WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

PDB ID : 3B04
Title : Crystal structure of Sulfolobus shibatae isopentenyl diphosphate isomerase in complex with oIPP.
Authors : Unno, H.; Nagai, T.; Hemmi, H.
Deposited on : 2011-06-03
Resolution : 2.30 Å(reported)

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 2.30 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.
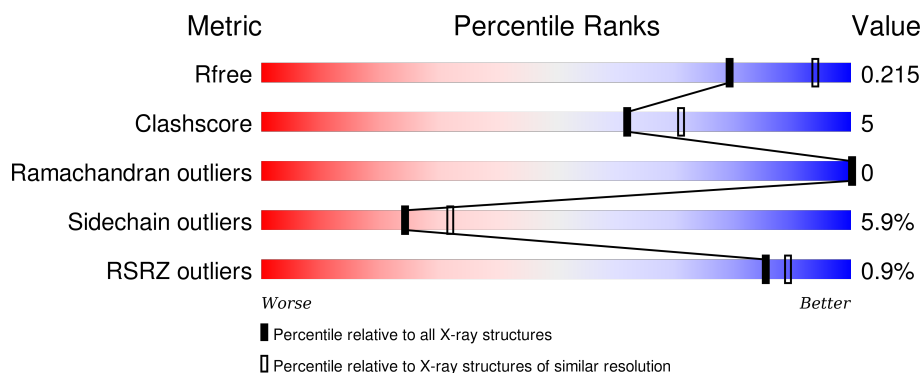
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	84% ... 12% .. .
1	B	368	86% ... 11% .. .
1	C	368	81% ... 15% .. .
1	D	368	85% ... 12% .. .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11828 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	362	Total 2796	C 1790	N 476	O 519	S 11	0	0	0
1	B	362	Total 2796	C 1790	N 476	O 519	S 11	0	0	0
1	C	362	Total 2796	C 1790	N 476	O 519	S 11	0	0	0
1	D	362	Total 2796	C 1790	N 476	O 519	S 11	0	0	0

- Molecule 2 is 1-DEOXY-1-[(4AR)-4A-[(2R)-1-HYDROXY-5-{[(S)-HYDROXY(PHOSPHO NOOXY)PHOSPHORYL]OXY}-3-METHYLIDENEPENTAN-2-YL]-7,8-DIMETHYL-2,4-DIOXO-3,4,4A,5-TETRAHYDROBENZO[G]PTERIDIN-10(2H)-YL]-5-O-PHOSPHONO-D-RIBITOL (three-letter code: OOP) (formula: $C_{23}H_{35}N_4O_{17}P_3$).
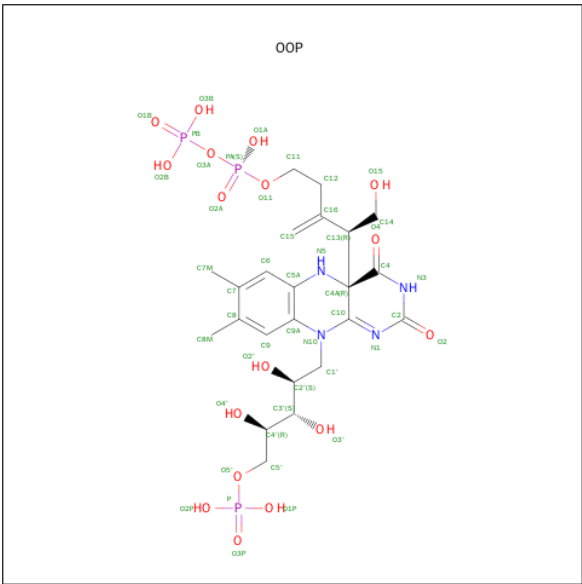
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 47	C 23	N 4	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			47	23	4	17	3		
2	C	1	Total	C	N	O	P	0	0
			47	23	4	17	3		
2	D	1	Total	C	N	O	P	0	0
			47	23	4	17	3		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	121	Total	O	0	0
			121	121		
4	C	112	Total	O	0	0
			112	112		
4	D	105	Total	O	0	0
			105	105		

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
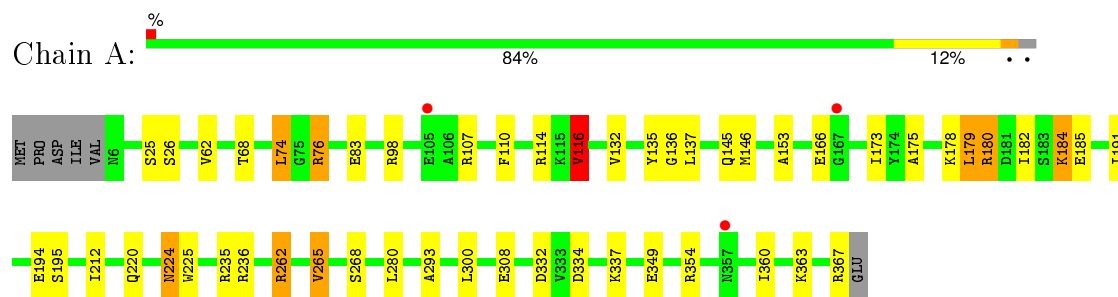
- Molecule 1: Isopentenyl-diphosphate delta-isomerase
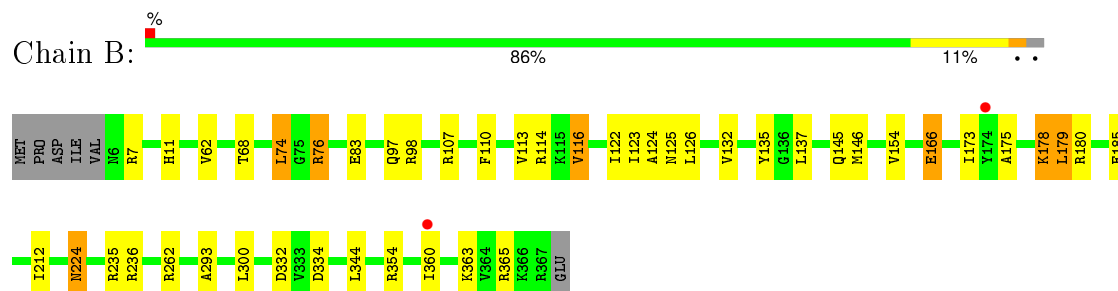
- Molecule 1: Isopentenyl-diphosphate delta-isomerase

- Molecule 1: Isopentenyl-diphosphate delta-isomerase
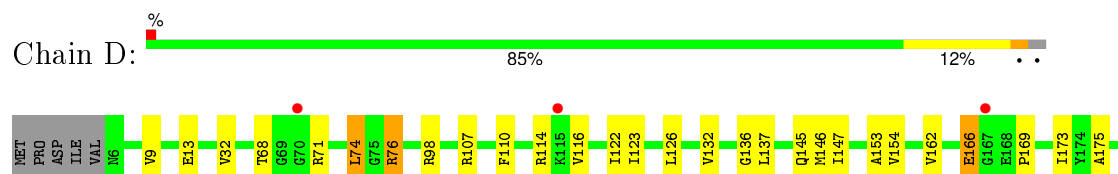
L179 R180 D181 I182 S183 K184 E185 I191 I212 R235 R236 R262 V265 P266 D267 S268 L280 K284 A287 L300 D334 I360 K363 V364 R365 K366 R367 GLU

4 Data and refinement statistics (i)

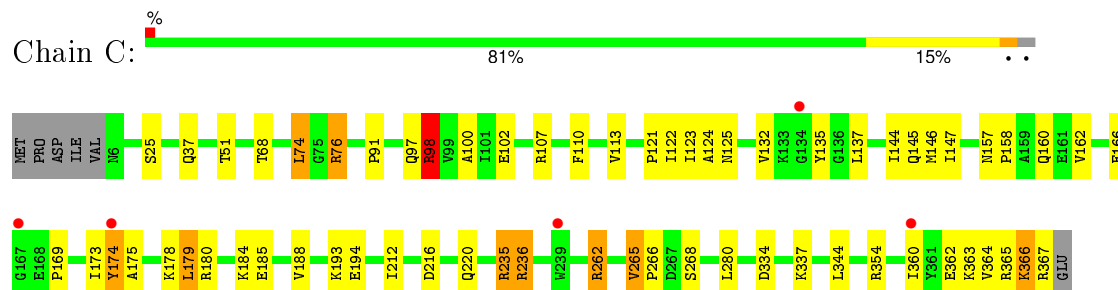| Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.23Å 101.23Å 337.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.30	Depositor
	48.48 – 2.30	EDS
% Data completeness	95.8 (48.48-2.30)	Depositor
(in resolution range)	95.8 (48.48-2.30)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.220	Depositor
