Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2021 – 04:06 PM EST

PDB ID	:	2AKZ
Title	:	Fluoride Inhibition of Enolase: Crystal Structure of the Inhibitory Complex
Authors	:	Qin, J.; Chai, G.; Brewer, J.M.; Lovelace, L.L.
Deposited on	:	2005-08-04
Resolution	:	1.36 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
https://www.wwpdb.org/validation/2017/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:

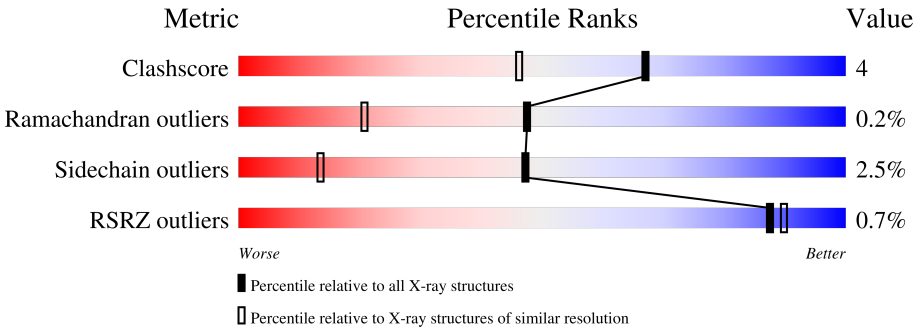
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

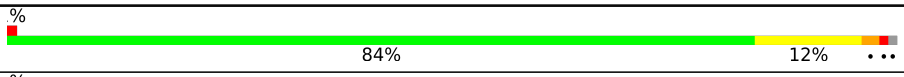
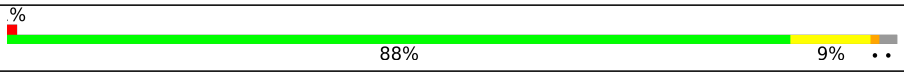
The reported resolution of this entry is 1.36 Å.

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))
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	439	
1	B	439	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7546 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 Gamma enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	6	0
			3295	2086	570	626	13			
1	B	432	Total	C	N	O	S	0	9	0
			3258	2062	564	619	13			

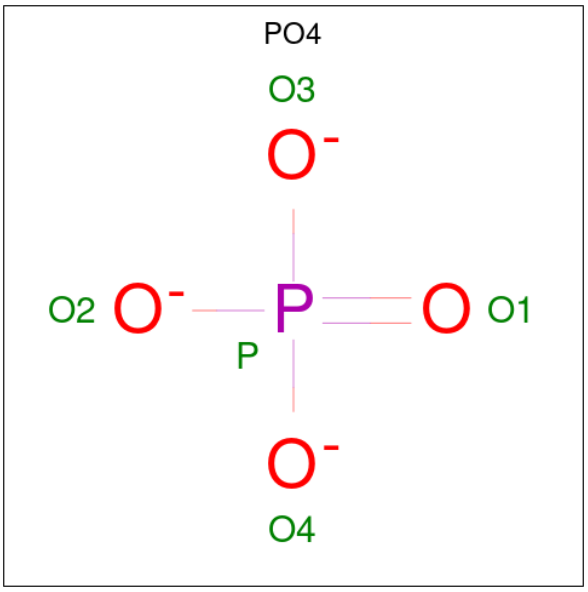
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	HIS	-	expression tag	UNP P09104
A	435	HIS	-	expression tag	UNP P09104
A	436	HIS	-	expression tag	UNP P09104
A	437	HIS	-	expression tag	UNP P09104
A	438	HIS	-	expression tag	UNP P09104
A	439	HIS	-	expression tag	UNP P09104
B	1434	HIS	-	expression tag	UNP P09104
B	1435	HIS	-	expression tag	UNP P09104
B	1436	HIS	-	expression tag	UNP P09104
B	1437	HIS	-	expression tag	UNP P09104
B	1438	HIS	-	expression tag	UNP P09104
B	1439	HIS	-	expression tag	UNP P09104

