OD1	-16.60	103.36	118.30
1	A	76	ARG	NE-CZ-NH2	15.91	128.26	120.30
1	C	98	ARG	NE-CZ-NH2	15.52	128.06	120.30
1	C	98	ARG	NE-CZ-NH1	-15.48	112.56	120.30
1	C	365	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	B	180	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	C	180	ARG	NE-CZ-NH1	-14.32	113.14	120.30
1	C	133	LYS	C-N-CA	-14.15	92.58	122.30
1	C	262	ARG	CD-NE-CZ	14.10	143.34	123.60
1	B	365	ARG	NE-CZ-NH1	14.09	127.35	120.30
1	D	180	ARG	NE-CZ-NH1	14.09	127.34	120.30
1	A	180	ARG	NE-CZ-NH2	-13.67	113.47	120.30
1	A	363	LYS	CD-CE-NZ	-13.55	80.54	111.70
1	D	365	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	B	170	GLU	OE1-CD-OE2	-12.68	108.09	123.30
1	C	235	ARG	CD-NE-CZ	11.89	140.25	123.60
1	A	166	GLU	CB-CA-C	-11.39	87.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	C	186	LEU	CB-CG-CD1	10.82	129.40	111.00
1	C	7	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	C	365	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	D	166	GLU	CB-CA-C	-10.38	89.63	110.40
1	C	235	ARG	CB-CG-CD	10.21	138.14	111.60
1	D	180	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	C	180	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	D	5	VAL	CG1-CB-CG2	-9.55	95.62	110.90
1	B	7	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	A	166	GLU	C-N-CA	-9.45	102.45	122.30
1	D	365	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	B	180	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	B	365	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	D	166	GLU	C-N-CA	-9.05	103.28	122.30
1	D	361	TYR	CB-CG-CD2	-9.04	115.58	121.00
1	A	236	ARG	NE-CZ-NH2	8.99	124.80	120.30
1	B	166	GLU	CB-CA-C	-8.98	92.43	110.40
1	D	186	LEU	CB-CG-CD1	8.95	126.21	111.00
1	B	292	ILE	CG1-CB-CG2	-8.69	92.28	111.40
1	A	179	LEU	CB-CG-CD2	8.45	125.37	111.00
1	D	236	ARG	NE-CZ-NH2	8.39	124.49	120.30
1	A	142	ASP	CB-CG-OD2	8.38	125.84	118.30
1	C	137	LEU	CB-CG-CD2	8.37	125.23	111.00
1	D	146	MET	CG-SD-CE	8.30	113.48	100.20
1	D	7	ARG	CB-CG-CD	-8.30	90.02	111.60
1	C	166	GLU	CB-CA-C	-8.17	94.06	110.40
1	A	236	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	146	MET	CG-SD-CE	8.13	113.21	100.20
1	B	71	ARG	CA-CB-CG	8.11	131.24	113.40
1	C	176	LEU	CB-CG-CD1	8.05	124.69	111.00
1	A	236	ARG	NH1-CZ-NH2	-7.89	110.72	119.40
1	B	332	ASP	CB-CG-OD2	7.77	125.30	118.30
1	C	133	LYS	O-C-N	-7.74	110.03	123.20
1	C	354	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	C	179	LEU	CB-CG-CD2	7.50	123.75	111.00
1	B	71	ARG	CB-CG-CD	7.50	131.09	111.60
1	A	161	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	C	174	TYR	CE1-CZ-OH	-7.23	100.58	120.10
1	C	267	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	267	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	137	LEU	CB-CG-CD2	7.12	123.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	249	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	265	VAL	CG1-CB-CG2	7.03	122.14	110.90
1	A	361	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	A	292	ILE	CB-CG1-CD1	-6.91	94.56	113.90
1	C	166	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	B	76	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	174	TYR	CG-CD1-CE1	-6.88	115.79	121.30
1	C	300	LEU	CB-CG-CD2	6.81	122.58	111.00
1	B	166	GLU	C-N-CA	-6.81	108.01	122.30
1	C	236	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	D	288	LEU	CB-CG-CD1	-6.71	99.59	111.00
1	D	201	MET	CG-SD-CE	-6.65	89.56	100.20
1	B	174	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	D	174	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	B	146	MET	CG-SD-CE	6.56	110.69	100.20
1	D	292	ILE	CB-CG1-CD1	-6.50	95.71	113.90
1	C	262	ARG	NH1-CZ-NH2	-6.46	112.30	119.40
1	A	365	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	76	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	71	ARG	CG-CD-NE	-6.39	98.38	111.80
1	C	174	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	A	166	GLU	N-CA-CB	-6.32	99.22	110.60
