Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:27 AM GMT

PDB ID	:	3OZE
Title	:	Crystal Structure of human 5'-deoxy-5'-methyladenosine phosphorylase
Authors	:	Ho, M.; Guan, R.; Almo, S.C.; Schramm, V.L.
Deposited on	:	2010-09-24
Resolution	:	2.00 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:

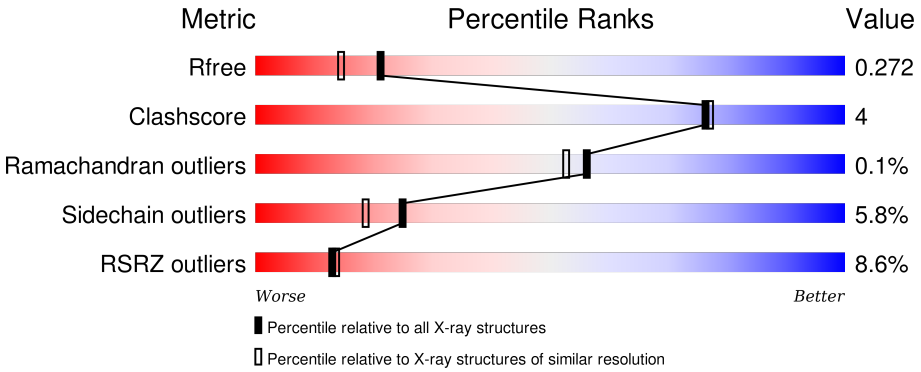
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	283	4% 83% 9% • 7%
1	B	283	10% 84% 9% • 5%
1	C	283	8% 80% 12% • 8%
1	D	283	7% 81% 11% • 7%
1	E	283	7% 81% 12% 7%

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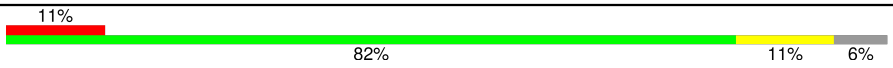
Mol	Chain	Length	Quality of chain
1	F	283	

2 Entry composition

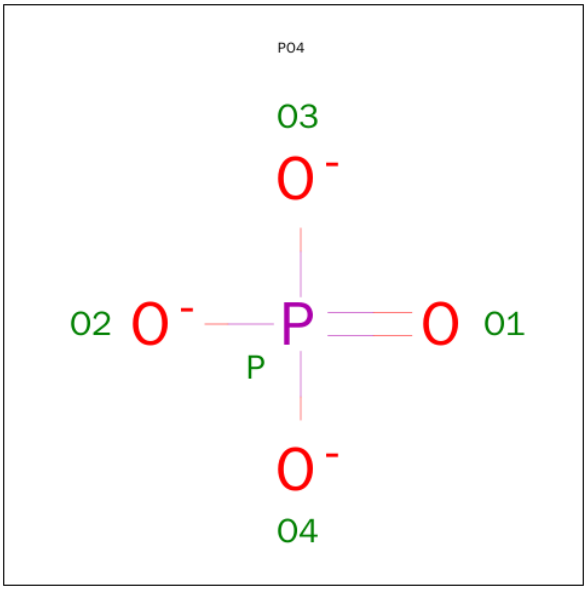
There are 3 unique types of molecules in this entry. The entry contains 12542 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-methyl-5'-thioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2031	1286	350	378	17			
1	B	268	Total	C	N	O	S	0	0	0
			2072	1309	358	388	17			
1	C	261	Total	C	N	O	S	0	0	0
			2016	1275	348	376	17			
1	D	263	Total	C	N	O	S	0	0	0
			2031	1286	350	378	17			
1	E	264	Total	C	N	O	S	0	0	0
			2043	1292	353	381	17			
1	F	265	Total	C	N	O	S	0	0	0
			2050	1296	355	382	17			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