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

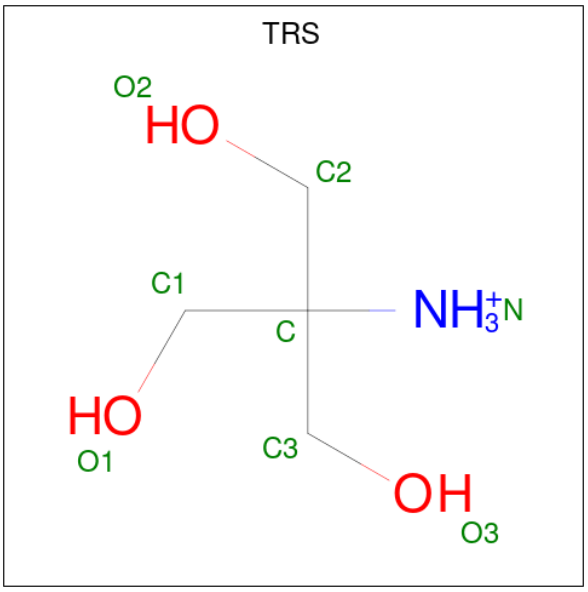


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total F 2 2	0	0
4	B	2	Total F 2 2	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is water.

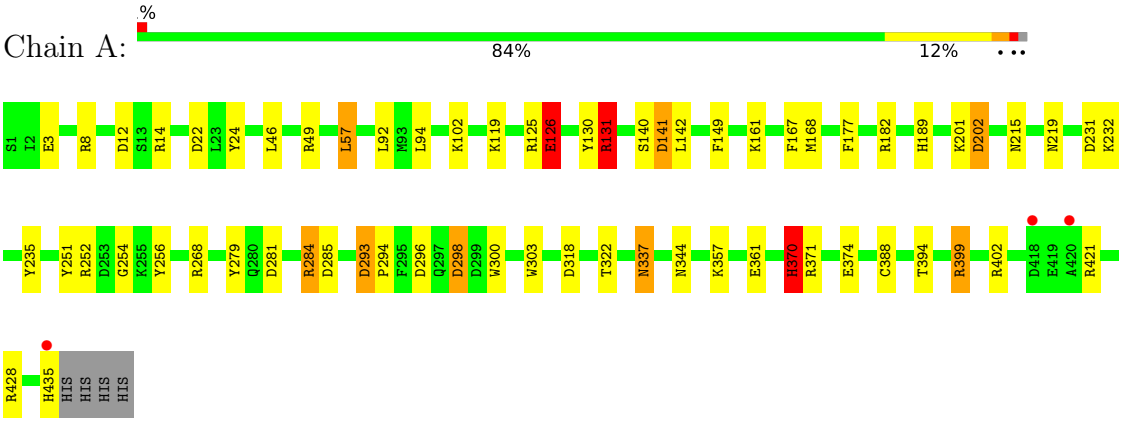
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	496	Total O 496 496	0	0
6	B	471	Total O 471 471	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

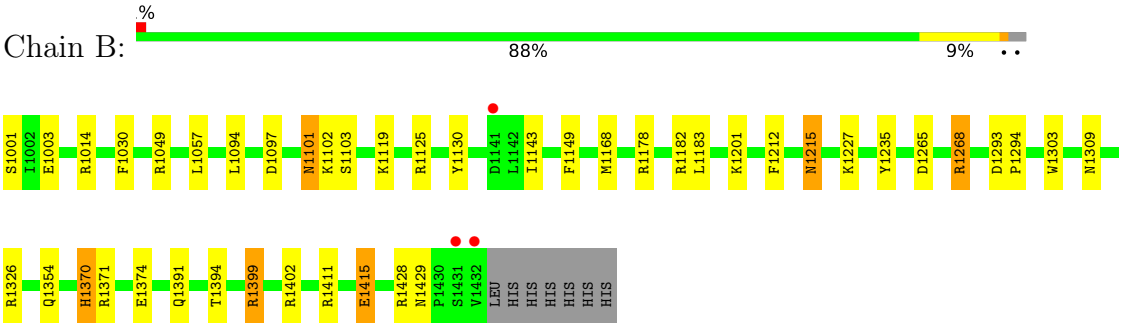
• Molecule 1: Gamma enolase

Chain A:



