



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:21 PM UTC

PDB ID : 6CA4 / pdb_00006ca4
Title : Crystal structure of humanized D. rerio TDP2 by 14 mutations
Authors : Shi, K.; Aihrrara, H.
Deposited on : 2018-01-29
Resolution : 1.62 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

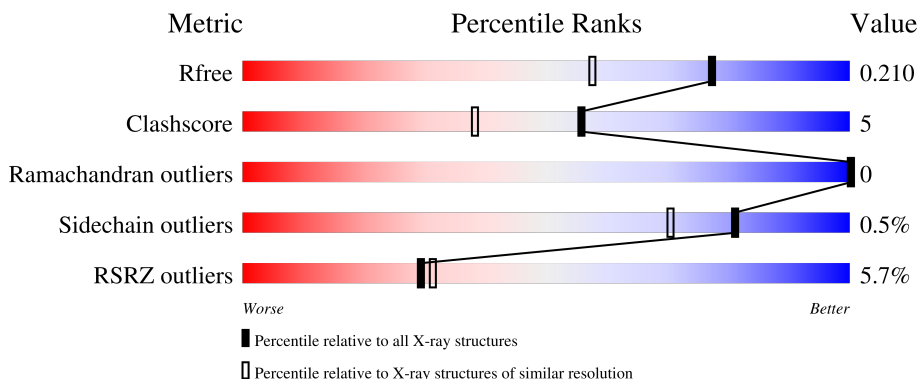
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	250	 5% 85% 12%
1	B	250	 5% 86% 11%
1	C	250	 6% 82% 10% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12087 atoms, of which 5807 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 Tyrosyl-DNA phosphodiesterase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	243	3905	1245	1945	336	365	14	0	4	0
1	B	244	3914	1248	1950	337	365	14	0	4	0
1	C	229	3669	1166	1838	313	340	12	0	2	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	SER	-	expression tag	UNP Q5XJA0
A	136	ASN	LEU	engineered mutation	UNP Q5XJA0
A	139	SER	ALA	engineered mutation	UNP Q5XJA0
A	239	THR	CYS	engineered mutation	UNP Q5XJA0
A	240	ARG	LYS	engineered mutation	UNP Q5XJA0
A	309	GLN	LYS	engineered mutation	UNP Q5XJA0
A	314	LEU	LYS	engineered mutation	UNP Q5XJA0
A	315	GLY	THR	engineered mutation	UNP Q5XJA0
A	316	ILE	VAL	engineered mutation	UNP Q5XJA0
A	317	THR	PRO	engineered mutation	UNP Q5XJA0
A	318	ALA	TYR	engineered mutation	UNP Q5XJA0
A	319	ALA	VAL	engineered mutation	UNP Q5XJA0
A	320	CYS	SER	engineered mutation	UNP Q5XJA0
A	321	LYS	ARG	engineered mutation	UNP Q5XJA0
A	322	LEU	CYS	engineered mutation	UNP Q5XJA0
B	120	SER	-	expression tag	UNP Q5XJA0
B	136	ASN	LEU	engineered mutation	UNP Q5XJA0
B	139	SER	ALA	engineered mutation	UNP Q5XJA0
B	239	THR	CYS	engineered mutation	UNP Q5XJA0
B	240	ARG	LYS	engineered mutation	UNP Q5XJA0
B	309	GLN	LYS	engineered mutation	UNP Q5XJA0
B	314	LEU	LYS	engineered mutation	UNP Q5XJA0
B	315	GLY	THR	engineered mutation	UNP Q5XJA0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	316	ILE	VAL	engineered mutation	UNP Q5XJA0
B	317	THR	PRO	engineered mutation	UNP Q5XJA0
B	318	ALA	TYR	engineered mutation	UNP Q5XJA0
B	319	ALA	VAL	engineered mutation	UNP Q5XJA0
B	320	CYS	SER	engineered mutation	UNP Q5XJA0
B	321	LYS	ARG	engineered mutation	UNP Q5XJA0
B	322	LEU	CYS	engineered mutation	UNP Q5XJA0
C	120	SER	-	expression tag	UNP Q5XJA0
C	136	ASN	LEU	engineered mutation	UNP Q5XJA0
C	139	SER	ALA	engineered mutation	UNP Q5XJA0
C	239	THR	CYS	engineered mutation	UNP Q5XJA0
C	240	ARG	LYS	engineered mutation	UNP Q5XJA0
C	309	GLN	LYS	engineered mutation	UNP Q5XJA0
C	314	LEU	LYS	engineered mutation	UNP Q5XJA0
C	315	GLY	THR	engineered mutation	UNP Q5XJA0
C	316	ILE	VAL	engineered mutation	UNP Q5XJA0
C	317	THR	PRO	engineered mutation	UNP Q5XJA0
C	318	ALA	TYR	engineered mutation	UNP Q5XJA0
C	319	ALA	VAL	engineered mutation	UNP Q5XJA0
C	320	CYS	SER	engineered mutation	UNP Q5XJA0
C	321	LYS	ARG	engineered mutation	UNP Q5XJA0
C	322	LEU	CYS	engineered mutation	UNP Q5XJA0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

