



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:11 PM UTC

PDB ID : 2AKZ / pdb_00002akz
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

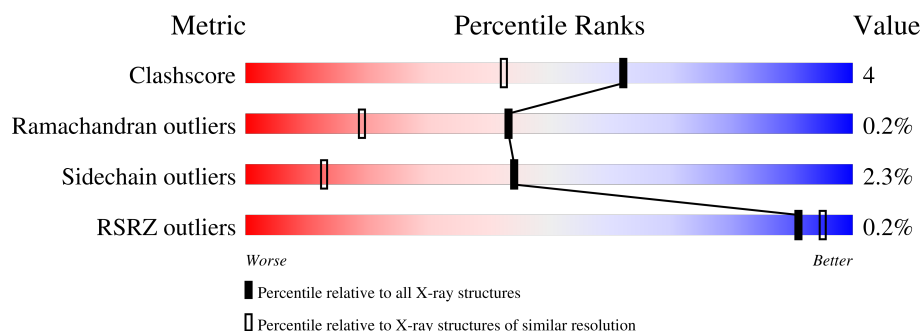
1 Overall quality at a glance

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	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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 $\leq 5\%$. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TRS	A	460	-	X	-	-

2 Entry composition

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			

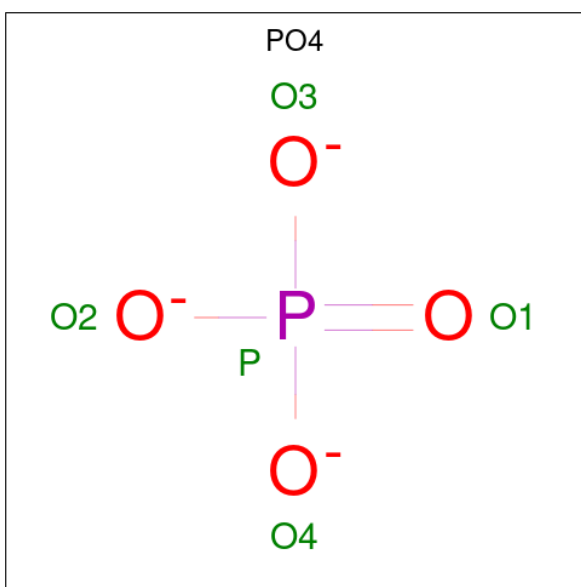
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: PO4) (formula: O₄P).

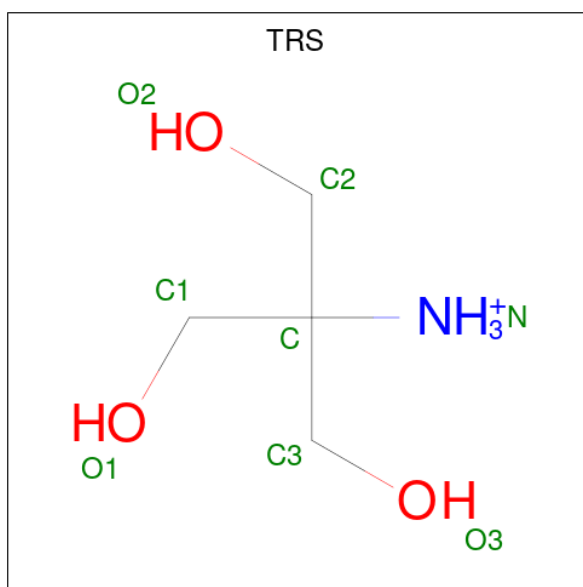


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLUORIDE ION (CCD ID: F) (formula: F).

