



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 12:45 PM EDT

PDB ID : 5TD9
Title : Structure of Human Enolase 2
Authors : Leonard, P.G.; Muller, F.L.
Deposited on : unknown
Resolution : 2.32 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

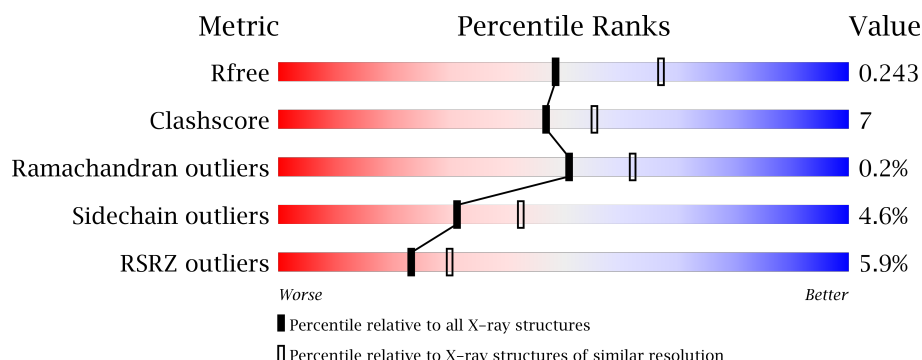
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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 $\leq 5\%$. 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	440	<div> <div>9%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	440	<div> <div>3%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6734 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	434	Total	C	N	O	S	0	0	0
			3322	2089	569	650	14			
1	B	434	Total	C	N	O	S	0	0	0
			3322	2089	569	650	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	440	HIS	-	expression tag	UNP P09104
B	435	HIS	-	expression tag	UNP P09104
B	436	HIS	-	expression tag	UNP P09104
B	437	HIS	-	expression tag	UNP P09104
B	438	HIS	-	expression tag	UNP P09104
B	439	HIS	-	expression tag	UNP P09104
B	440	HIS	-	expression tag	UNP P09104

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0

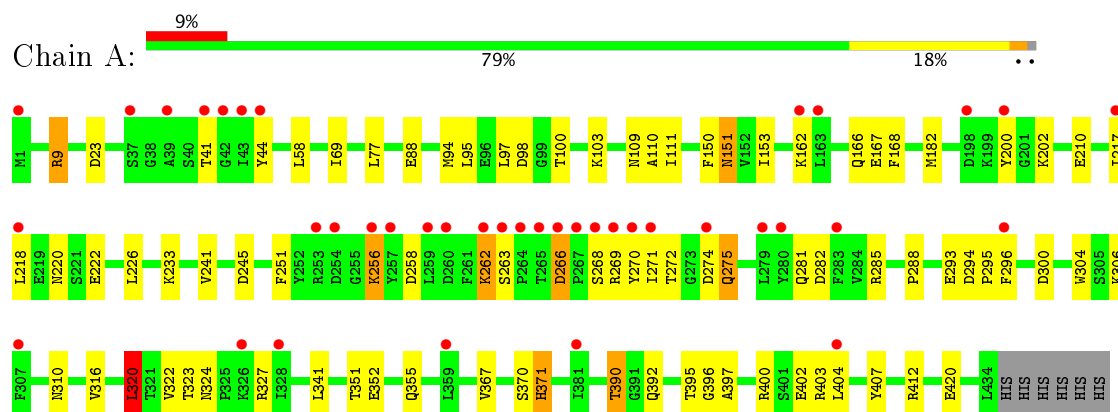
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total 41	O 41	0	0
4	B	45	Total 45	O 45	0	0