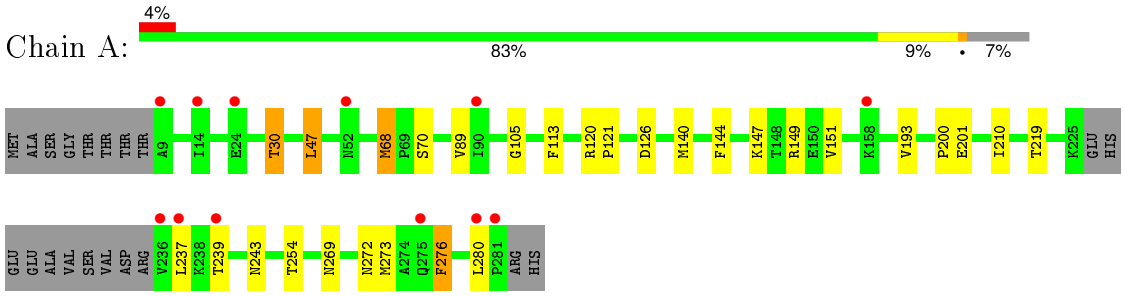
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 71 71	0	0
3	B	35	Total O 35 35	0	0
3	C	38	Total O 38 38	0	0
3	D	45	Total O 45 45	0	0
3	E	41	Total O 41 41	0	0
3	F	39	Total O 39 39	0	0

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.

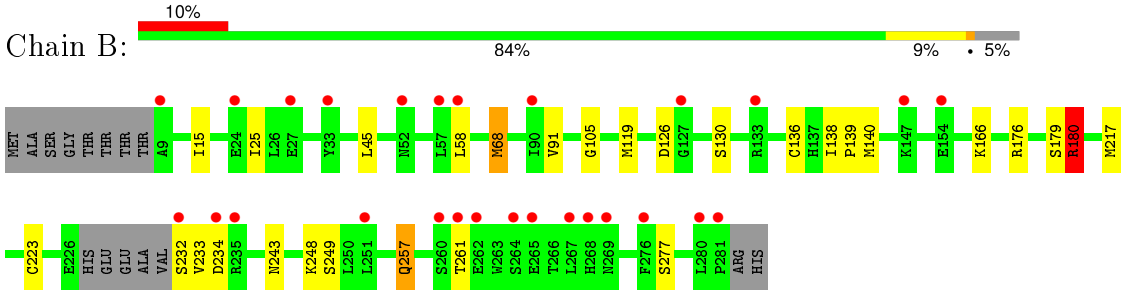
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain A:



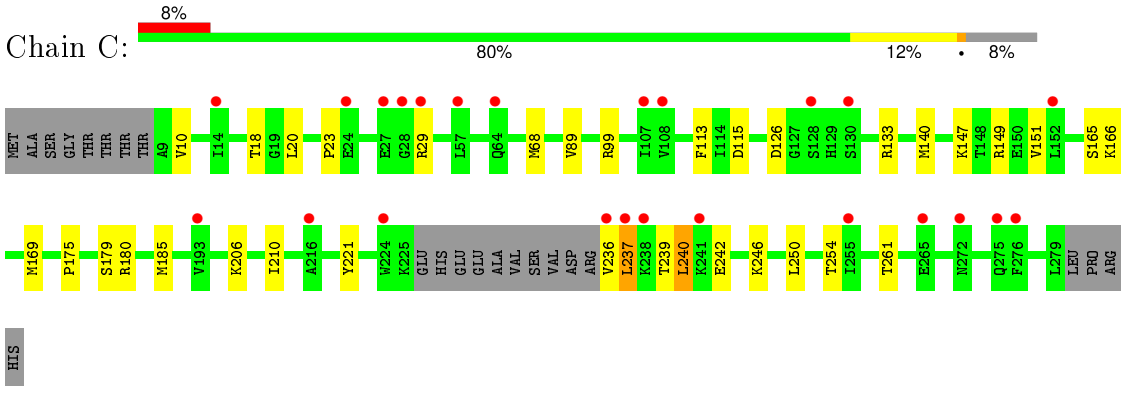
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain B:



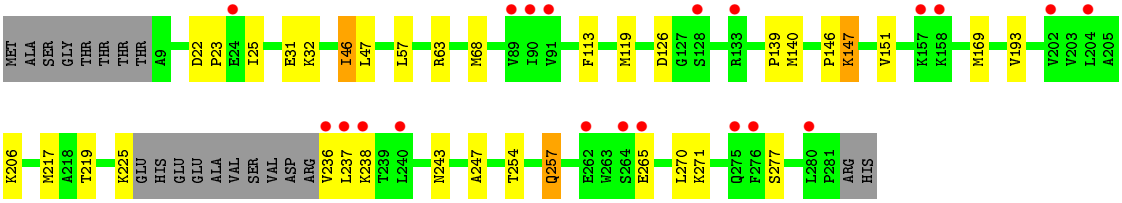
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain C:



