



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 08:58 AM GMT

PDB ID : 1XYM
Title : THE ROLE OF THE DIVALENT METAL ION IN SUGAR BINDING,
RING OPENING, AND ISOMERIZATION BY D-XYLOSE ISOMERASE:
REPLACEMENT OF A CATALYTIC METAL BY AN AMINO-ACID
Authors : Allen, K.N.; Lavie, A.; Petsko, G.A.; Ringe, D.
Deposited on : 1993-12-07
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

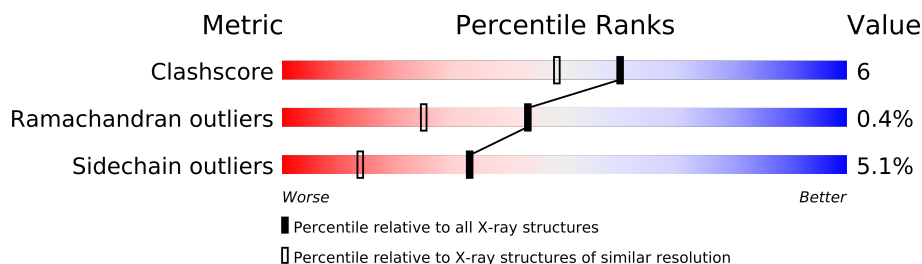
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8862 atoms, of which 2314 are hydrogens and 0 are deuterium.

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.

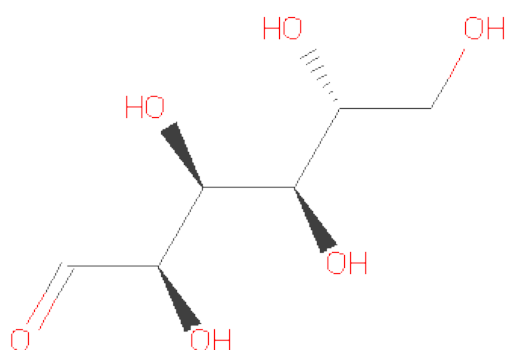
- Molecule 1 is a protein called XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	H	N	O	S	0	0	0
			3696	1905	672	541	570	8			
1	B	386	Total	C	H	N	O	S	0	0	0
			3696	1905	672	541	570	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LYS	GLU	CONFLICT	UNP P15587
B	680	LYS	GLU	CONFLICT	UNP P15587

- Molecule 2 is SUGAR (D-GLUCOSE IN LINEAR FORM) (three-letter code: GLO) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	12	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			24	6	12	6		

- 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		

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	H	O	0	0
			2	1	1		
4	B	1	Total	H	O	0	0
			2	1	1		

- Molecule 5 is water.

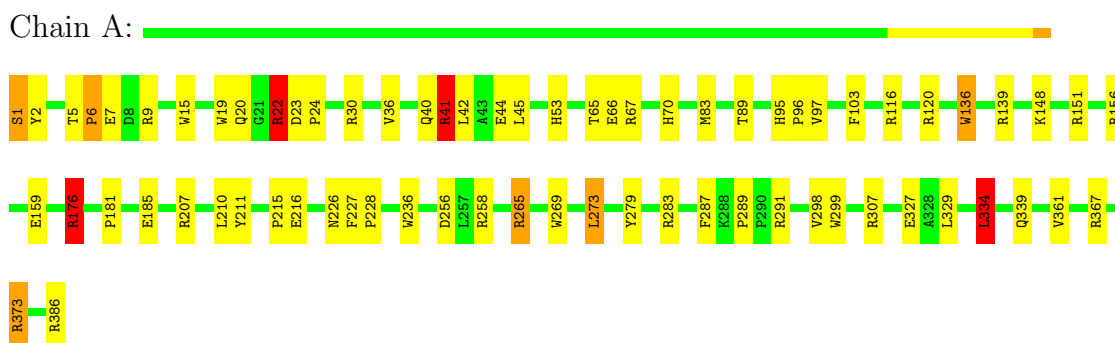
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	247	Total	H	O	0	0
			741	494	247		
5	B	225	Total	H	O	0	0
			675	450	225		