1	D	98	ARG	CB-CG-CD	-6.30	95.23	111.60
1	B	361	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	174	TYR	CE1-CZ-OH	-6.22	103.31	120.10
1	A	43	SER	N-CA-CB	-6.12	101.31	110.50
1	C	332	ASP	CB-CG-OD2	6.03	123.73	118.30
1	D	181	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	7	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	C	361	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	B	170	GLU	CG-CD-OE2	5.98	130.26	118.30
1	C	292	ILE	CB-CG1-CD1	-5.97	97.19	113.90
1	B	74	LEU	CB-CG-CD1	5.96	121.13	111.00
1	B	133	LYS	C-N-CA	-5.96	109.79	122.30
1	B	358	LEU	CB-CG-CD2	5.95	121.12	111.00
1	A	98	ARG	CB-CG-CD	-5.91	96.23	111.60
1	B	292	ILE	CB-CA-C	-5.90	99.81	111.60
1	A	332	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	55	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	74	LEU	CB-CG-CD1	5.86	120.96	111.00
1	D	74	LEU	CB-CG-CD1	5.86	120.96	111.00
1	C	76	ARG	NE-CZ-NH2	-5.84	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	363	LYS	CA-CB-CG	-5.84	100.55	113.40
1	C	166	GLU	C-N-CA	-5.81	110.10	122.30
1	D	361	TYR	CB-CG-CD1	5.81	124.48	121.00
1	B	98	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	186	LEU	CB-CG-CD1	5.79	120.83	111.00
1	C	232	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	267	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	7	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	C	174	TYR	OH-CZ-CE2	5.70	135.49	120.10
1	C	249	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	146	MET	CG-SD-CE	5.60	109.16	100.20
1	B	5	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	C	235	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
1	C	74	LEU	CB-CG-CD1	5.54	120.42	111.00
1	A	76	ARG	CG-CD-NE	-5.54	100.18	111.80
1	A	292	ILE	CA-CB-CG2	5.49	121.88	110.90
1	B	362	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	D	174	TYR	OH-CZ-CE2	-5.48	105.30	120.10
1	B	179	LEU	CB-CG-CD2	5.45	120.27	111.00
1	C	321	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	A	358	LEU	CB-CG-CD2	5.42	120.22	111.00
1	C	170	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	B	265	VAL	CA-CB-CG1	5.40	119.00	110.90
1	A	361	TYR	OH-CZ-CE2	-5.38	105.58	120.10
1	D	232	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	137	LEU	CB-CG-CD2	5.38	120.14	111.00
1	D	267	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	71	ARG	CB-CG-CD	5.33	125.45	111.60
1	D	7	ARG	CA-CB-CG	5.32	125.10	113.40
1	B	319	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	B	98	ARG	CB-CG-CD	-5.31	97.80	111.60
1	B	332	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	C	315	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	180	ARG	CB-CG-CD	-5.27	97.90	111.60
1	D	265	VAL	CA-CB-CG1	5.26	118.78	110.90
1	B	134	GLY	N-CA-C	5.25	126.22	113.10
1	B	76	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	98	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	7	ARG	CB-CA-C	-5.20	99.99	110.40
1	D	361	TYR	OH-CZ-CE2	-5.19	106.09	120.10
1	D	361	TYR	CG-CD1-CE1	-5.17	117.16	121.30
1	A	361	TYR	CG-CD1-CE1	-5.16	117.17	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	GLU	N-CA-C	5.16	124.93	111.00
1	D	76	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	174	TYR	OH-CZ-CE2	-5.11	106.31	120.10
1	D	7	ARG	CG-CD-NE	5.06	122.42	111.80
1	D	133	LYS	CD-CE-NZ	5.06	123.33	111.70
1	C	7	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	A	114	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	300	LEU	CB-CG-CD2	5.03	119.54	111.00
1	A	133	LYS	CD-CE-NZ	5.01	123.22	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	GLY	Peptide
1	B	166	GLU	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	2800	0	2886	29	0
1	B	2800	0	2886	33	0
1	C	2800	0	2886	63	0
1	D	2800	0	2886	41	1
2	A	31	0	22	3	0
2	B	31	0	22	2	0
2	C	31	0	22	1	0
2	D	31	0	22	0	0
3	A	163	0	0	7	0
3	B	174	0	0	4	0
3	C	207	0	0	14	1
3	D	180	0	0	7	0
All	All	12048	0	11632	169	1

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 7.