• Molecule 1: Gamma enolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.01Å 118.52Å 67.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.36 9.97 – 1.36	Depositor EDS
% Data completeness (in resolution range)	88.9 (10.00-1.36) 88.9 (9.97-1.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 1.36Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.110 , 0.144 0.120 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 86.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7546	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, MG, F, 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	1.38	3/3386 (0.1%)	1.49	41/4584 (0.9%)
1	B	0.69	1/3366 (0.0%)	1.32	18/4559 (0.4%)
All	All	1.09	4/6752 (0.1%)	1.41	59/9143 (0.6%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLU	CD-OE2	70.04	2.02	1.25
1	A	3	GLU	CD-OE2	8.29	1.34	1.25
1	B	1003	GLU	CD-OE2	6.22	1.32	1.25
1	A	402	ARG	CZ-NH1	-5.39	1.26	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	GLU	OE1-CD-OE2	-32.56	84.23	123.30
1	A	131[A]	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	A	131[B]	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	B	1402	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	B	1399	ARG	NE-CZ-NH1	12.79	126.69	120.30
1	B	1428	ARG	CD-NE-CZ	11.27	139.38	123.60
1	B	1428	ARG	NE-CZ-NH1	-11.11	114.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	8	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	B	1411	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	B	1411	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	399	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	126	GLU	CG-CD-OE2	-9.38	99.55	118.30
1	A	202	ASP	CB-CG-OD1	9.06	126.45	118.30
1	A	131[A]	ARG	CD-NE-CZ	8.96	136.15	123.60
1	A	131[B]	ARG	CD-NE-CZ	8.96	136.15	123.60
1	B	1125[A]	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	B	1125[B]	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	231	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	125	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	A	252	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	177	PHE	CB-CG-CD1	-7.75	115.38	120.80
1	A	131[A]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	131[B]	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	1030	PHE	CB-CG-CD1	-7.59	115.48	120.80
1	B	1268	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	252	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	300	TRP	CE3-CZ3-CH2	6.94	128.84	121.20
1	A	12	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	268	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	B	1014	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	293	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	421	ARG	CA-CB-CG	6.62	127.95	113.40
1	A	141	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	421	ARG	N-CA-CB	6.51	122.33	110.60
1	A	14	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	125	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	A	141	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	B	1212	PHE	CB-CG-CD2	-5.99	116.61	120.80
1	B	1399	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	402	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	22	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	428	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	1326	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	92	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	1049	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	1402	ARG	CD-NE-CZ	5.46	131.25	123.60
1	B	1268	ARG	NH1-CZ-NH2	-5.45	113.41	119.40
1	A	279	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	A	24	TYR	CD1-CE1-CZ	-5.38	114.96	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	370	HIS	CG-ND1-CE1	5.36	115.71	108.20
1	A	298	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	318	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	167	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	A	167	PHE	CE1-CZ-CE2	5.28	129.49	120.00
1	A	219	ASN	CB-CG-OD1	5.24	132.08	121.60
1	A	49	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	296	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	A	256	TYR	CB-CG-CD1	5.01	124.01	121.00
1	B	1178	ARG	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	GLU	Sidechain

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	3295	0	3239	31	0
1	B	3258	0	3185	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	12	0	0
6	A	496	0	0	8	0
6	B	471	0	0	8	0
All	All	7546	0	6436	51	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 4.