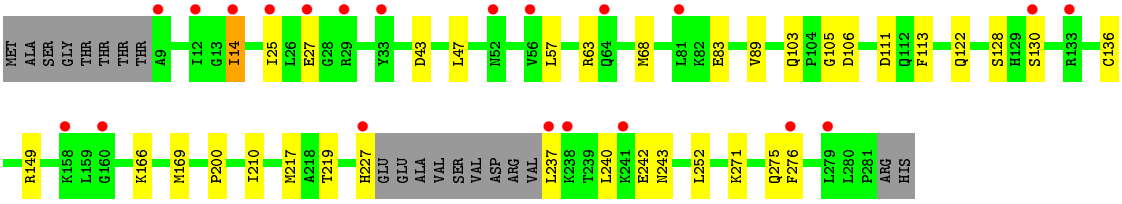
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain D:



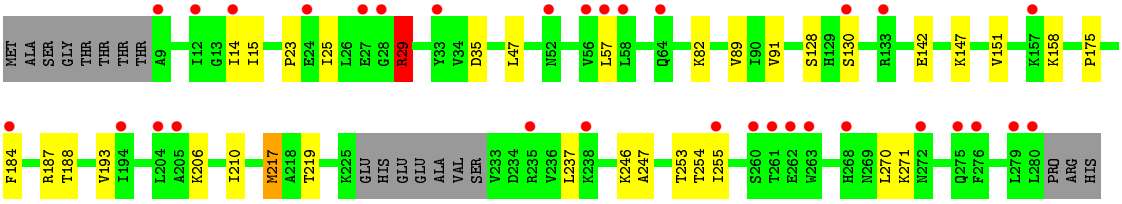
• Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain E:



• Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.52Å 81.81Å 130.28Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.00) 99.2 (19.89-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.262 0.226 , 0.272	Depositor DCC
R_{free} test set	5598 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.0	EDS
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.010 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 111658 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12542	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: PO4

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	0.82	0/2070	0.78	0/2802
1	B	0.71	1/2111 (0.0%)	0.74	3/2857 (0.1%)
1	C	0.67	0/2054	0.70	1/2779 (0.0%)
1	D	0.73	0/2070	0.74	0/2802
1	E	0.66	0/2083	0.71	0/2819
1	F	0.63	0/2088	0.69	0/2825
All	All	0.71	1/12476 (0.0%)	0.73	4/16884 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	SER	CB-OG	5.75	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	176	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	B	180	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	C	115	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	180	ARG	NE-CZ-NH2	5.47	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2031	0	2063	14	0
1	B	2072	0	2100	14	1
1	C	2016	0	2045	21	0
1	D	2031	0	2063	22	0
1	E	2043	0	2067	17	0
1	F	2050	0	2082	18	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	71	0	0	0	0
3	B	35	0	0	0	0
3	C	38	0	0	0	0
3	D	45	0	0	1	0
3	E	41	0	0	0	1
3	F	39	0	0	1	0
All	All	12542	0	12420	94	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 4.