All (169) 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:C:134:GLY:N	1:C:134:GLY:CA	1.69	1.56
1:A:361:TYR:HE1	3:A:614:HOH:O	1.05	1.32
1:C:133:LYS:O	1:C:134:GLY:HA3	1.30	1.25
1:C:90:ILE:CG1	3:C:593:HOH:O	1.71	1.24
1:C:133:LYS:O	1:C:134:GLY:CA	1.82	1.23
1:C:90:ILE:HB	3:C:593:HOH:O	1.26	1.17
1:C:133:LYS:C	1:C:134:GLY:CA	2.13	1.17
1:C:130:GLN:NE2	3:C:657:HOH:O	1.80	1.14
1:C:30:ASN:OD1	3:C:598:HOH:O	1.68	1.12
1:B:366:LYS:HD3	3:B:586:HOH:O	1.52	1.07
1:A:361:TYR:CE1	3:A:614:HOH:O	1.82	1.07
1:C:90:ILE:CD1	3:C:593:HOH:O	1.90	1.06
1:C:90:ILE:HD12	3:C:593:HOH:O	1.50	1.06
1:C:100:ALA:HB1	1:C:146:MET:HE3	1.37	1.06
1:C:130:GLN:HG2	3:C:579:HOH:O	1.54	1.06
1:C:130:GLN:OE1	3:C:579:HOH:O	1.84	0.94
1:D:100:ALA:HB1	1:D:146:MET:HE3	1.47	0.94
1:C:107:ARG:HA	1:C:146:MET:CE	1.99	0.93
1:B:107:ARG:NH1	3:B:576:HOH:O	2.01	0.90
1:B:338:LYS:HG2	1:B:366:LYS:HB3	1.55	0.88
1:A:184:LYS:HA	1:A:184:LYS:HE2	1.54	0.87
1:D:366:LYS:O	3:D:656:HOH:O	1.93	0.86
1:D:137:LEU:HD11	1:D:185:GLU:HG2	1.56	0.86
1:A:338:LYS:HG2	1:A:366:LYS:HB3	1.58	0.86
1:C:100:ALA:HB1	1:C:146:MET:CE	2.05	0.85
1:D:180:ARG:HD2	3:D:543:HOH:O	1.76	0.85
1:C:235:ARG:HD2	3:C:605:HOH:O	1.77	0.83
1:D:100:ALA:HB1	1:D:146:MET:CE	2.07	0.83
1:C:184:LYS:HE2	1:C:184:LYS:HA	1.61	0.82
1:C:107:ARG:HA	1:C:146:MET:HE2	1.61	0.82
1:D:265:VAL:HG23	1:D:268:SER:HB3	1.63	0.81
1:D:100:ALA:CB	1:D:146:MET:HE1	2.15	0.76
1:C:130:GLN:CG	3:C:579:HOH:O	2.21	0.76
1:D:100:ALA:CB	1:D:146:MET:CE	2.63	0.76
1:A:180:ARG:HD2	3:A:598:HOH:O	1.86	0.75
1:C:97:GLN:HE21	1:C:125:ASN:H	1.34	0.75
1:D:107:ARG:HA	1:D:146:MET:CE	2.16	0.74
1:C:90:ILE:CB	3:C:593:HOH:O	1.77	0.73
1:A:184:LYS:HE2	1:A:184:LYS:CA	2.19	0.72
1:D:338:LYS:HG2	1:D:366:LYS:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:VAL:CG2	1:D:268:SER:HB3	2.20	0.72
1:D:97:GLN:HE21	1:D:125:ASN:H	1.36	0.71
1:B:97:GLN:HE21	1:B:125:ASN:H	1.38	0.71
1:B:265:VAL:HG22	1:B:268:SER:HB3	1.72	0.71
1:A:97:GLN:HE21	1:A:125:ASN:H	1.39	0.70
1:C:308:GLU:HG2	3:C:530:HOH:O	1.89	0.70
1:A:137:LEU:HD11	1:A:185:GLU:HG2	1.73	0.70
1:B:184:LYS:HE2	1:B:184:LYS:HA	1.73	0.70
1:C:107:ARG:CA	1:C:146:MET:HE2	2.20	0.70
1:C:97:GLN:HE22	1:C:124:ALA:HB1	1.57	0.69
1:C:170:GLU:OE2	3:C:655:HOH:O	2.13	0.67
1:C:107:ARG:HG2	1:C:146:MET:CE	2.25	0.66