	0.181 , 0.215	DCC
R_{free} test set	3793 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Outliers	1 of 75569 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11828	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OOP

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	1.06	2/2843 (0.1%)	1.08	18/3828 (0.5%)
1	B	1.06	0/2843	1.03	17/3828 (0.4%)
1	C	1.09	2/2843 (0.1%)	1.11	20/3828 (0.5%)
1	D	1.10	3/2843 (0.1%)	1.05	15/3828 (0.4%)
All	All	1.08	7/11372 (0.1%)	1.07	70/15312 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ARG	CZ-NH1	-9.65	1.20	1.33
1	D	262	ARG	CZ-NH2	-9.30	1.21	1.33
1	C	174	TYR	CD1-CE1	6.91	1.49	1.39
1	C	236	ARG	CZ-NH1	-5.82	1.25	1.33
1	D	262	ARG	CZ-NH1	-5.72	1.25	1.33
1	D	235	ARG	CZ-NH1	-5.72	1.25	1.33
1	A	308	GLU	CG-CD	5.62	1.60	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	ARG	NE-CZ-NH2	18.40	129.50	120.30
1	C	235	ARG	NE-CZ-NH1	17.68	129.14	120.30
1	B	235	ARG	NE-CZ-NH1	16.13	128.37	120.30
1	C	98	ARG	NE-CZ-NH2	15.71	128.16	120.30
1	A	76	ARG	NE-CZ-NH1	-15.58	112.51	120.30
1	A	236	ARG	NE-CZ-NH2	15.44	128.02	120.30
1	A	76	ARG	NE-CZ-NH2	15.06	127.83	120.30
1	C	98	ARG	NE-CZ-NH1	-13.90	113.35	120.30
1	C	262	ARG	NE-CZ-NH2	13.29	126.94	120.30
1	A	262	ARG	NE-CZ-NH2	13.27	126.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	235	ARG	NE-CZ-NH2	12.87	126.74	120.30
1	C	180	ARG	NE-CZ-NH2	12.07	126.33	120.30
1	C	236	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	C	180	ARG	NE-CZ-NH1	-11.20	114.70	120.30
1	D	236	ARG	NE-CZ-NH1	-10.31	115.15	120.30
1	B	235	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	D	235	ARG	NH1-CZ-NH2	-9.55	108.90	119.40
1	B	236	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	D	262	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	A	236	ARG	NH1-CZ-NH2	-8.60	109.94	119.40
1	A	180	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	236	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	B	180	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	D	262	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	235	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	C	236	ARG	CD-NE-CZ	8.12	134.97	123.60
1	D	235	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	D	262	ARG	NH1-CZ-NH2	-7.94	110.67	119.40
1	C	236	ARG	CG-CD-NE	-7.87	95.28	111.80
1	C	235	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	354	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	B	236	ARG	CD-NE-CZ	7.35	133.88	123.60