All (94) 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:217:MET:HE3	1:D:247:ALA:HB2	1.30	1.14
1:E:14:ILE:HD11	1:E:57:LEU:HD13	1.42	1.00
1:D:217:MET:CE	1:D:247:ALA:HB2	2.05	0.86
1:A:30:THR:HG22	1:A:47:LEU:HB2	1.59	0.85
1:D:126:ASP:HA	1:E:68:MET:HE1	1.62	0.81
1:F:29:ARG:HB2	1:F:29:ARG:HH11	1.45	0.81
1:F:29:ARG:CB	1:F:29:ARG:HH11	1.95	0.79
1:C:236:VAL:HG13	1:C:237:LEU:H	1.49	0.77
1:A:89:VAL:HG23	1:A:210:ILE:HG21	1.70	0.74
1:A:126:ASP:HA	1:B:68:MET:HE1	1.67	0.74
1:A:105:GLY:HA2	1:A:243:ASN:HD21	1.53	0.72
1:E:14:ILE:CD1	1:E:57:LEU:HD13	2.18	0.70
1:D:225:LYS:O	1:D:225:LYS:HG3	1.90	0.70
1:F:29:ARG:CG	1:F:29:ARG:HH11	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ASP:HA	1:C:68:MET:HE1	1.74	0.68
1:C:89:VAL:HG23	1:C:210:ILE:HG21	1.76	0.68
1:F:14:ILE:HD11	1:F:255:ILE:CD1	2.25	0.66
1:E:105:GLY:HA2	1:E:243:ASN:HD21	1.60	0.66
1:E:14:ILE:HD11	1:E:57:LEU:CD1	2.24	0.65
1:B:126:ASP:HA	1:C:68:MET:CE	2.26	0.65
1:D:126:ASP:HA	1:E:68:MET:CE	2.26	0.64
1:F:29:ARG:NH1	1:F:29:ARG:HB2	2.12	0.64
1:F:29:ARG:NH1	1:F:29:ARG:CB	2.62	0.62
1:F:151:VAL:HG12	1:F:254:THR:HG23	1.81	0.62
1:E:89:VAL:HG23	1:E:210:ILE:HG21	1.84	0.60
1:D:217:MET:CE	1:D:247:ALA:CB	2.79	0.60
1:D:217:MET:HE3	1:D:247:ALA:CB	2.21	0.59
1:D:217:MET:CE	1:D:243:ASN:O	2.51	0.59
1:B:15:ILE:HB	1:B:91:VAL:HG12	1.84	0.58
1:D:257:GLN:HA	1:D:257:GLN:NE2	2.18	0.57
1:D:217:MET:HE2	1:D:243:ASN:O	2.04	0.57
1:D:151:VAL:HG12	1:D:254:THR:HG23	1.86	0.57
1:A:68:MET:CE	1:C:126:ASP:HA	2.34	0.56
1:C:236:VAL:HG13	1:C:237:LEU:N	2.19	0.56
1:B:180:ARG:HD2	1:B:223:CYS:O	2.05	0.56
1:C:242:GLU:O	1:C:246:LYS:HG3	2.08	0.54
1:E:25:ILE:HG12	1:E:252:LEU:HD21	1.90	0.53
1:A:68:MET:HE1	1:C:126:ASP:HA	1.91	0.53
1:B:25:ILE:HD11	1:B:248:LYS:HB3	1.91	0.52
1:E:111:ASP:HB3	1:E:149:ARG:NH2	2.24	0.52
1:D:225:LYS:O	1:D:225:LYS:CG	2.58	0.52
1:F:217:MET:HE1	1:F:247:ALA:HB2	1.91	0.52
1:F:89:VAL:HG23	1:F:210:ILE:HG21	1.91	0.52
1:A:144:PHE:HB2	1:A:149:ARG:HD2	1.92	0.50
1:D:139:PRO:HD3	1:D:277:SER:OG	2.11	0.50
1:E:14:ILE:CD1	1:E:57:LEU:CD1	2.88	0.50
1:E:271:LYS:O	1:E:275:GLN:HB2	2.11	0.50
1:C:140:MET:HE1	1:C:206:LYS:HG3	1.93	0.50
1:C:140:MET:CE	1:C:206:LYS:HG3	2.42	0.50
1:F:29:ARG:HG3	1:F:29:ARG:HH11	1.75	0.49
1:B:45:LEU:HD23	1:B:58:LEU:HD13	1.93	0.49
1:A:140:MET:O	1:B:179:SER:HA	2.12	0.48
1:E:136:CYS:O	1:F:175:PRO:HB2	2.13	0.48
1:F:142:GLU:O	1:F:206:LYS:NZ	2.48	0.47
1:D:46:ILE:HB	1:D:57:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:THR:HG22	1:C:240:LEU:HD11	1.96	0.46
1:B:136:CYS:O	1:C:175:PRO:HB2	2.14	0.46
1:D:113:PHE:HA	1:D:169:MET:O	2.15	0.46
1:F:23:PRO:HD2	1:F:57:LEU:HD21	1.97	0.46
1:C:23:PRO:O	1:C:29:ARG:NH1	2.47	0.46
1:D:31:GLU:HG2	1:D:46:ILE:HD13	1.98	0.46
1:F:15:ILE:HB	1:F:91:VAL:HG12	1.97	0.46
1:E:113:PHE:HA	1:E:169:MET:O	2.16	0.46
1:A:200:PRO:O	1:A:201:GLU:C	2.54	0.45
1:C:250:LEU:O	1:C:254:THR:OG1	2.28	0.45
1:A:113:PHE:CD1	1:A:113:PHE:C	2.89	0.45
1:E:43:ASP:OD1	1:E:63:ARG:NH2	2.49	0.45
1:F:14:ILE:HD11	1:F:255:ILE:HD11	1.98	0.45
1:A:120:ARG:HA	1:A:121:PRO:HD2	1.86	0.44
1:C:236:VAL:CG1	1:C:237:LEU:H	2.24	0.44
1:B:138:ILE:HA	1:B:139:PRO:HD3	1.88	0.44
1:D:146:PRO:HG2	1:D:147:LYS:HE2	1.99	0.44
1:B:257:GLN:HE21	1:B:257:GLN:HA	1.82	0.44
1:A:151:VAL:HG12	1:A:254:THR:HG23	2.00	0.44
1:B:139:PRO:HD3	1:B:277:SER:OG	2.18	0.43
1:C:149:ARG:NH2	1:C:165:SER:O	2.51	0.43
1:A:272:ASN:O	1:A:276:PHE:HB2	2.17	0.43
1:E:111:ASP:HB3	1:E:149:ARG:CZ	2.49	0.43
1:F:184:PHE:O	1:F:188:THR:HG23	2.19	0.43
1:C:151:VAL:HG12	1:C:254:THR:HG23	2.01	0.42
1:D:22:ASP:HB2	1:D:63:ARG:HG2	2.01	0.42
1:D:219:THR:HG22	1:D:243:ASN:HD22	1.84	0.42
1:D:140:MET:CE	1:D:206:LYS:HG3	2.50	0.42
1:A:68:MET:HE2	1:C:126:ASP:HA	2.00	0.42
1:D:206:LYS:HG2	3:D:299:HOH:O	2.20	0.42
1:B:140:MET:O	1:C:179:SER:HA	2.20	0.42
1:E:122:GLN:HG2	1:E:200:PRO:HB3	2.02	0.41
1:E:103:GLN:O	1:E:106:ASP:HB2	2.21	0.41
1:F:184:PHE:O	1:F:187:ARG:HB2	2.21	0.40
1:B:105:GLY:HA2	1:B:243:ASN:OD1	2.21	0.40
1:C:99:ARG:O	1:C:221:TYR:HE1	2.04	0.40
1:D:23:PRO:HD2	1:D:57:LEU:HD21	2.04	0.40
1:C:113:PHE:HA	1:C:169:MET:O	2.20	0.40
1:F:246:LYS:NZ	3:F:319:HOH:O	2.51	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:B:234:ASP:OD2	3:E:323:HOH:O[2_546]	2.10	0.10