1:D:107:ARG:HG2	1:D:146:MET:HE3	1.79	0.64
1:C:231:ILE:HG22	1:C:235:ARG:HD3	1.78	0.64
1:B:107:ARG:CZ	3:B:576:HOH:O	2.39	0.64
1:B:79:LYS:O	1:B:83:GLU:HG2	1.98	0.63
1:C:262:ARG:HD2	1:C:289:GLY:O	1.97	0.63
1:C:141:GLN:HG2	3:C:548:HOH:O	1.98	0.63
1:C:107:ARG:HG2	1:C:146:MET:HE3	1.80	0.62
1:D:308:GLU:HG2	3:D:579:HOH:O	1.98	0.62
1:B:107:ARG:NE	3:B:576:HOH:O	2.31	0.62
1:D:137:LEU:CD1	1:D:185:GLU:HG2	2.29	0.62
1:C:132:VAL:HG12	1:C:175:ALA:HB2	1.82	0.62
1:B:137:LEU:CD2	1:B:185:GLU:HG2	2.30	0.62
1:D:107:ARG:HA	1:D:146:MET:HE2	1.82	0.61
1:B:68:THR:OG1	1:B:74:LEU:HG	2.00	0.61
1:C:107:ARG:CB	1:C:146:MET:HE2	2.31	0.60
1:A:97:GLN:HE22	1:A:124:ALA:HB1	1.67	0.60
1:C:100:ALA:CB	1:C:146:MET:CE	2.79	0.60
1:A:365:ARG:O	1:A:366:LYS:HB2	2.02	0.58
1:D:265:VAL:O	1:D:265:VAL:HG23	2.03	0.58
1:C:231:ILE:CG2	1:C:235:ARG:HD3	2.34	0.58
1:D:365:ARG:O	1:D:366:LYS:HB2	2.03	0.57
1:A:129:PRO:O	1:A:132:VAL:HG22	2.05	0.57
1:A:71:ARG:HB2	1:A:74:LEU:HD22	1.86	0.57
1:D:184:LYS:HB2	3:D:616:HOH:O	2.05	0.57
1:C:100:ALA:CB	1:C:146:MET:HE3	2.25	0.56
1:B:174:TYR:CD2	1:B:174:TYR:C	2.79	0.56
1:D:68:THR:OG1	1:D:74:LEU:HG	2.06	0.55
1:C:97:GLN:NE2	1:C:125:ASN:H	2.05	0.55
1:A:308:GLU:HG2	3:A:516:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:H	1:A:220:GLN:HE21	1.55	0.55
1:C:107:ARG:HA	1:C:146:MET:HE1	1.89	0.54
1:A:68:THR:OG1	1:A:74:LEU:HG	2.09	0.53
1:C:68:THR:OG1	1:C:74:LEU:HG	2.08	0.53
1:C:338:LYS:HG2	1:C:366:LYS:HB3	1.90	0.52
1:B:97:GLN:NE2	1:B:125:ASN:H	2.08	0.51
1:A:97:GLN:NE2	1:A:125:ASN:H	2.05	0.51
1:D:107:ARG:HA	1:D:146:MET:HE3	1.92	0.51
1:B:137:LEU:HD21	1:B:185:GLU:HG2	1.92	0.51
1:D:26:SER:H	1:D:220:GLN:HE21	1.58	0.51
1:D:97:GLN:HE22	1:D:124:ALA:HB1	1.76	0.51
1:D:265:VAL:HG23	1:D:268:SER:CB	2.39	0.50
1:B:137:LEU:HD22	1:B:185:GLU:HG2	1.92	0.50
1:D:265:VAL:O	1:D:265:VAL:CG2	2.60	0.50
1:B:26:SER:H	1:B:220:GLN:HE21	1.58	0.49
1:B:287:ALA:O	1:B:365:ARG:HD2	2.12	0.49
1:D:184:LYS:HA	1:D:184:LYS:HE2	1.95	0.49
1:A:107:ARG:HG2	1:A:146:MET:HE2	1.94	0.48
1:B:184:LYS:HE2	1:B:184:LYS:CA	2.40	0.48
1:C:174:TYR:C	1:C:174:TYR:CD2	2.87	0.48
1:D:71:ARG:HG3	1:D:74:LEU:HD22	1.96	0.48
1:C:26:SER:H	1:C:220:GLN:HE21	1.62	0.47
2:A:401:FNR:H9	2:A:401:FNR:H6	1.96	0.47
1:C:62:VAL:HA	1:C:293:ALA:O	2.15	0.47