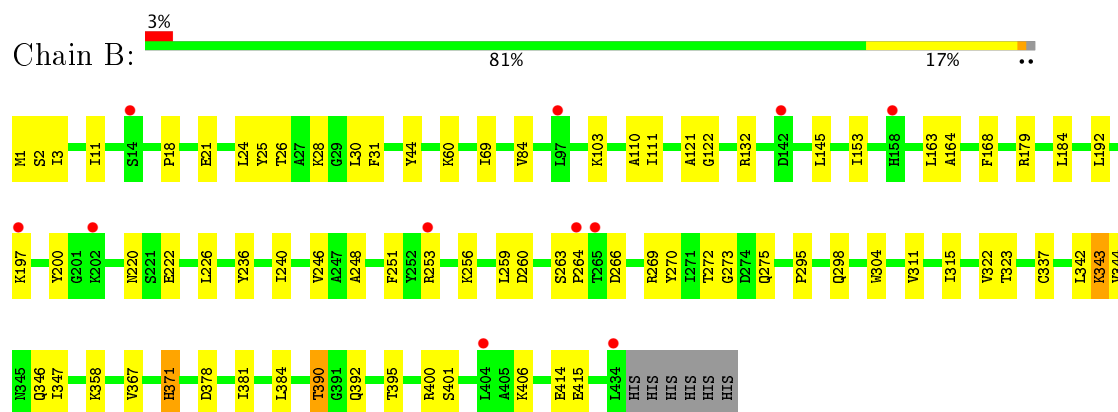
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	68.32Å 112.87Å 119.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.51 – 2.32 43.51 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.51-2.32) 95.7 (43.51-2.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.76 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155-000	Depositor
R, R_{free}	0.200 , 0.245 0.196 , 0.243	Depositor DCC
R_{free} test set	1920 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: MG, CL

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	0.27	0/3377	0.47	1/4568 (0.0%)
1	B	0.27	0/3377	0.46	0/4568
All	All	0.27	0/6754	0.46	1/9136 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	LEU	CA-CB-CG	6.10	129.32	115.30

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	3322	0	3299	50	0
1	B	3322	0	3299	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	41	0	0	0	0
4	B	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6734	0	6598	94	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 7.