3 Residue-property plots

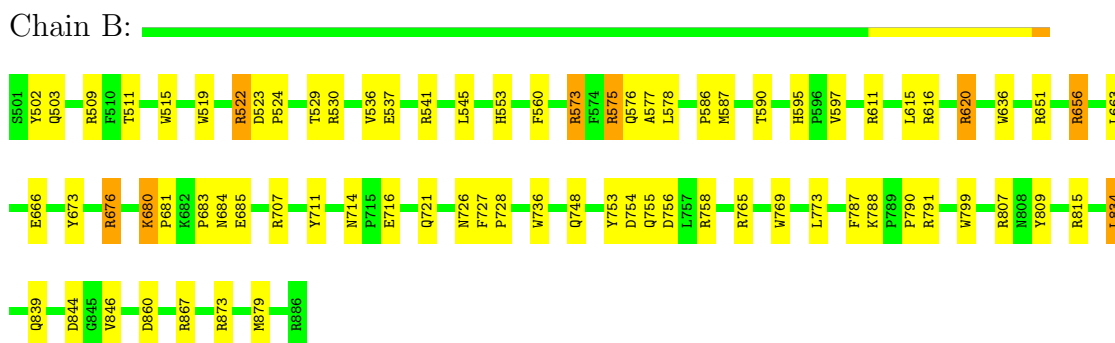
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: XYLOSE ISOMERASE



• Molecule 1: XYLOSE ISOMERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.12Å 99.53Å 94.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8862	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.80	0/3096	1.41	46/4196 (1.1%)
1	B	0.79	0/3096	1.43	53/4196 (1.3%)
All	All	0.80	0/6192	1.42	99/8392 (1.2%)