2:C:401:FNR:H9	2:C:401:FNR:H6	1.96	0.47
1:D:184:LYS:HG3	3:D:616:HOH:O	2.14	0.47
1:B:134:GLY:HA2	1:B:178:LYS:NZ	2.30	0.47
1:D:287:ALA:O	1:D:365:ARG:HD2	2.15	0.47
1:D:193:LYS:HB3	1:D:216:ASP:HB3	1.96	0.47
1:C:295:MET:HE1	1:C:313:PHE:HE1	1.79	0.47
1:D:110:PHE:CD1	1:D:146:MET:HE1	2.51	0.46
1:C:184:LYS:CA	1:C:184:LYS:HE2	2.40	0.46
1:C:107:ARG:CG	1:C:146:MET:CE	2.92	0.45
1:D:97:GLN:NE2	1:D:125:ASN:H	2.09	0.45
1:B:121:PRO:HA	1:B:150:ASP:OD2	2.16	0.45
1:C:266:PRO:HB3	1:C:364:VAL:HG13	1.99	0.45
1:B:295:MET:HE2	1:B:295:MET:HB2	1.75	0.45
1:B:193:LYS:HB3	1:B:216:ASP:HB3	1.97	0.45
2:B:401:FNR:H6	2:B:401:FNR:H9	1.98	0.45
1:D:308:GLU:CD	1:D:308:GLU:H	2.20	0.45
1:A:121:PRO:HA	1:A:150:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:O	1:C:83:GLU:HG3	2.17	0.45
1:C:179:LEU:HD22	1:C:190:ILE:HD13	2.00	0.44
1:B:365:ARG:O	1:B:366:LYS:HB2	2.16	0.44
1:A:292:ILE:HD13	1:A:292:ILE:HG21	1.79	0.44
1:A:180:ARG:CD	3:A:598:HOH:O	2.58	0.44
1:B:134:GLY:HA2	1:B:178:LYS:HZ2	1.82	0.44
1:B:193:LYS:NZ	2:B:401:FNR:HN1	2.16	0.44
1:B:62:VAL:HA	1:B:293:ALA:O	2.18	0.43
1:C:25:SER:HB2	1:C:220:GLN:HE21	1.82	0.43
1:A:365:ARG:HG3	1:A:366:LYS:N	2.33	0.43
1:D:180:ARG:CD	3:D:543:HOH:O	2.50	0.43
1:C:107:ARG:HG2	1:C:146:MET:HE2	1.99	0.43
1:D:91:PRO:HB3	1:D:121:PRO:HB2	2.01	0.43
1:A:266:PRO:HB3	1:A:364:VAL:HG13	2.00	0.43
1:D:26:SER:H	1:D:220:GLN:NE2	2.17	0.42
1:B:113:VAL:CG1	1:B:122:ILE:HD12	2.48	0.42
1:B:86:GLU:OE2	1:B:119:THR:HG23	2.19	0.42
1:A:263:TYR:HE1	1:A:360:ILE:HG13	1.83	0.42
1:B:105:GLU:CD	1:B:105:GLU:H	2.22	0.42
1:A:193:LYS:NZ	2:A:401:FNR:HN1	2.17	0.42
1:A:287:ALA:O	1:A:365:ARG:HD2	2.19	0.42
1:C:365:ARG:O	1:C:366:LYS:HB2	2.19	0.42
1:D:184:LYS:CB	3:D:616:HOH:O	2.66	0.42
1:C:292:ILE:HD13	1:C:292:ILE:HG21	1.54	0.42
1:B:279:GLY:HA3	1:B:320:GLU:HB2	2.01	0.42
1:C:107:ARG:CG	1:C:146:MET:HE2	2.50	0.41
1:C:97:GLN:HE22	1:C:124:ALA:CB	2.30	0.41
1:B:174:TYR:HE2	1:B:178:LYS:HD2	1.85	0.41
1:A:193:LYS:HZ1	2:A:401:FNR:HN1	1.68	0.41
1:B:358:LEU:O	1:B:359:SER:C	2.58	0.41
1:C:287:ALA:O	1:C:365:ARG:HD2	2.20	0.41
1:C:179:LEU:HD13	1:C:212:ILE:HD11	2.03	0.41
1:A:86:GLU:OE2	1:A:119:THR:HG23	2.21	0.41
1:C:333:VAL:HG12	1:C:337:LYS:HE3	2.03	0.41
1:C:126:LEU:O	1:C:154:VAL:HA	2.20	0.41