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:A:256:LYS:HD2	1:A:270:TYR:HB2	1.60	0.83
1:A:245:ASP:HA	1:A:293:GLU:HB3	1.69	0.73
1:A:162:LYS:HG3	1:A:218:LEU:HA	1.69	0.72
1:B:26:THR:HG23	1:B:28:LYS:H	1.55	0.71
1:B:103:LYS:HG2	1:B:111:ILE:HD12	1.72	0.71
1:A:390:THR:HG22	1:A:392:GLN:H	1.57	0.69
1:A:200:TYR:OH	1:A:222:GLU:OE1	2.13	0.67
1:A:153:ILE:HB	1:A:168:PHE:HB2	1.78	0.66
1:A:150:PHE:HZ	1:A:182:MET:HE2	1.61	0.64
1:B:84:VAL:HG13	1:B:122:GLY:HA2	1.80	0.64
1:A:9:ARG:NH2	1:A:23:ASP:OD1	2.30	0.63
1:B:390:THR:HG22	1:B:392:GLN:H	1.66	0.59
1:A:256:LYS:HB2	1:A:270:TYR:HB3	1.85	0.59
1:A:282:ASP:HA	1:A:285:ARG:HG2	1.85	0.58
1:B:272:THR:HG23	1:B:275:GLN:H	1.66	0.58
1:A:367:VAL:O	1:A:390:THR:HG23	2.03	0.58
1:A:98:ASP:OD2	1:A:100:THR:OG1	2.15	0.58
1:B:179:ARG:HH21	1:B:414:GLU:HG2	1.68	0.58
1:A:167:GLU:HB2	1:A:245:ASP:HB3	1.85	0.58
1:B:11:ILE:HD13	1:B:21:GLU:HB2	1.85	0.57
1:A:88:GLU:HG3	1:A:351:THR:HG21	1.86	0.56
1:A:371:HIS:CG	1:A:395:THR:HA	2.42	0.55
1:A:241:VAL:HG23	1:A:288:PRO:HB2	1.89	0.55
1:A:294:ASP:HA	1:A:304:TRP:CH2	2.42	0.54
1:A:272:THR:HG22	1:A:274:ASP:H	1.73	0.54
1:A:295:PRO:HD2	1:A:304:TRP:CH2	2.43	0.54
1:B:153:ILE:HD11	1:B:192:LEU:HD21	1.90	0.54
1:A:271:ILE:HD12	1:A:275:GLN:HB2	1.90	0.53
1:B:256:LYS:HB2	1:B:270:TYR:HB3	1.90	0.53
1:B:371:HIS:CG	1:B:395:THR:HA	2.43	0.53
1:A:95:LEU:HD21	1:A:103:LYS:HE3	1.90	0.53
1:B:200:TYR:OH	1:B:222:GLU:OE1	2.19	0.53
1:B:323:THR:HG23	1:B:342:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD11	1:B:220:ASN:HA	1.92	0.51
1:B:367:VAL:O	1:B:390:THR:HG23	2.10	0.51
1:A:182:MET:SD	1:A:407:TYR:HB3	2.50	0.51
1:A:9:ARG:NH1	1:B:415:GLU:OE1	2.44	0.51
1:B:84:VAL:HG21	1:B:121:ALA:HB3	1.93	0.51
1:A:300:ASP:O	1:A:304:TRP:HD1	1.93	0.50
1:B:378:ASP:O	1:B:406:LYS:NZ	2.35	0.50
1:B:18:PRO:HG2	1:B:60:LYS:O	2.11	0.50
1:A:396:GLY:HA3	1:A:403:ARG:HD2	1.94	0.50
1:A:166:GLN:HG2	1:A:167:GLU:HG3	1.94	0.50
1:B:44:TYR:HB2	1:B:322:VAL:HG21	1.94	0.49
1:B:266:ASP:O	1:B:269:ARG:HG2	2.12	0.49
1:B:343:LYS:HB2	1:B:346:GLN:HB2	1.93	0.49
1:A:44:TYR:HB2	1:A:322:VAL:HG21	1.95	0.49
1:B:260:ASP:HB3	1:B:269:ARG:HD2	1.95	0.48
1:B:1:MET:HG3	1:B:2:SER:H	1.78	0.48
1:B:367:VAL:O	1:B:392:GLN:HG3	2.14	0.48
1:B:11:ILE:O	1:B:18:PRO:HA	2.14	0.48
1:B:153:ILE:HB	1:B:168:PHE:HB2	1.95	0.48
1:A:69:ILE:HD11	1:A:110:ALA:HA	1.96	0.47
1:A:294:ASP:HA	1:A:304:TRP:HH2	1.77	0.47
1:B:295:PRO:HD2	1:B:304:TRP:CH2	2.49	0.47
1:B:248:ALA:HA	1:B:251:PHE:CE1	2.50	0.46
1:B:253:ARG:HA	1:B:253:ARG:HD3	1.73	0.46
1:B:164:ALA:HB2	1:B:259:LEU:O	2.16	0.45
1:A:162:LYS:HG2	1:A:162:LYS:H	1.56	0.45
1:B:272:THR:HG22	1:B:275:GLN:OE1	2.16	0.45
1:A:402:GLU:HB3	1:B:401:SER:HB2	1.99	0.45
1:B:69:ILE:HD11	1:B:110:ALA:HA	1.99	0.45
1:A:251:PHE:HB2	1:A:258:ASP:O	2.18	0.44
1:A:168:PHE:HZ	1:A:220:ASN:HB3	1.82	0.44
1:B:25:TYR:CZ	1:B:30:LEU:HD12	2.52	0.43
1:A:341:LEU:HD11	1:A:370:SER:HB2	2.00	0.43
1:A:200:TYR:CZ	1:A:217:ILE:HD11	2.53	0.43
1:B:260:ASP:O	1:B:263:SER:HB2	2.18	0.43
1:A:296:PHE:HB2	1:A:304:TRP:NE1	2.33	0.43
1:B:26:THR:HG22	1:B:31:PHE:HE2	1.83	0.42
1:A:266:ASP:OD1	1:A:268:SER:HB3	2.19	0.42
1:A:103:LYS:HB3	1:A:111:ILE:HD12	2.01	0.42
1:A:151:ASN:O	1:A:397:ALA:HB2	2.19	0.42
1:B:358:LYS:HD3	1:B:358:LYS:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LEU:O	1:A:327:ARG:HD3	2.19	0.42
1:A:109:ASN:N	1:A:109:ASN:OD1	2.51	0.42
1:A:77:LEU:HD11	1:A:94:MET:SD	2.60	0.42
1:B:256:LYS:CB	1:B:270:TYR:HB3	2.49	0.41
1:B:263:SER:HB3	1:B:264:PRO:HD2	2.01	0.41
1:B:344:VAL:HG23	4:B:607:HOH:O	2.20	0.41
1:A:322:VAL:HG23	1:A:324:ASN:HB2	2.03	0.41
1:B:184:LEU:HB3	1:B:240:ILE:HD11	2.02	0.41
1:B:272:THR:OG1	1:B:273:GLY:N	2.53	0.41
1:B:381:ILE:HA	1:B:384:LEU:HB3	2.03	0.41
1:A:352:GLU:HA	1:A:355:GLN:HG2	2.03	0.41
1:B:315:ILE:O	1:B:337:CYS:HB2	2.21	0.41
1:A:222:GLU:O	1:A:226:LEU:HB2	2.20	0.41
1:A:341:LEU:HA	1:A:341:LEU:HD12	1.94	0.41
1:A:200:TYR:OH	1:A:217:ILE:HD11	2.21	0.41
1:A:262:LYS:NZ	1:A:263:SER:HB3	2.36	0.41
1:B:184:LEU:HD22	1:B:236:TYR:CZ	2.56	0.41
1:A:281:GLN:NE2	1:A:310:ASN:OD1	2.53	0.41
1:A:412:ARG:NH2	1:B:21:GLU:OE2	2.35	0.40
1:B:3:ILE:HD13	1:B:24:LEU:HD11	2.04	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	432/440 (98%)	419 (97%)	12 (3%)	1 (0%)	51	62
1	B	432/440 (98%)	415 (96%)	16 (4%)	1 (0%)	51	62
All	All	864/880 (98%)	834 (96%)	28 (3%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	B	400	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	351/357 (98%)	330 (94%)	21 (6%)	22	30
1	B	351/357 (98%)	340 (97%)	11 (3%)	45	61
All	All	702/714 (98%)	670 (95%)	32 (5%)	31	42