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	A	307	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	765	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	265	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	B	765	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	265	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	758	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	B	616	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	A	15	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	B	575	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	B	515	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	B	573	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	807	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	519	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	B	799	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	A	367	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	236	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	176	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	867	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	799	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	B	758	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	15	TRP	CE2-CD2-CG	-7.47	101.33	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	651	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	386	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	519	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	B	636	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	A	299	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	30	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	515	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	B	736	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	19	TRP	CD1-CG-CD2	7.07	111.96	106.30
1	B	530	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	736	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	A	41	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	867	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	136	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	B	636	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	A	236	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	136	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	307	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	834	LEU	CA-CB-CG	-6.79	99.69	115.30
1	A	299	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	B	711	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	A	19	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	B	620	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	769	TRP	CD1-CG-CD2	6.46	111.47	106.30
1	A	367	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	269	TRP	CD1-CG-CD2	6.41	111.43	106.30
1	A	283	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	673	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	B	879	MET	CG-SD-CE	-6.33	90.07	100.20
1	A	269	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	41	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	736	TRP	CG-CD2-CE3	6.24	139.52	133.90
1	B	502	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	B	807	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	22	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	815	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	258	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	769	TRP	CE2-CD2-CG	-6.09	102.42	107.30
1	B	616	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	176	ARG	CG-CD-NE	6.03	124.46	111.80
1	A	386	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	373	ARG	NE-CZ-NH1	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	754	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	334	LEU	CA-CB-CG	-5.83	101.88	115.30
1	A	44	GLU	CA-CB-CG	-5.81	100.62	113.40
1	A	273	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	299	TRP	CB-CG-CD1	-5.77	119.50	127.00
1	B	611	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	299	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	B	656	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	22	ARG	CA-CB-CG	5.68	125.89	113.40
1	B	620	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	799	TRP	CB-CG-CD1	-5.57	119.76	127.00
1	B	522	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	15	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	A	116	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	515	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	A	151	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	156	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	211	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	236	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	B	515	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	B	575	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	136	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	279	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	B	519	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	B	736	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	B	799	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	B	515	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	B	636	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	B	753	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	809	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	B	537	GLU	CA-CB-CG	5.03	124.46	113.40
1	B	676	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	587	MET	CA-CB-CG	5.01	121.83	113.30
1	A	283	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	116	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3024	672	2244	40	0
1	B	3024	672	2244	34	0
2	A	12	12	0	1	0
2	B	12	12	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	1	0	0	0
4	B	1	1	0	0	0
5	A	247	494	0	21	0
5	B	225	450	0	22	0
All	All	6548	2314	4488	72	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:GLN:HB2	1:A:22:ARG:HH12	1.60	0.66
1:B:681:PRO:HA	5:B:1186:HOH:H1	1.63	0.64
1:B:680:LYS:HG2	1:B:714:ASN:O	1.99	0.63
1:A:291:ARG:HH12	5:A:1200:HOH:H2	1.47	0.62
1:A:1:SER:HB2	1:A:2:TYR:HD1	1.66	0.60
1:B:523:ASP:HB2	1:B:524:PRO:HD2	1.83	0.60
1:B:620:ARG:HH11	5:B:1174:HOH:H2	1.49	0.59
1:B:873:ARG:HH11	5:B:1394:HOH:H2	1.50	0.59
1:A:1:SER:HB2	1:A:2:TYR:CD1	2.37	0.59
5:A:1055:HOH:H1	1:B:791:ARG:HH12	1.51	0.59
1:A:22:ARG:HB3	1:A:22:ARG:HH11	1.68	0.58
1:A:70:HIS:HE1	5:A:1436:HOH:O	1.87	0.57
1:B:683:PRO:HD3	5:B:1124:HOH:H1	1.70	0.57
1:B:873:ARG:H	5:B:1218:HOH:H2	1.52	0.56
1:A:265:ARG:HG3	5:A:1094:HOH:O	2.04	0.56
1:A:216:GLU:H	5:A:1258:HOH:H2	1.51	0.56
1:B:595:HIS:HD2	1:B:597:VAL:H	1.54	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:620:ARG:HD3	5:B:1174:HOH:H2	1.71	0.54
1:B:716:GLU:H	5:B:1127:HOH:H1	1.55	0.53
1:A:120:ARG:HH12	5:A:1503:HOH:H1	1.56	0.53
1:B:522:ARG:HB3	5:B:1104:HOH:H1	1.73	0.52
1:A:96:PRO:HB3	1:B:529:THR:HG22	1.91	0.51
1:A:207:ARG:HE	5:A:1257:HOH:H2	1.57	0.51
1:B:575:ARG:NH1	5:B:1168:HOH:H2	2.09	0.51
1:B:860:ASP:H	5:B:1545:HOH:H1	1.58	0.50
1:B:511:THR:HG21	1:B:586:PRO:HG2	1.94	0.50
1:B:726:ASN:H	5:B:1383:HOH:H2	1.58	0.50
1:A:83:MET:SD	5:A:1540:HOH:O	2.70	0.49
1:A:181:PRO:HA	5:A:1037:HOH:H1	1.77	0.49
1:A:159:GLU:HA	5:A:1441:HOH:H2	1.77	0.48
1:B:615:LEU:HD11	5:B:1142:HOH:H2	1.77	0.48
1:B:790:PRO:HA	5:B:1320:HOH:H2	1.78	0.48
1:A:136:TRP:CD2	2:A:950:GLO:H2	2.49	0.48
1:B:536:VAL:HG13	1:B:577:ALA:HB2	1.96	0.48
1:A:103:PHE:H	5:A:1300:HOH:H1	1.60	0.47
1:A:289:PRO:HG2	1:A:298:VAL:HG13	1.96	0.47
1:A:226:ASN:H	5:A:1050:HOH:H1	1.63	0.47
1:A:36:VAL:O	1:A:40:GLN:HG2	2.15	0.47
1:B:560:PHE:H	5:B:1340:HOH:H2	1.63	0.47
1:B:684:ASN:HD21	5:B:1225:HOH:H1	1.63	0.46
1:A:339:GLN:HB3	5:A:1445:HOH:H1	1.77	0.46
1:A:329:LEU:HD22	1:A:334:LEU:HD13	1.97	0.46
1:B:707:ARG:HH11	5:B:1125:HOH:H2	1.61	0.46
1:A:95:HIS:CD2	1:A:97:VAL:H	2.34	0.46
1:A:7:GLU:HG2	5:A:1500:HOH:O	2.16	0.45
1:A:41:ARG:HE	1:A:41:ARG:HA	1.81	0.45
1:A:256:ASP:HB3	1:A:287:PHE:HA	1.98	0.45
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.98	0.45
1:A:24:PRO:HD3	1:B:524:PRO:HB3	1.99	0.45
1:B:727:PHE:HB3	1:B:728:PRO:HD3	1.98	0.44
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.52	0.44
1:A:227:PHE:HB3	1:A:228:PRO:HD3	1.99	0.44
1:B:788:LYS:HG3	5:B:1332:HOH:H1	1.82	0.44
1:A:95:HIS:HD2	1:A:97:VAL:H	1.66	0.44
1:A:20:GLN:HB2	1:A:22:ARG:HH22	1.83	0.43
1:A:176:ARG:HB2	1:A:176:ARG:HH11	1.83	0.43
1:B:721:GLN:HE22	1:B:748:GLN:HB3	1.83	0.43
1:B:755:GLN:HE21	5:B:1080:HOH:H2	1.66	0.43
1:A:67:ARG:HH21	5:A:1283:HOH:H2	1.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:656:ARG:HH12	5:B:1150:HOH:H1	1.65	0.43
1:A:20:GLN:HG2	5:A:1234:HOH:O	2.19	0.43
1:A:327:GLU:HG3	5:A:1029:HOH:H2	1.84	0.42
1:B:620:ARG:HD3	5:B:1174:HOH:O	2.19	0.42
1:A:7:GLU:HG2	5:A:1500:HOH:H1	1.84	0.42
1:B:553:HIS:CE1	2:B:960:GLO:H5	2.55	0.41
1:A:139:ARG:H	5:A:1036:HOH:H2	1.68	0.41
1:B:707:ARG:H	5:B:1128:HOH:H2	1.67	0.41
1:A:148:LYS:HE3	5:A:1034:HOH:H1	1.86	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.95	0.41
1:B:839:GLN:HE21	5:B:1157:HOH:H1	1.68	0.41
1:A:215:PRO:HA	5:A:1258:HOH:H2	1.84	0.41
1:B:756:ASP:HB3	1:B:787:PHE:HA	2.04	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	384/386 (100%)	369 (96%)	13 (3%)	2 (0%)	38	19
1	B	384/386 (100%)	370 (96%)	13 (3%)	1 (0%)	50	31
All	All	768/772 (100%)	739 (96%)	26 (3%)	3 (0%)	43	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	185	GLU
1	B	685	GLU