All (51) 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:A:126:GLU:OE2	1:A:126:GLU:CD	2.02	0.97
1:B:1130:TYR:OH	1:B:1415:GLU:OE1	1.82	0.97
1:B:1265:ASP:O	1:B:1268:ARG:HG2	1.85	0.76
1:A:201:LYS:HE2	6:A:680:HOH:O	1.98	0.63
1:B:1143:ILE:HG13	1:B:1143:ILE:O	2.02	0.59
1:A:142:LEU:O	1:A:435:HIS:HE1	1.86	0.58
1:B:1094:LEU:HD13	6:B:696:HOH:O	2.03	0.57
1:A:189:HIS:HD2	6:A:624:HOH:O	1.86	0.56
1:A:337:ASN:HD22	1:A:337:ASN:C	2.10	0.55
1:A:130:TYR:CE1	1:A:131[B]:ARG:HG3	2.44	0.53
1:A:126:GLU:OE2	1:A:126:GLU:OE1	2.28	0.52
1:A:131[A]:ARG:HD3	6:A:899:HOH:O	2.10	0.50
1:A:284:ARG:HG3	1:A:285:ASP:N	2.26	0.50
1:A:370:HIS:CG	1:A:394:THR:HA	2.46	0.50
1:A:294:PRO:HD2	1:A:303:TRP:CH2	2.47	0.49
1:B:1294:PRO:HD2	1:B:1303:TRP:CH2	2.47	0.49
1:A:57:LEU:HD22	6:B:822:HOH:O	2.12	0.49
1:A:149:PHE:O	1:A:168:MET:HA	2.13	0.48
1:B:1149:PHE:O	1:B:1168:MET:HA	2.14	0.48
1:B:1119:LYS:HE2	6:B:821:HOH:O	2.13	0.48
1:A:298:ASP:HB2	6:A:610:HOH:O	2.14	0.47
1:B:1293:ASP:HA	1:B:1303:TRP:CH2	2.49	0.47
1:A:293:ASP:HA	1:A:303:TRP:CH2	2.49	0.46
1:A:182[B]:ARG:NH2	1:A:235:TYR:OH	2.49	0.45
1:B:1001:SER:N	6:B:295:HOH:O	2.49	0.45
1:B:1354:GLN:NE2	6:B:776:HOH:O	2.49	0.45
1:A:281:ASP:OD1	1:A:284:ARG:NH1	2.50	0.45
1:B:1309:ASN:ND2	6:B:572:HOH:O	2.50	0.45
1:B:1101:ASN:ND2	1:B:1103:SER:OG	2.49	0.45
1:A:142:LEU:HA	1:A:388:CYS:SG	2.56	0.45
1:A:94:LEU:CD2	1:A:102:LYS:HE3	2.47	0.44
1:B:1371:ARG:O	1:B:1374:GLU:HG2	2.17	0.44
1:B:1370:HIS:CG	1:B:1394:THR:HA	2.52	0.44
1:B:1215:ASN:ND2	6:B:666:HOH:O	2.49	0.44
1:A:371:ARG:O	1:A:374:GLU:HG2	2.17	0.44
1:A:131[A]:ARG:NH2	1:A:140:SER:O	2.49	0.43
1:B:1094:LEU:CD2	1:B:1102:LYS:HE3	2.48	0.43
1:B:1182[A]:ARG:NH1	1:B:1235:TYR:OH	2.50	0.43
1:B:1183:LEU:HD22	1:B:1235:TYR:CZ	2.53	0.43
1:B:1057:LEU:HD12	1:B:1057:LEU:N	2.34	0.42
1:A:251:TYR:CZ	1:A:254:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HE2	6:A:853:HOH:O	2.17	0.42
1:A:57:LEU:HD23	1:A:57:LEU:N	2.35	0.41
1:A:357:LYS:O	1:A:361:GLU:HG3	2.20	0.41
1:B:1227[B]:LYS:HE2	6:B:557:HOH:O	2.20	0.41
1:A:141:ASP:HB3	1:A:435:HIS:CD2	2.55	0.41
1:A:182[B]:ARG:NH1	6:A:759:HOH:O	2.49	0.41
1:A:161:LYS:HA	1:B:1201[B]:LYS:NZ	2.36	0.41
1:A:232:LYS:HE3	6:A:911:HOH:O	2.21	0.40
1:A:322:THR:HG22	1:A:322:THR:O	2.22	0.40
1:A:361:GLU:HG3	6:A:749:HOH:O	2.20	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	439/439 (100%)	431 (98%)	7 (2%)	1 (0%)	47	21
1	B	439/439 (100%)	429 (98%)	9 (2%)	1 (0%)	47	21
All	All	878/878 (100%)	860 (98%)	16 (2%)	2 (0%)	47	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	B	1399	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	335/356 (94%)	325 (97%)	10 (3%)	41 9
1	B	330/356 (93%)	322 (98%)	8 (2%)	49 15
All	All	665/712 (93%)	647 (97%)	18 (3%)	47 12