1	B	76	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	354	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	A	76	ARG	CD-NE-CZ	7.14	133.60	123.60
1	B	76	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	C	98	ARG	CD-NE-CZ	6.98	133.37	123.60
1	A	98	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	235	ARG	CD-NE-CZ	6.74	133.04	123.60
1	D	76	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	262	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	A	180	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	C	76	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	98	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	280	LEU	CD1-CG-CD2	-6.16	92.02	110.50
1	D	236	ARG	CD-NE-CZ	6.14	132.20	123.60
1	C	236	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	D	180	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	98	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	262	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	180	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	116	VAL	CG1-CB-CG2	5.78	120.14	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	354	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	C	365	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	262	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	236	ARG	CG-CD-NE	-5.65	99.93	111.80
1	C	280	LEU	CD1-CG-CD2	-5.64	93.57	110.50
1	D	280	LEU	CD1-CG-CD2	-5.62	93.63	110.50
1	D	98	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	C	235	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	235	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	365	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	365	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	D	98	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	98	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	344	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	332	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	76	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	180	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	354	ARG	NE-CZ-NH2	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2796	0	2879	26	0
1	B	2796	0	2879	24	0
1	C	2796	0	2879	36	0
1	D	2796	0	2879	26	0
2	A	47	0	30	7	0
2	B	47	0	30	4	0
2	C	47	0	30	4	0
2	D	47	0	30	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	114	0	0	2	0
4	B	121	0	0	1	0
4	C	112	0	0	4	0
4	D	105	0	0	3	0
All	All	11828	0	11636	124	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 5.