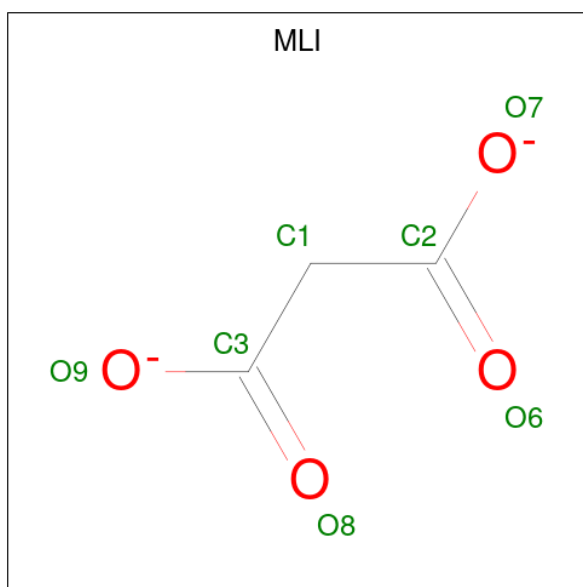
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	A	1	10	2	6	2	0	0
3	B	1	10	2	6	2	0	0
3	B	1	10	2	6	2	0	0
3	C	1	10	2	6	2	0	0
3	C	1	10	2	6	2	0	0

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	B	1	9	3	2	4	0	0

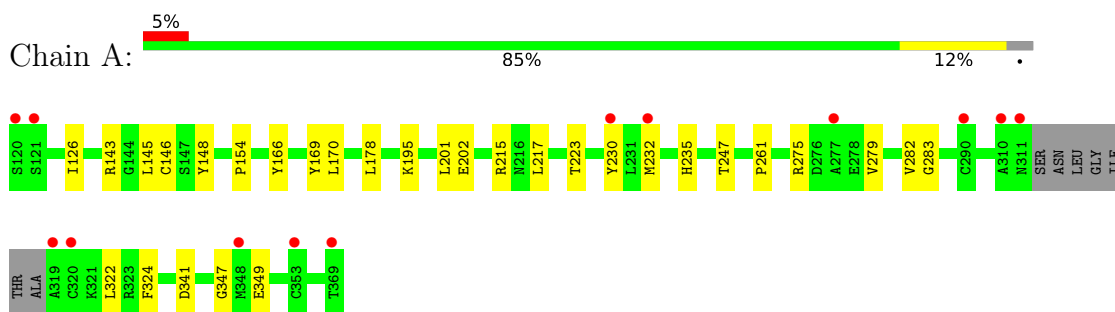
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total	O	0	0
			171	171		
5	B	142	Total	O	0	0
			142	142		
5	C	152	Total	O	0	2
			154	154		

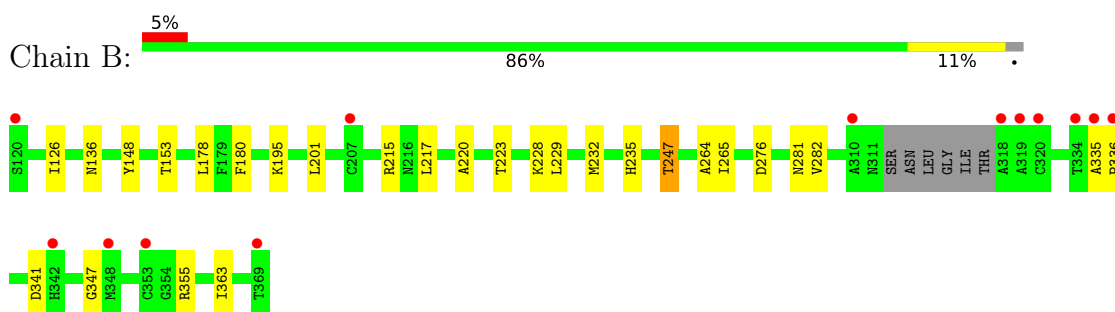
3 Residue-property plots [i](#)

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.