1:C:97:GLN:NE2	1:C:124:ALA:HB1	2.30	0.41
1:B:26:SER:H	1:B:220:GLN:NE2	2.19	0.41
1:D:292:ILE:HD13	1:D:292:ILE:HG21	1.78	0.41
1:D:62:VAL:HA	1:D:293:ALA:O	2.21	0.40
1:C:71:ARG:HG3	1:C:74:LEU:HD22	2.03	0.40
1:C:295:MET:HE1	1:C:313:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PRO:HB3	1:D:364:VAL:HG13	2.03	0.40
1:C:100:ALA:CB	1:C:146:MET:HE1	2.51	0.40
1:A:137:LEU:HD13	3:A:567:HOH:O	2.21	0.40
1:C:128:MET:N	1:C:129:PRO:CD	2.84	0.40
1:A:7:ARG:NH2	3:A:639:HOH:O	2.54	0.40
1:D:168:GLU:HA	1:D:169:PRO:HD2	1.85	0.40

All (1) 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)
1:D:55:ARG:NH2	3:C:643:HOH:O[6_565]	2.04	0.16

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	361/368 (98%)	349 (97%)	12 (3%)	0	100	100
1	B	361/368 (98%)	350 (97%)	11 (3%)	0	100	100
1	C	361/368 (98%)	352 (98%)	9 (2%)	0	100	100
1	D	361/368 (98%)	354 (98%)	7 (2%)	0	100	100
All	All	1444/1472 (98%)	1405 (97%)	39 (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	297/302 (98%)	282 (95%)	15 (5%)	29 10
1	B	297/302 (98%)	280 (94%)	17 (6%)	25 8
1	C	297/302 (98%)	283 (95%)	14 (5%)	32 12
1	D	297/302 (98%)	286 (96%)	11 (4%)	41 18
All	All	1188/1208 (98%)	1131 (95%)	57 (5%)	31 12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	71	ARG
1	A	74	LEU
1	A	137	LEU
1	A	142	ASP
1	A	145	GLN
1	A	157	ASN
1	A	166	GLU
1	A	179	LEU
1	A	185	GLU
1	A	194	GLU
1	A	300	LEU
1	A	334	ASP
1	A	360	ILE
1	A	366	LYS
1	B	5	VAL
1	B	9	VAL
1	B	74	LEU
1	B	99	VAL
1	B	138	LYS
1	B	145	GLN
1	B	157	ASN
1	B	166	GLU
1	B	174	TYR
1	B	179	LEU
1	B	186	LEU
1	B	194	GLU
1	B	201	MET
1	B	300	LEU
1	B	334	ASP

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Mol	Chain	Res	Type
1	B	360	ILE
1	B	366	LYS
1	C	5	VAL
1	C	74	LEU
1	C	130	GLN
1	C	137	LEU
1	C	157	ASN
1	C	176	LEU
1	C	179	LEU
1	C	186	LEU
1	C	194	GLU
1	C	262	ARG
1	C	300	LEU
1	C	334	ASP
1	C	360	ILE
1	C	363	LYS
1	D	7	ARG
1	D	74	LEU
1	D	137	LEU
1	D	186	LEU
1	D	194	GLU
1	D	300	LEU
1	D	334	ASP
1	D	359	SER
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	145	GLN
1	A	157	ASN
1	A	197	ASN
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

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Mol	Chain	Res	Type
1	B	246	ASN
1	C	30	ASN
1	C	97	GLN
1	C	130	GLN
1	C	145	GLN
1	C	157	ASN
1	C	164	GLN