All (124) 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)
2:A:669:OOP:H14A	2:A:669:OOP:C11	1.60	1.23
2:A:669:OOP:C14	2:A:669:OOP:H11	1.69	1.23
2:B:669:OOP:H11A	2:B:669:OOP:H14A	1.38	1.04
1:D:107:ARG:HA	1:D:146:MET:HE3	1.49	0.92
1:D:184:LYS:HB2	4:D:457:HOH:O	1.69	0.91
1:C:107:ARG:HA	1:C:146:MET:HE3	1.55	0.88
1:A:107:ARG:HA	1:A:146:MET:HE3	1.56	0.86
1:B:107:ARG:HA	1:B:146:MET:HE3	1.59	0.83
1:C:132:VAL:HG13	1:C:175:ALA:HB2	1.64	0.79
1:A:265:VAL:HG22	1:A:268:SER:HB3	1.66	0.78
1:C:110:PHE:CD1	1:C:146:MET:HE1	2.20	0.77
1:C:265:VAL:HG22	1:C:268:SER:HB3	1.67	0.77
1:D:265:VAL:HG22	1:D:268:SER:HB3	1.68	0.76
2:B:669:OOP:C11	2:B:669:OOP:H14A	2.13	0.73
1:C:97:GLN:HE22	1:C:124:ALA:HB1	1.51	0.73
1:D:110:PHE:CD1	1:D:146:MET:HE1	2.24	0.72
1:B:97:GLN:HE21	1:B:125:ASN:H	1.39	0.71
1:A:110:PHE:CD1	1:A:146:MET:HE1	2.25	0.71
1:B:132:VAL:HG13	1:B:175:ALA:HB2	1.72	0.70
1:D:180:ARG:HD2	4:D:462:HOH:O	1.91	0.70
1:A:225:TRP:CZ2	2:A:669:OOP:H15A	2.29	0.68
1:C:362:GLU:O	1:C:366:LYS:HG2	1.93	0.67
1:A:225:TRP:CH2	2:A:669:OOP:C15	2.78	0.66
1:B:110:PHE:HB2	1:B:146:MET:HE2	1.77	0.66
1:C:235:ARG:HD2	4:C:426:HOH:O	1.96	0.66
1:B:97:GLN:HE22	1:B:124:ALA:HB1	1.60	0.65
1:B:110:PHE:CD1	1:B:146:MET:HE1	2.31	0.65
1:C:135:TYR:O	1:C:178:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:O	1:B:178:LYS:HE2	1.96	0.64
1:C:97:GLN:HE21	1:C:125:ASN:H	1.43	0.64
1:D:179:LEU:HD13	1:D:212:ILE:HD11	1.80	0.64
1:C:107:ARG:HA	1:C:146:MET:CE	2.27	0.63
1:A:225:TRP:CH2	2:A:669:OOP:H15A	2.33	0.62
1:C:25:SER:HB2	1:C:220:GLN:HE21	1.65	0.61
1:D:107:ARG:HA	1:D:146:MET:CE	2.29	0.60
1:D:184:LYS:CB	4:D:457:HOH:O	2.40	0.59
1:C:337:LYS:HD3	4:C:461:HOH:O	2.02	0.59
1:C:179:LEU:HD13	1:C:212:ILE:HD11	1.84	0.58
2:C:669:OOP:O11	2:C:669:OOP:H15	2.04	0.57
1:A:179:LEU:HD13	1:A:212:ILE:HD11	1.87	0.57
1:C:174:TYR:HB3	4:C:459:HOH:O	2.05	0.57
2:A:669:OOP:H14A	2:A:669:OOP:H11	0.72	0.57
1:A:107:ARG:HA	1:A:146:MET:CE	2.34	0.56
1:B:107:ARG:HA	1:B:146:MET:CE	2.35	0.55
1:D:110:PHE:HB2	1:D:146:MET:HE2	1.88	0.55
1:D:32:VAL:O	1:D:284:LYS:HE2	2.08	0.53
1:B:179:LEU:HD13	1:B:212:ILE:HD11	1.89	0.53
1:D:68:THR:OG1	1:D:74:LEU:HG	2.09	0.52
1:A:110:PHE:HB2	1:A:146:MET:HE2	1.91	0.52
1:B:135:TYR:O	1:B:178:LYS:CE	2.59	0.51
1:A:337:LYS:HD3	4:A:391:HOH:O	2.10	0.51
1:C:97:GLN:NE2	1:C:124:ALA:HB1	2.23	0.51