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	302/302 (100%)	287 (95%)	15 (5%)	34	14
1	B	302/302 (100%)	286 (95%)	16 (5%)	32	13
All	All	604/604 (100%)	573 (95%)	31 (5%)	33	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	THR
1	A	6	PRO
1	A	9	ARG
1	A	22	ARG
1	A	41	ARG
1	A	45	LEU
1	A	65	THR
1	A	66	GLU
1	A	176	ARG
1	A	210	LEU
1	A	273	LEU
1	A	334	LEU
1	A	361	VAL
1	A	373	ARG
1	B	503	GLN
1	B	509	ARG
1	B	541	ARG
1	B	545	LEU
1	B	573	ARG
1	B	576	GLN
1	B	578	LEU
1	B	590	THR
1	B	663	LEU
1	B	666	GLU
1	B	676	ARG
1	B	680	LYS
1	B	773	LEU
1	B	834	LEU

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Mol	Chain	Res	Type
1	B	844	ASP
1	B	846	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	76	GLN
1	A	95	HIS
1	A	308	ASN
1	A	326	GLN
1	B	503	GLN
1	B	595	HIS
1	B	721	GLN
1	B	808	ASN
1	B	839	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 2 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	GLO	A	950	-	11,11,11	1.34	1 (9%)	14,14,14	1.81	3 (21%)
2	GLO	B	960	-	11,11,11	1.38	1 (9%)	14,14,14	1.80	4 (28%)

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	GLO	A	950	-	-	0/15/16/16	0/0/0/0
2	GLO	B	960	-	-	0/15/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	GLO	C3-C2	2.85	1.57	1.53
2	B	960	GLO	C3-C2	2.64	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	GLO	C5-C4-C3	4.46	119.70	112.43
2	B	960	GLO	C4-C3-C2	-4.04	106.46	113.67
2	A	950	GLO	O4-C4-C5	-3.12	100.85	108.74
2	A	950	GLO	C4-C3-C2	-2.88	108.54	113.67
2	B	960	GLO	C5-C4-C3	2.56	116.61	112.43
2	B	960	GLO	O3-C3-C2	2.49	113.30	108.86
2	B	960	GLO	O4-C4-C5	-2.20	103.17	108.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.