1	C	197	ASN
1	C	220	GLN
1	D	97	GLN
1	D	164	GLN
1	D	197	ASN
1	D	220	GLN
1	D	312	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	401	-	30,33,33	1.93	8 (26%)	33,50,50	2.49	6 (18%)
2	FNR	B	401	-	30,33,33	1.74	4 (13%)	33,50,50	3.47	9 (27%)
2	FNR	C	401	-	30,33,33	1.85	8 (26%)	33,50,50	2.41	9 (27%)
2	FNR	D	401	-	30,33,33	1.82	6 (20%)	33,50,50	2.62	8 (24%)

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	401	-	-	0/18/18/18	0/3/3/3
2	FNR	B	401	-	-	0/18/18/18	0/3/3/3
2	FNR	C	401	-	-	0/18/18/18	0/3/3/3
2	FNR	D	401	-	-	0/18/18/18	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FNR	C9A-C5A	-2.30	1.38	1.42
2	C	401	FNR	C9-C8	2.04	1.43	1.37
2	C	401	FNR	C4-C4A	2.16	1.45	1.41
2	D	401	FNR	C5'-C4'	2.22	1.55	1.51
2	A	401	FNR	C7M-C7	2.44	1.55	1.51
2	C	401	FNR	C4A-CAA	2.50	1.45	1.41
2	A	401	FNR	C4A-CAA	2.59	1.45	1.41
2	B	401	FNR	C4-C4A	2.63	1.46	1.41
2	A	401	FNR	C4-N3	2.78	1.38	1.33
2	D	401	FNR	C4-C4A	2.79	1.46	1.41
2	D	401	FNR	C9-C8	2.81	1.45	1.37
2	C	401	FNR	C4-N3	2.93	1.38	1.33
2	D	401	FNR	C4A-N5	2.95	1.38	1.33
2	B	401	FNR	C4A-CAA	2.97	1.46	1.41
2	A	401	FNR	C9-C8	3.13	1.46	1.37
2	A	401	FNR	C4-C4A	3.36	1.48	1.41
2	B	401	FNR	C9A-N10	3.41	1.43	1.38
2	D	401	FNR	C4A-CAA	3.56	1.47	1.41
2	C	401	FNR	C5'-C4'	3.56	1.57	1.51
2	A	401	FNR	C4A-N5	4.09	1.39	1.33
2	C	401	FNR	C9A-N10	4.09	1.44	1.38
2	A	401	FNR	C5'-C4'	4.18	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FNR	C4A-N5	4.29	1.40	1.33
2	A	401	FNR	C9A-N10	4.45	1.44	1.38
2	D	401	FNR	C9A-N10	4.77	1.45	1.38
2	B	401	FNR	C4A-N5	5.36	1.41	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FNR	C4-C4A-CAA	-8.98	114.19	119.94
2	B	401	FNR	C4-C4A-CAA	-7.89	114.89	119.94
2	D	401	FNR	C4-C4A-CAA	-7.11	115.39	119.94
2	B	401	FNR	C4A-C4-N3	-6.37	114.88	123.59
2	B	401	FNR	C4A-CAA-N10	-5.20	117.46	120.52
2	D	401	FNR	C4A-C4-N3	-5.12	116.59	123.59
2	C	401	FNR	C4-C4A-CAA	-4.87	116.83	119.94
2	A	401	FNR	C4A-CAA-N10	-2.98	118.77	120.52
2	A	401	FNR	C4A-C4-N3	-2.97	119.52	123.59
2	C	401	FNR	O3'-C3'-C4'	-2.63	102.13	108.75
2	C	401	FNR	C4A-C4-N3	-2.41	120.29	123.59
2	D	401	FNR	C4A-CAA-N10	-2.30	119.16	120.52
2	B	401	FNR	C4A-N5-C5A	-2.29	114.13	116.76
2	C	401	FNR	O2'-C2'-C3'	-2.15	103.60	109.02
2	D	401	FNR	C9-C8-C7	-2.07	116.09	120.04