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	259/283 (92%)	254 (98%)	5 (2%)	0	100	100
1	B	264/283 (93%)	253 (96%)	11 (4%)	0	100	100
1	C	257/283 (91%)	248 (96%)	9 (4%)	0	100	100
1	D	259/283 (92%)	255 (98%)	4 (2%)	0	100	100
1	E	260/283 (92%)	254 (98%)	6 (2%)	0	100	100
1	F	261/283 (92%)	253 (97%)	7 (3%)	1 (0%)	39	33
All	All	1560/1698 (92%)	1517 (97%)	42 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	29	ARG

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	225/242 (93%)	212 (94%)	13 (6%)	25	19
1	B	230/242 (95%)	220 (96%)	10 (4%)	35	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	223/242 (92%)	212 (95%)	11 (5%)	31	25
1	D	225/242 (93%)	210 (93%)	15 (7%)	20	14
1	E	226/242 (93%)	212 (94%)	14 (6%)	23	16
1	F	227/242 (94%)	211 (93%)	16 (7%)	19	12
All	All	1356/1452 (93%)	1277 (94%)	79 (6%)	25	19

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	47	LEU
1	A	68	MET
1	A	70	SER
1	A	147	LYS
1	A	193	VAL
1	A	219	THR
1	A	237	LEU
1	A	239	THR
1	A	269	ASN
1	A	273	MET
1	A	276	PHE
1	A	280	LEU
1	B	68	MET
1	B	119	MET
1	B	130	SER
1	B	166	LYS
1	B	180	ARG
1	B	217	MET
1	B	233	VAL
1	B	249	SER
1	B	257	GLN
1	B	261	THR
1	C	10	VAL
1	C	20	LEU
1	C	133	ARG
1	C	147	LYS
1	C	166	LYS
1	C	180	ARG
1	C	185	MET
1	C	237	LEU
1	C	239	THR