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	57	LEU
1	A	131[A]	ARG
1	A	131[B]	ARG
1	A	202	ASP
1	A	215	ASN
1	A	284	ARG
1	A	337	ASN
1	A	344	ASN
1	A	370	HIS
1	B	1097	ASP
1	B	1101	ASN
1	B	1215	ASN
1	B	1370	HIS
1	B	1391	GLN
1	B	1415	GLU
1	B	1429[A]	ASN
1	B	1429[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	150	ASN
1	A	189	HIS
1	A	215	ASN
1	A	337	ASN
1	A	434	HIS
1	A	435	HIS
1	B	1101	ASN
1	B	1150	ASN

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Mol	Chain	Res	Type
1	B	1165	GLN
1	B	1309	ASN
1	B	1345	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	TRS	A	460	-	7,7,7	26.71	3 (42%)	9,9,9	7.41	5 (55%)
3	PO4	A	442	2	4,4,4	3.01	3 (75%)	6,6,6	0.62	0
3	PO4	B	1442	2	4,4,4	2.91	3 (75%)	6,6,6	0.65	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
5	TRS	A	460	-	-	1/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	460	TRS	C3-C	57.33	3.31	1.53
5	A	460	TRS	O3-C3	41.14	2.79	1.42
3	B	1442	PO4	P-O2	-4.24	1.41	1.54
3	A	442	PO4	P-O1	-4.02	1.41	1.50
5	A	460	TRS	C-N	3.36	1.60	1.49
3	B	1442	PO4	P-O4	-3.18	1.45	1.54
3	A	442	PO4	P-O2	-3.10	1.45	1.54
3	A	442	PO4	P-O4	-2.84	1.46	1.54
3	B	1442	PO4	P-O3	-2.17	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	460	TRS	O3-C3-C	-18.26	53.13	111.00
5	A	460	TRS	C3-C-C2	-10.00	79.80	110.81
5	A	460	TRS	O1-C1-C	-5.73	92.85	111.00
5	A	460	TRS	C2-C-C1	4.47	124.67	110.81
5	A	460	TRS	C1-C-N	2.07	114.17	107.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	460	TRS	N-C-C1-O1

There are no ring outliers.

No monomer is involved in short contacts.

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	435/439 (99%)	-0.50	3 (0%)	87	90	9, 14, 29, 42	0
1	B	432/439 (98%)	-0.51	3 (0%)	87	90	9, 14, 28, 45	0
All	All	867/878 (98%)	-0.51	6 (0%)	87	90	9, 14, 29, 45	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	HIS	2.6
1	B	1431	SER	2.3
1	A	418	ASP	2.3
1	B	1432	VAL	2.2
1	B	1141	ASP	2.1
1	A	420	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
5	TRS	A	460	8/8	0.95	0.09	16,19,28,74	0
4	F	B	1445	1/1	0.99	0.04	13,13,13,13	0
4	F	A	445	1/1	0.99	0.07	14,14,14,14	0
2	MG	B	1441	1/1	1.00	0.02	9,9,9,9	0
3	PO4	A	442	5/5	1.00	0.03	9,9,10,10	0
3	PO4	B	1442	5/5	1.00	0.03	8,9,10,10	0
4	F	A	444	1/1	1.00	0.05	10,10,10,10	0
2	MG	A	440	1/1	1.00	0.01	11,11,11,11	0
4	F	B	1444	1/1	1.00	0.01	9,9,9,9	0
2	MG	A	441	1/1	1.00	0.01	10,10,10,10	0
2	MG	B	1440	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.