1:C:91:PRO:HB3	1:C:121:PRO:HB2	1.92	0.51
1:B:97:GLN:NE2	1:B:124:ALA:HB1	2.26	0.50
1:B:68:THR:OG1	1:B:74:LEU:HG	2.12	0.50
1:C:110:PHE:HD1	1:C:146:MET:HE1	1.76	0.50
1:A:26:SER:H	1:A:220:GLN:HE21	1.58	0.50
1:C:113:VAL:CG1	1:C:122:ILE:HD12	2.42	0.49
1:D:123:ILE:HD12	1:D:123:ILE:N	2.28	0.49
1:A:110:PHE:HB2	1:A:146:MET:CE	2.43	0.49
1:C:162:VAL:HG23	1:C:169:PRO:HG3	1.93	0.49
1:B:123:ILE:N	1:B:123:ILE:HD12	2.28	0.49
1:C:97:GLN:NE2	1:C:125:ASN:H	2.09	0.48
1:C:123:ILE:HD12	1:C:123:ILE:N	2.28	0.48
2:A:669:OOP:C2	2:A:669:OOP:H14	2.43	0.48
1:D:166:GLU:HG2	1:D:166:GLU:O	2.14	0.48
2:C:669:OOP:H2'	2:C:669:OOP:H9	1.95	0.48
2:B:669:OOP:H9	2:B:669:OOP:H2'	1.96	0.47
1:A:132:VAL:HG13	1:A:175:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:VAL:HG23	1:D:169:PRO:HG3	1.96	0.47
1:B:126:LEU:O	1:B:154:VAL:HA	2.14	0.47
1:A:180:ARG:HD2	4:A:425:HOH:O	2.15	0.47
1:B:62:VAL:HA	1:B:293:ALA:O	2.15	0.46
1:B:113:VAL:CG1	1:B:122:ILE:HD12	2.45	0.46
1:C:25:SER:HB2	1:C:220:GLN:NE2	2.29	0.46
2:D:669:OOP:H12A	2:D:669:OOP:C4	2.46	0.46
1:C:100:ALA:HB1	1:C:146:MET:HE3	1.97	0.46
1:C:110:PHE:HB2	1:C:146:MET:HE2	1.98	0.46
1:A:68:THR:OG1	1:A:74:LEU:HG	2.16	0.46
1:C:68:THR:OG1	1:C:74:LEU:HG	2.16	0.46
1:C:174:TYR:CB	4:C:459:HOH:O	2.62	0.46
2:C:669:OOP:O11	2:C:669:OOP:C15	2.61	0.45
1:D:122:ILE:CG2	1:D:147:ILE:HD12	2.46	0.45
1:A:62:VAL:HA	1:A:293:ALA:O	2.17	0.45
1:C:135:TYR:O	1:C:178:LYS:CE	2.64	0.45
1:D:132:VAL:HG13	1:D:175:ALA:HB2	1.99	0.44
1:A:114:ARG:HA	1:A:114:ARG:HD3	1.78	0.44
1:D:126:LEU:O	1:D:154:VAL:HA	2.18	0.44
1:A:224:ASN:HD22	1:A:224:ASN:C	2.21	0.44
1:C:37:GLN:HA	1:C:37:GLN:NE2	2.33	0.44
1:D:110:PHE:HB2	1:D:146:MET:CE	2.47	0.44
1:B:114:ARG:HD3	1:B:114:ARG:HA	1.78	0.43
1:D:122:ILE:HG22	1:D:147:ILE:HD12	2.00	0.43
1:D:114:ARG:HA	1:D:114:ARG:HD3	1.79	0.43
2:B:669:OOP:H12A	2:B:669:OOP:C4	2.48	0.43
1:D:9:VAL:O	1:D:13:GLU:HG3	2.18	0.43
1:A:349:GLU:HB2	1:B:344:LEU:HD22	2.01	0.43
1:A:136:GLY:HA2	1:A:182:ILE:HD11	2.01	0.43
1:A:25:SER:HB2	1:A:220:GLN:HE21	1.84	0.42
1:C:122:ILE:HG22	1:C:147:ILE:HD12	2.01	0.42
1:A:83:GLU:HB3	1:A:116:VAL:HG13	2.01	0.42
1:B:224:ASN:C	1:B:224:ASN:HD22	2.23	0.42
1:A:184:LYS:HD2	1:A:184:LYS:HA	1.93	0.42
1:B:7:ARG:HG2	1:B:11:HIS:CE1	2.54	0.42
1:C:160:GLN:OE1	2:C:669:OOP:O15	2.38	0.42