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

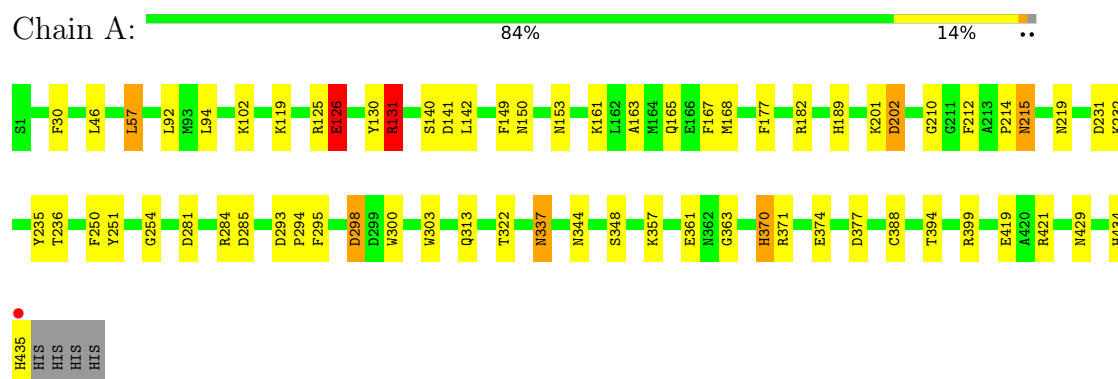
- Molecule 6 is water.

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

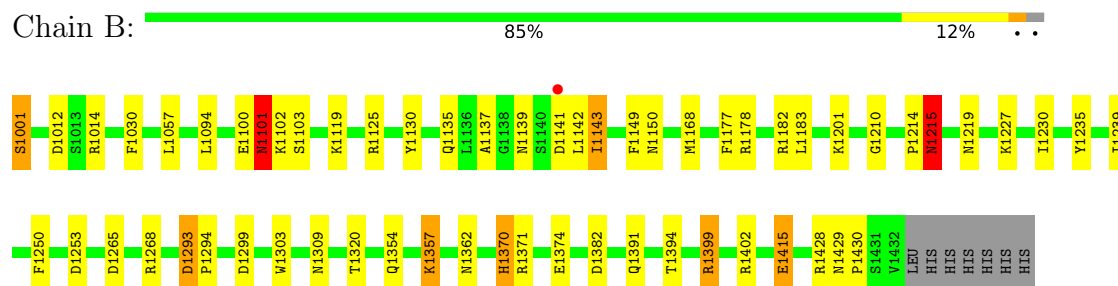
3 Residue-property plots

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



• Molecule 1: Gamma enolase



4 Data and refinement statistics

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 10.00 – 1.36	Depositor EDS
% Data completeness (in resolution range)	88.9 (10.00-1.36) 88.6 (10.00-1.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.41 , 82.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, F, MG, TRS

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	1.16	1/3386 (0.0%)	1.58	41/4584 (0.9%)
1	B	0.93	1/3366 (0.0%)	1.54	42/4559 (0.9%)
All	All	1.05	2/6752 (0.0%)	1.56	83/9143 (0.9%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLU	CD-OE2	40.71	2.02	1.25
1	B	1293	ASP	C-O	-6.96	1.20	1.23