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Mol	Chain	Res	Type
1	C	240	LEU
1	C	261	THR
1	D	25	ILE
1	D	32	LYS
1	D	46	ILE
1	D	47	LEU
1	D	68	MET
1	D	119	MET
1	D	147	LYS
1	D	193	VAL
1	D	236	VAL
1	D	237	LEU
1	D	238	LYS
1	D	257	GLN
1	D	265	GLU
1	D	270	LEU
1	D	271	LYS
1	E	14	ILE
1	E	27	GLU
1	E	47	LEU
1	E	83	GLU
1	E	128	SER
1	E	130	SER
1	E	166	LYS
1	E	217	MET
1	E	219	THR
1	E	227	HIS
1	E	237	LEU
1	E	240	LEU
1	E	242	GLU
1	E	276	PHE
1	F	25	ILE
1	F	29	ARG
1	F	35	ASP
1	F	47	LEU
1	F	82	LYS
1	F	128	SER
1	F	130	SER
1	F	147	LYS
1	F	158	LYS
1	F	193	VAL
1	F	217	MET

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Mol	Chain	Res	Type
1	F	219	THR
1	F	237	LEU
1	F	253	THR
1	F	270	LEU
1	F	271	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	A	269	ASN
1	B	257	GLN
1	B	269	ASN
1	B	272	ASN
1	C	269	ASN
1	D	257	GLN
1	D	269	ASN
1	D	272	ASN
1	E	243	ASN
1	E	245	ASN
1	E	269	ASN
1	E	272	ASN
1	F	245	ASN
1	F	269	ASN
1	F	272	ASN

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 (i)