1:B:83:GLU:HB3	1:B:116:VAL:HG13	2.02	0.42
1:D:136:GLY:HA2	1:D:182:ILE:HD11	2.00	0.42
1:C:98:ARG:HD3	1:C:102:GLU:OE2	2.19	0.42
1:C:193:LYS:HB3	1:C:216:ASP:HB3	2.01	0.42
1:C:144:ILE:HD13	1:C:188:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:O	1:B:166:GLU:HG2	2.20	0.42
1:A:135:TYR:O	1:A:178:LYS:HE2	2.18	0.42
1:D:153:ALA:HA	1:D:191:ILE:O	2.20	0.42
1:D:287:ALA:O	1:D:365:ARG:HD2	2.20	0.42
1:B:332:ASP:HB2	4:B:372:HOH:O	2.20	0.42
1:A:153:ALA:HA	1:A:191:ILE:O	2.19	0.42
1:C:37:GLN:HE21	1:C:37:GLN:HA	1.84	0.41
1:D:71:ARG:CG	1:D:74:LEU:HD22	2.51	0.41
1:D:266:PRO:HB3	1:D:364:VAL:HG13	2.03	0.41
1:C:266:PRO:HB3	1:C:364:VAL:HG13	2.02	0.41
1:B:97:GLN:NE2	1:B:125:ASN:H	2.11	0.41
2:D:669:OOP:H14A	2:D:669:OOP:H11A	2.03	0.41
1:A:25:SER:HB2	1:A:220:GLN:NE2	2.36	0.40
1:C:157:ASN:N	1:C:158:PRO:CD	2.84	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	360/368 (98%)	343 (95%)	17 (5%)	0	100	100
1	B	360/368 (98%)	347 (96%)	13 (4%)	0	100	100
1	C	360/368 (98%)	348 (97%)	12 (3%)	0	100	100
1	D	360/368 (98%)	347 (96%)	13 (4%)	0	100	100
All	All	1440/1472 (98%)	1385 (96%)	55 (4%)	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	296/302 (98%)	276 (93%)	20 (7%)	20	25
1	B	296/302 (98%)	281 (95%)	15 (5%)	29	39
1	C	296/302 (98%)	276 (93%)	20 (7%)	20	25
1	D	296/302 (98%)	281 (95%)	15 (5%)	29	39
All	All	1184/1208 (98%)	1114 (94%)	70 (6%)	24	32

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	76	ARG
1	A	116	VAL
1	A	137	LEU
1	A	145	GLN
1	A	166	GLU
1	A	173	ILE
1	A	179	LEU
1	A	184	LYS
1	A	185	GLU
1	A	194	GLU
1	A	195	SER
1	A	224	ASN
1	A	262	ARG
1	A	265	VAL
1	A	300	LEU
1	A	334	ASP
1	A	360	ILE
1	A	363	LYS
1	A	367	ARG
1	B	74	LEU
1	B	76	ARG
1	B	116	VAL
1	B	137	LEU

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Mol	Chain	Res	Type
1	B	145	GLN
1	B	166	GLU
1	B	173	ILE
1	B	178	LYS
1	B	179	LEU
1	B	185	GLU
1	B	224	ASN
1	B	300	LEU
1	B	334	ASP
1	B	360	ILE
1	B	363	LYS
1	C	51	THR
1	C	74	LEU
1	C	76	ARG
1	C	98	ARG
1	C	137	LEU
1	C	145	GLN
1	C	166	GLU
1	C	173	ILE
1	C	179	LEU
1	C	184	LYS
1	C	185	GLU
1	C	194	GLU
1	C	236	ARG
1	C	262	ARG
1	C	265	VAL
1	C	334	ASP
1	C	360	ILE
1	C	363	LYS
1	C	366	LYS
1	C	367	ARG
1	D	74	LEU
1	D	76	ARG
1	D	116	VAL
1	D	137	LEU
1	D	145	GLN
1	D	166	GLU
1	D	173	ILE
1	D	179	LEU
1	D	184	LYS
1	D	185	GLU
1	D	265	VAL