2	B	401	FNR	C1'-C2'-C3'	2.02	115.59	109.82
2	C	401	FNR	C8M-C8-C7	2.10	125.34	120.73
2	B	401	FNR	C4-C4A-N5	2.26	121.46	118.72
2	C	401	FNR	C4-C4A-N5	2.75	122.06	118.72
2	D	401	FNR	C4-C4A-N5	2.95	122.30	118.72
2	D	401	FNR	C5A-C9A-N10	3.02	119.91	117.62
2	D	401	FNR	C1'-N10-C9A	3.56	122.86	118.86
2	A	401	FNR	C1'-N10-C9A	3.59	122.89	118.86
2	C	401	FNR	C4-N3-C2	3.85	118.57	115.25
2	A	401	FNR	C4-C4A-N5	4.18	123.79	118.72
2	B	401	FNR	C1'-N10-C9A	4.18	123.56	118.86
2	B	401	FNR	C5A-C9A-N10	5.30	121.65	117.62
2	C	401	FNR	C5A-C9A-N10	5.73	121.97	117.62
2	A	401	FNR	C4-N3-C2	7.13	121.41	115.25
2	C	401	FNR	C1'-N10-C9A	8.10	127.96	118.86
2	D	401	FNR	C4-N3-C2	9.24	123.24	115.25
2	B	401	FNR	C4-N3-C2	13.64	127.03	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	FNR	3	0
2	B	401	FNR	2	0
2	C	401	FNR	1	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	363/368 (98%)	-0.08	10 (2%) 56 61	14, 21, 38, 50	0
1	B	363/368 (98%)	-0.04	16 (4%) 38 42	14, 21, 38, 50	0
1	C	363/368 (98%)	-0.07	8 (2%) 65 70	14, 20, 37, 50	0
1	D	363/368 (98%)	-0.08	9 (2%) 61 65	14, 21, 38, 50	0
All	All	1452/1472 (98%)	-0.07	43 (2%) 54 58	14, 21, 38, 50	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	4.8
1	D	166	GLU	4.7
1	C	360	ILE	4.1
1	B	360	ILE	4.0
1	A	166	GLU	3.7
1	B	166	GLU	3.5
1	A	360	ILE	3.4
1	B	174	TYR	3.4
1	D	72	ASN	3.3
1	B	4	ILE	3.3
1	C	5	VAL	3.3
1	A	71	ARG	3.3
1	B	72	ASN	3.1
1	C	4	ILE	3.0
1	C	166	GLU	2.9
1	A	363	LYS	2.9
1	B	363	LYS	2.8
1	B	7	ARG	2.8
1	D	360	ILE	2.8
1	B	134	GLY	2.8
1	C	363	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	2.7
1	C	72	ASN	2.7
1	A	72	ASN	2.7
1	A	73	GLU	2.6
1	B	6	ASN	2.6
1	B	168	GLU	2.5
1	D	363	LYS	2.4
1	A	7	ARG	2.4
1	A	103	LYS	2.3
1	B	364	VAL	2.3
1	D	76	ARG	2.2
1	B	71	ARG	2.2
1	D	71	ARG	2.2
1	B	76	ARG	2.2
1	B	359	SER	2.1
1	A	154	VAL	2.1
1	D	6	ASN	2.1
1	C	76	ARG	2.1
1	D	105	GLU	2.0
1	B	357	ASN	2.0
1	C	358	LEU	2.0
1	D	184	LYS	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
2	FNR	B	401	31/31	0.98	0.10	-0.23	13,17,20,22	0
2	FNR	D	401	31/31	0.98	0.09	-0.40	15,16,20,23	0
2	FNR	A	401	31/31	0.98	0.09	-0.42	14,17,20,21	0
2	FNR	C	401	31/31	0.98	0.09	-0.44	13,15,19,20	0

6.5 Other polymers (i)

There are no such residues in this entry.