6 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	PO4	A	284	-	4,4,4	0.30	0	6,6,6	0.29	0
2	PO4	B	284	-	4,4,4	0.44	0	6,6,6	0.27	0
2	PO4	C	284	-	4,4,4	0.50	0	6,6,6	0.31	0
2	PO4	D	284	-	4,4,4	0.68	0	6,6,6	0.30	0
2	PO4	E	284	-	4,4,4	0.43	0	6,6,6	0.30	0
2	PO4	F	284	-	4,4,4	0.55	0	6,6,6	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	284	-	-	0/0/0/0	0/0/0/0
2	PO4	B	284	-	-	0/0/0/0	0/0/0/0
2	PO4	C	284	-	-	0/0/0/0	0/0/0/0
2	PO4	D	284	-	-	0/0/0/0	0/0/0/0
2	PO4	E	284	-	-	0/0/0/0	0/0/0/0
2	PO4	F	284	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	263/283 (92%)	0.21	12 (4%) 36 38	30, 42, 59, 68	0
1	B	268/283 (94%)	0.58	27 (10%) 9 10	27, 51, 78, 86	0
1	C	261/283 (92%)	0.57	24 (9%) 11 12	35, 52, 71, 78	0
1	D	263/283 (92%)	0.41	20 (7%) 17 18	31, 46, 65, 75	0
1	E	264/283 (93%)	0.49	21 (7%) 15 16	34, 53, 67, 79	0
1	F	265/283 (93%)	0.71	32 (12%) 6 6	35, 54, 76, 83	0
All	All	1584/1698 (93%)	0.50	136 (8%) 13 14	27, 50, 71, 86	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	280	LEU	6.9
1	B	280	LEU	6.8
1	E	276	PHE	6.2
1	B	281	PRO	5.7
1	F	276	PHE	5.6
1	D	276	PHE	5.5
1	F	261	THR	5.2
1	A	9	ALA	5.2
1	E	9	ALA	4.9
1	C	276	PHE	4.4
1	C	238	LYS	4.4
1	B	9	ALA	4.3
1	B	276	PHE	4.3
1	D	237	LEU	4.2
1	F	9	ALA	4.2
1	D	280	LEU	4.1
1	F	52	ASN	4.0
1	B	264	SER	4.0
1	B	235	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	3.9
1	E	227	HIS	3.8
1	C	27	GLU	3.8
1	F	262	GLU	3.8
1	C	130	SER	3.5
1	C	237	LEU	3.4
1	F	64	GLN	3.4
1	D	158	LYS	3.4
1	F	235	ARG	3.4
1	F	263	TRP	3.4
1	A	280	LEU	3.3
1	E	52	ASN	3.3
1	B	234	ASP	3.3
1	F	268	HIS	3.2
1	F	184	PHE	3.2
1	B	267	LEU	3.2
1	C	29	ARG	3.2
1	D	24	GLU	3.1
1	D	236	VAL	3.1
1	F	28	GLY	3.1
1	B	262	GLU	3.1
1	B	52	ASN	3.1
1	B	265	GLU	3.1
1	D	240	LEU	3.0
1	D	275	GLN	3.0
1	E	33	TYR	3.0
1	F	24	GLU	3.0
1	F	275	GLN	3.0
1	E	237	LEU	2.9
1	A	239	THR	2.9
1	B	27	GLU	2.9
1	E	238	LYS	2.8
1	F	14	ILE	2.8
1	B	58	LEU	2.8
1	D	157	LYS	2.8
1	C	275	GLN	2.8
1	D	262	GLU	2.8
1	A	24	GLU	2.8
1	B	90	ILE	2.8
1	B	232	SER	2.7
1	F	57	LEU	2.7
1	C	193	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	2.7
1	E	25	ILE	2.6
1	A	52	ASN	2.6
1	D	133	ARG	2.6
1	F	279	LEU	2.6
1	E	130	SER	2.6
1	F	27	GLU	2.6
1	F	130	SER	2.6
1	C	14	ILE	2.6
1	F	33	TYR	2.6
1	A	236	VAL	2.6
1	C	255	ILE	2.6
1	B	133	ARG	2.6
1	C	57	LEU	2.5
1	C	28	GLY	2.5
1	E	133	ARG	2.5
1	D	238	LYS	2.5
1	B	260	SER	2.5
1	C	108	VAL	2.5
1	C	107	ILE	2.5
1	D	202	VAL	2.5
1	B	33	TYR	2.5
1	D	204	LEU	2.5
1	F	194	ILE	2.5
1	C	64	GLN	2.4
1	E	241	LYS	2.4
1	D	264	SER	2.4
1	D	90	ILE	2.4
1	F	157	LYS	2.4
1	E	64	GLN	2.4
1	E	279	LEU	2.4
1	B	154	GLU	2.4
1	F	58	LEU	2.4
1	E	14	ILE	2.3
1	B	147	LYS	2.3
1	F	238	LYS	2.3
1	A	158	LYS	2.3
1	C	241	LYS	2.3
1	F	260	SER	2.3
1	F	204	LEU	2.3
1	D	89	VAL	2.2
1	D	265	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	12	ILE	2.2
1	B	24	GLU	2.2
1	F	133	ARG	2.2
1	F	205	ALA	2.2
1	B	261	THR	2.2
1	C	152	LEU	2.1
1	E	56	VAL	2.1
1	E	160	GLY	2.1
1	C	224	TRP	2.1
1	C	24	GLU	2.1
1	A	275	GLN	2.1
1	A	14	ILE	2.1
1	F	12	ILE	2.1
1	F	255	ILE	2.1
1	A	281	PRO	2.1
1	B	269	ASN	2.1
1	E	27	GLU	2.1
1	E	29	ARG	2.1
1	C	236	VAL	2.1
1	E	158	LYS	2.1
1	A	90	ILE	2.1
1	B	251	LEU	2.1
1	E	81	LEU	2.1
1	C	272	ASN	2.1
1	C	128	SER	2.1
1	B	57	LEU	2.0
1	F	272	ASN	2.0
1	C	265	GLU	2.0
1	D	91	VAL	2.0
1	B	268	HIS	2.0
1	D	128	SER	2.0
1	C	216	ALA	2.0
1	F	56	VAL	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

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	PO4	E	284	5/5	0.96	0.12	0.49	38,39,41,42	0
2	PO4	D	284	5/5	0.98	0.10	0.14	37,40,42,46	0
2	PO4	B	284	5/5	0.98	0.07	-1.11	38,41,41,43	0
2	PO4	C	284	5/5	0.98	0.08	-1.43	42,46,48,49	0
2	PO4	A	284	5/5	0.98	0.07	-1.59	32,32,35,37	0
2	PO4	F	284	5/5	0.98	0.09	-3.11	39,41,42,43	0

6.5 Other polymers

There are no such residues in this entry.