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Mol	Chain	Res	Type
1	D	300	LEU
1	D	334	ASP
1	D	360	ILE
1	D	363	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	145	GLN
1	A	197	ASN
1	A	220	GLN
1	A	224	ASN
1	B	11	HIS
1	B	97	GLN
1	B	145	GLN
1	B	197	ASN
1	B	224	ASN
1	C	6	ASN
1	C	11	HIS
1	C	37	GLN
1	C	97	GLN
1	C	145	GLN
1	C	197	ASN
1	C	220	GLN
1	D	6	ASN
1	D	11	HIS
1	D	145	GLN
1	D	197	ASN

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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	OOP	A	669	3	44,49,49	1.17	6 (13%)	53,76,76	1.61	10 (18%)
2	OOP	B	669	3	44,49,49	1.28	4 (9%)	53,76,76	1.55	9 (16%)
2	OOP	C	669	3	44,49,49	1.06	3 (6%)	53,76,76	1.44	6 (11%)
2	OOP	D	669	3	44,49,49	0.96	3 (6%)	53,76,76	1.61	13 (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	OOP	A	669	3	-	0/39/76/76	0/3/3/3
2	OOP	B	669	3	-	0/39/76/76	0/3/3/3
2	OOP	C	669	3	-	0/39/76/76	0/3/3/3
2	OOP	D	669	3	-	0/39/76/76	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	669	OOP	C4A-C4	-4.31	1.50	1.54
2	B	669	OOP	C5A-N5	-4.16	1.32	1.39
2	A	669	OOP	C4A-C4	-2.95	1.51	1.54
2	A	669	OOP	C5A-N5	-2.95	1.34	1.39
2	A	669	OOP	C4A-N5	-2.82	1.44	1.46
2	B	669	OOP	C4A-N5	-2.64	1.44	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	669	OOP	C4A-N5	-2.38	1.44	1.46
2	D	669	OOP	C5A-N5	-2.36	1.35	1.39
2	A	669	OOP	C8M-C8	2.02	1.55	1.51
2	D	669	OOP	C5'-C4'	2.03	1.54	1.51
2	A	669	OOP	C1'-C2'	2.05	1.55	1.52
2	B	669	OOP	C5'-C4'	2.30	1.55	1.51
2	D	669	OOP	C10-N10	2.37	1.42	1.37
2	C	669	OOP	C5'-C4'	2.55	1.55	1.51
2	C	669	OOP	C10-N10	2.67	1.42	1.37
2	A	669	OOP	C5'-C4'	2.67	1.55	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	669	OOP	C13-C16-C15	-4.28	116.86	124.12
2	C	669	OOP	O3A-PA-O11	-4.12	92.00	102.94
2	B	669	OOP	O4-C4-C4A	-3.57	118.78	124.29
2	A	669	OOP	O4-C4-C4A	-3.56	118.80	124.29
2	C	669	OOP	C13-C16-C15	-3.51	118.17	124.12
2	D	669	OOP	O4-C4-C4A	-3.42	119.01	124.29
2	B	669	OOP	C6-C5A-N5	-3.40	115.63	120.68
2	A	669	OOP	PA-O3A-PB	-3.23	121.83	132.67
2	D	669	OOP	O15-C14-C13	-3.22	100.01	112.02
2	D	669	OOP	PA-O3A-PB	-3.10	122.27	132.67
2	D	669	OOP	C7M-C7-C6	-2.70	114.46	119.49
2	B	669	OOP	O15-C14-C13	-2.70	101.97	112.02
2	C	669	OOP	O2-C2-N1	-2.48	117.29	121.79
2	A	669	OOP	O2-C2-N1	-2.48	117.30	121.79