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLU	OE1-CD-OE2	-16.11	84.23	122.90
1	B	1215	ASN	CA-CB-CG	11.28	123.88	112.60
1	B	1428	ARG	CD-NE-CZ	10.70	139.38	124.40
1	A	215	ASN	CA-CB-CG	10.45	123.05	112.60
1	B	1215	ASN	OD1-CG-ND2	-9.74	112.86	122.60
1	A	30	PHE	CA-CB-CG	-8.76	105.04	113.80
1	B	1402	ARG	NE-CZ-NH2	8.59	126.93	119.20
1	B	1030	PHE	CA-CB-CG	-8.39	105.41	113.80
1	B	1100	GLU	CA-C-O	8.35	129.40	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLU	CG-CD-OE2	-8.20	99.55	118.40
1	B	1101	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	A	214	PRO	CA-C-N	7.97	134.01	122.21
1	A	214	PRO	C-N-CA	7.97	134.01	122.21
1	B	1012	ASP	CA-CB-CG	7.96	120.56	112.60
1	B	1214	PRO	CA-C-N	7.92	133.92	122.21
1	B	1214	PRO	C-N-CA	7.92	133.92	122.21
1	B	1250	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	313	GLN	CA-C-N	7.74	133.39	123.10
1	A	313	GLN	C-N-CA	7.74	133.39	123.10
1	A	421	ARG	N-CA-CB	7.36	122.33	110.77
1	A	210	GLY	CA-C-N	7.32	127.29	120.34
1	A	210	GLY	C-N-CA	7.32	127.29	120.34
1	B	1362	ASN	CA-CB-CG	-7.31	105.29	112.60
1	A	370	HIS	CB-CG-CD2	7.03	140.34	131.20
1	A	421	ARG	CA-CB-CG	6.93	127.95	114.10
1	B	1135	GLN	OE1-CD-NE2	6.82	129.42	122.60
1	B	1299	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	1428	ARG	NE-CZ-NH1	-6.76	114.74	121.50
1	B	1230	ILE	O-C-N	6.70	128.47	121.91
1	A	219	ASN	CB-CG-ND2	-6.69	106.37	116.40
1	B	1215	ASN	CB-CG-ND2	6.59	126.28	116.40
1	B	1177	PHE	CA-CB-CG	-6.54	107.26	113.80
1	A	153	ASN	CB-CG-ND2	-6.52	106.62	116.40
1	B	1370	HIS	CB-CG-CD2	6.49	139.63	131.20
1	B	1142	LEU	CA-C-N	-6.47	113.39	122.71
1	B	1142	LEU	C-N-CA	-6.47	113.39	122.71
1	A	177	PHE	CA-CB-CG	-6.46	107.33	113.80
1	A	377	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	434	HIS	CA-C-N	6.42	133.25	121.70
1	A	434	HIS	C-N-CA	6.42	133.25	121.70
1	B	1101	ASN	CB-CG-ND2	6.41	126.01	116.40
1	A	429	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	A	298	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	313	GLN	O-C-N	-6.26	115.71	123.04
1	B	1014	ARG	CD-NE-CZ	6.11	132.95	124.40
1	B	1430	PRO	CA-C-N	6.07	129.02	120.28
1	B	1430	PRO	C-N-CA	6.07	129.02	120.28
1	B	1125[A]	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	B	1125[B]	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	A	300	TRP	CE3-CZ3-CH2	5.95	128.84	121.10
1	A	131[A]	ARG	NE-CZ-NH1	-5.92	115.58	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131[B]	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	B	1362	ASN	OD1-CG-ND2	5.92	128.51	122.60
1	B	1178	ARG	CA-CB-CG	-5.85	102.39	114.10
1	A	219	ASN	CB-CG-OD1	5.64	132.08	120.80
1	A	165	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	B	1239	ILE	O-C-N	5.58	129.23	123.20
1	A	348	SER	O-C-N	5.58	129.63	123.33
1	A	163	ALA	CA-C-N	5.57	128.78	120.87
1	A	163	ALA	C-N-CA	5.57	128.78	120.87
1	A	150	ASN	CA-CB-CG	5.54	118.14	112.60
1	A	212	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	202	ASP	CA-CB-CG	-5.50	107.10	112.60
1	B	1357	LYS	CB-CG-CD	5.42	123.77	111.30
1	B	1139	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	1001	SER	CA-C-O	5.31	129.83	120.80
1	A	250	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	125	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	A	419	GLU	N-CA-CB	5.28	118.75	110.46
1	A	167	PHE	CE1-CZ-CE2	5.28	129.49	120.00
1	A	421	ARG	CB-CA-C	-5.26	101.72	110.14
1	B	1210	GLY	O-C-N	-5.22	115.80	122.43
1	B	1150	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	1399	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	B	1219	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	B	1382	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	295	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	1141	ASP	O-C-N	5.10	128.75	122.84
1	A	370	HIS	ND1-CG-CD2	-5.04	101.06	106.10
1	B	1253	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	1139	ASN	CA-C-N	5.01	131.07	122.09
1	B	1139	ASN	C-N-CA	5.01	131.07	122.09
1	A	363	GLY	CA-C-O	5.01	125.24	119.13