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	41	THR
1	A	58	LEU
1	A	97	LEU
1	A	151	ASN
1	A	202	LYS
1	A	210	GLU
1	A	233	LYS
1	A	256	LYS
1	A	262	LYS
1	A	266	ASP
1	A	269	ARG
1	A	275	GLN
1	A	306	LYS
1	A	316	VAL
1	A	320	LEU
1	A	323	THR
1	A	371	HIS
1	A	390	THR
1	A	404	LEU
1	A	420	GLU
1	B	132	ARG

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Mol	Chain	Res	Type
1	B	145	LEU
1	B	197	LYS
1	B	226	LEU
1	B	246	VAL
1	B	298	GLN
1	B	311	VAL
1	B	343	LYS
1	B	347	ILE
1	B	371	HIS
1	B	390	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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, 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	434/440 (98%)	0.49	40 (9%) 10 13	28, 56, 111, 178	0
1	B	434/440 (98%)	0.03	11 (2%) 58 65	29, 47, 79, 118	0
All	All	868/880 (98%)	0.26	51 (5%) 23 30	28, 52, 101, 178	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	5.1
1	A	271	ILE	5.0
1	A	268	SER	4.6
1	A	43	ILE	4.5
1	A	267	PRO	4.2
1	A	254	ASP	4.2
1	A	162	LYS	4.0
1	A	264	PRO	3.9
1	A	163	LEU	3.9
1	A	259	LEU	3.9
1	A	262	LYS	3.8
1	A	218	LEU	3.8
1	A	307	PHE	3.7
1	A	217	ILE	3.7
1	B	264	PRO	3.7
1	A	41	THR	3.4
1	A	274	ASP	3.3
1	A	269	ARG	3.3
1	A	265	THR	3.3
1	A	296	PHE	3.2
1	A	266	ASP	3.1
1	A	263	SER	3.1
1	A	326	LYS	3.0
1	A	283	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	3.0
1	A	42	GLY	2.8
1	B	142	ASP	2.8
1	A	381	ILE	2.8
1	B	97	LEU	2.8
1	A	279	LEU	2.7
1	B	14	SER	2.7
1	A	1	MET	2.6
1	A	280	TYR	2.6
1	A	404	LEU	2.6
1	B	265	THR	2.5
1	A	270	TYR	2.5
1	A	253	ARG	2.5
1	A	39	ALA	2.5
1	A	198	ASP	2.5
1	A	37	SER	2.4
1	B	202	LYS	2.4
1	A	359	LEU	2.3
1	B	434	LEU	2.3
1	A	256	LYS	2.3
1	A	328	ILE	2.3
1	A	44	TYR	2.3
1	B	158	HIS	2.3
1	A	200	TYR	2.1
1	B	197	LYS	2.1
1	B	404	LEU	2.1
1	B	253	ARG	2.1

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(\AA^2)	Q<0.9
2	MG	A	501	1/1	0.90	0.10	-1.50	74,74,74,74	0
2	MG	B	501	1/1	0.95	0.07	-1.84	47,47,47,47	0
3	CL	B	502	1/1	0.91	0.43	-	83,83,83,83	0
3	CL	A	502	1/1	0.93	0.34	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.