2	D	669	OOP	C13-C16-C15	-2.43	120.00	124.12
2	B	669	OOP	PA-O3A-PB	-2.43	124.53	132.67
2	A	669	OOP	C9A-N10-C10	-2.35	116.56	120.57
2	D	669	OOP	O4'-C4'-C5'	-2.28	105.22	110.19
2	C	669	OOP	C6-C5A-N5	-2.12	117.54	120.68
2	D	669	OOP	O3A-PA-O11	-2.12	97.32	102.94
2	D	669	OOP	O2B-PB-O3A	-2.12	95.49	105.09
2	A	669	OOP	O1P-P-O5'	-2.07	100.59	106.56
2	A	669	OOP	C7M-C7-C6	-2.05	115.68	119.49
2	B	669	OOP	O2-C2-N1	-2.02	118.13	121.79
2	D	669	OOP	O2'-C2'-C1'	2.08	115.38	110.45
2	C	669	OOP	C9A-C5A-N5	2.09	122.15	119.59
2	D	669	OOP	O1A-PA-O2A	2.17	124.26	112.53
2	B	669	OOP	O3B-PB-O2B	2.43	116.64	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	669	OOP	O3B-PB-O2B	2.56	117.14	107.38
2	A	669	OOP	O3B-PB-O2B	2.58	117.19	107.38
2	B	669	OOP	C10-C4A-N5	2.67	109.35	106.41
2	B	669	OOP	C1'-N10-C9A	3.13	125.94	120.47
2	A	669	OOP	C4A-C4-N3	3.24	119.06	110.69
2	C	669	OOP	C4A-C4-N3	3.53	119.80	110.69
2	B	669	OOP	C4A-C4-N3	4.00	121.01	110.69
2	D	669	OOP	C10-C4A-N5	4.34	111.20	106.41
2	A	669	OOP	C10-C4A-N5	4.66	111.55	106.41
2	D	669	OOP	C4A-C4-N3	4.98	123.54	110.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	669	OOP	7	0
2	B	669	OOP	4	0
2	C	669	OOP	4	0
2	D	669	OOP	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	362/368 (98%)	-0.38	3 (0%)	87	90	21, 31, 51, 62	0
1	B	362/368 (98%)	-0.39	2 (0%)	90	93	21, 31, 50, 62	0
1	C	362/368 (98%)	-0.36	5 (1%)	78	83	22, 31, 51, 64	0
1	D	362/368 (98%)	-0.40	3 (0%)	87	90	22, 31, 51, 62	0
All	All	1448/1472 (98%)	-0.38	13 (0%)	85	89	21, 31, 51, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	3.0
1	B	360	ILE	2.9
1	D	70	GLY	2.7
1	C	134	GLY	2.7
1	C	174	TYR	2.4
1	D	167	GLY	2.4
1	D	115	LYS	2.3
1	A	105	GLU	2.3
1	C	360	ILE	2.3
1	C	167	GLY	2.2
1	C	239	TRP	2.1
1	A	357	ASN	2.0
1	B	174	TYR	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, 95th 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	OOP	A	669	47/47	0.96	0.10	-0.02	22,30,71,71	0
2	OOP	B	669	47/47	0.96	0.10	-0.06	19,29,65,68	0
2	OOP	D	669	47/47	0.96	0.10	-0.18	23,30,69,72	0
3	MG	D	1002	1/1	0.91	0.09	-0.21	63,63,63,63	0
2	OOP	C	669	47/47	0.97	0.10	-0.26	23,32,66,67	0
3	MG	B	1002	1/1	0.92	0.15	-	76,76,76,76	0
3	MG	A	1002	1/1	0.86	0.13	-	74,74,74,74	0
3	MG	C	1002	1/1	0.76	0.15	-	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.