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 ⓘ

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	32	0
1	B	3258	0	3185	22	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	53	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 (53) 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	1.00
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:A:337:ASN:HD22	1:A:337:ASN:C	2.10	0.59
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:130:TYR:CE1	1:A:131[B]:ARG:HG3	2.44	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:GLU:OE2	1:A:126:GLU:OE1	2.28	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:1137:ALA:O	1:B:1357:LYS:NZ	2.49	0.43
1:A:231:ASP:OD2	1:A:236:THR:OG1	2.30	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
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

5.3.1 Protein backbone

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%)	43	19
1	B	439/439 (100%)	429 (98%)	9 (2%)	1 (0%)	43	19
All	All	878/878 (100%)	860 (98%)	16 (2%)	2 (0%)	43	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	B	1399	ARG

5.3.2 Protein sidechains

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%)	326 (97%)	9 (3%)	39	9
1	B	330/356 (93%)	322 (98%)	8 (2%)	43	12
All	All	665/712 (93%)	648 (97%)	17 (3%)	44	9

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	57	LEU
1	A	92	LEU
1	A	131[A]	ARG

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Mol	Chain	Res	Type
1	A	131[B]	ARG
1	A	202	ASP
1	A	215	ASN
1	A	337	ASN
1	A	344	ASN
1	B	1101	ASN
1	B	1143	ILE
1	B	1215	ASN
1	B	1320	THR
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	165	GLN
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	1165	GLN
1	B	1345	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 oligosaccharides 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	30.14	3 (42%)	9,9,9	8.46	6 (66%)
3	PO4	A	442	2	4,4,4	3.08	3 (75%)	6,6,6	0.65	0
3	PO4	B	1442	2	4,4,4	3.01	3 (75%)	6,6,6	0.69	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	-	-	3/9/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	460	TRS	C3-C	67.09	3.31	1.53
5	A	460	TRS	O3-C3	42.90	2.79	1.42
3	B	1442	PO4	P-O2	-4.39	1.41	1.54
3	A	442	PO4	P-O1	-4.04	1.41	1.50
5	A	460	TRS	C-N	3.52	1.60	1.49
3	B	1442	PO4	P-O4	-3.29	1.45	1.54
3	A	442	PO4	P-O2	-3.21	1.45	1.54
3	A	442	PO4	P-O4	-2.94	1.46	1.54
3	B	1442	PO4	P-O3	-2.25	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	460	TRS	O3-C3-C	-20.72	53.13	110.88
5	A	460	TRS	C3-C-C2	-11.59	79.80	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	460	TRS	O1-C1-C	-6.47	92.85	110.88
5	A	460	TRS	C2-C-C1	5.26	124.67	110.66
5	A	460	TRS	C1-C-N	2.35	114.17	108.17
5	A	460	TRS	C2-C-N	2.08	113.47	108.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	460	TRS	N-C-C1-O1
5	A	460	TRS	C3-C-C1-O1
5	A	460	TRS	N-C-C3-O3

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 [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(Å ²)	Q<0.9
1	A	435/439 (99%)	-0.42	1 (0%) 91 95	9, 14, 29, 42	6 (1%)
1	B	432/439 (98%)	-0.42	1 (0%) 91 95	9, 14, 27, 45	8 (1%)
All	All	867/878 (98%)	-0.42	2 (0%) 91 95	9, 14, 28, 45	14 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1141	ASP	2.4
1	A	435	HIS	2.2

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	TRS	A	460	8/8	0.94	0.08	16,19,28,74	0
4	F	A	445	1/1	0.98	0.08	14,14,14,14	0
4	F	B	1445	1/1	0.99	0.04	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	1441	1/1	1.00	0.01	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	0.03	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	0.02	9,9,9,9	0
2	MG	A	441	1/1	1.00	0.02	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.