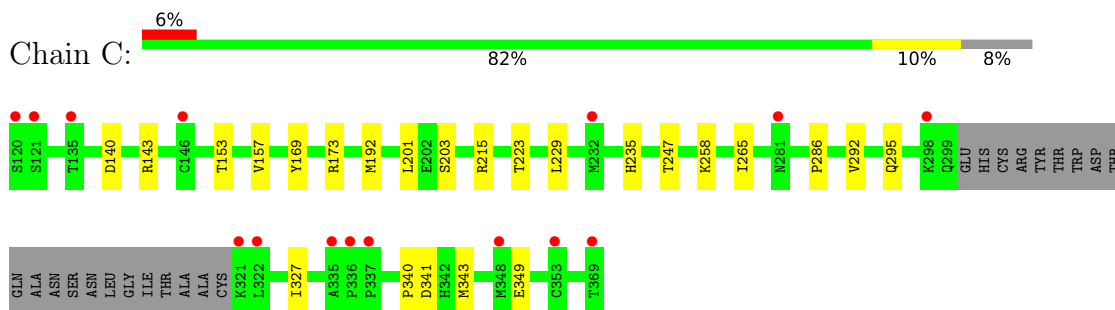
- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



- Molecule 1: Tyrosyl-DNA phosphodiesterase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 98.26Å 134.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.39 – 1.62 79.39 – 1.62	Depositor EDS
% Data completeness (in resolution range)	98.3 (79.39-1.62) 98.3 (79.39-1.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.63Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.183 , 0.209 0.186 , 0.210	Depositor DCC
R_{free} test set	4749 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtrriage
Anisotropy	0.457	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12087	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/2020	0.44	0/2732
1	B	0.23	0/2025	0.44	0/2738
1	C	0.24	0/1878	0.43	0/2537
All	All	0.23	0/5923	0.44	0/8007

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1960	1945	1925	19	0
1	B	1964	1950	1935	21	0
1	C	1831	1838	1830	17	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	32	48	48	2	0
3	B	8	12	12	0	0
3	C	8	12	12	0	0
4	B	7	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	171	0	0	1	6
5	B	142	0	0	2	2
5	C	154	0	0	3	6
All	All	6280	5807	5764	55	8

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 5.

All (55) 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:C:349:GLU:OE2	5:C:501:HOH:O	1.86	0.92
1:C:341:ASP:OD1	5:C:502:HOH:O	1.99	0.80
1:B:180[B]:PHE:CZ	1:B:220:ALA:HB2	2.25	0.71
1:B:136:ASN:O	1:B:355:ARG:NH2	2.24	0.71
1:A:341:ASP:OD2	3:A:402:EDO:O1	2.08	0.69
1:B:341:ASP:OD1	5:B:501:HOH:O	2.13	0.66
1:A:146:CYS:SG	1:A:170:LEU:HD23	2.37	0.65
1:A:283:GLY:O	5:A:501:HOH:O	2.15	0.65
1:B:276:ASP:OD2	5:B:502:HOH:O	2.15	0.64
1:C:169:TYR:OH	1:C:173:ARG:NH1	2.30	0.64
1:A:217:LEU:HD21	1:A:232:MET:HE3	1.79	0.62
1:B:217:LEU:HD21	1:B:232:MET:HE3	1.82	0.61
1:B:281:ASN:HD21	1:C:247:THR:HG21	1.69	0.58
1:A:247:THR:HG23	1:A:282:VAL:CG1	2.35	0.57
1:B:201:LEU:HD11	1:B:223:THR:HG23	1.86	0.57
1:A:217:LEU:HD21	1:A:232:MET:CE	2.37	0.55
1:B:228:LYS:HD2	1:B:264:ALA:HB2	1.88	0.55
1:C:292:VAL:HG13	1:C:340:PRO:HB3	1.89	0.53
1:A:322:LEU:HD13	1:A:324:PHE:CZ	2.44	0.53
1:B:217:LEU:HD11	1:B:232:MET:HE3	1.91	0.52
1:C:201:LEU:HD11	1:C:223:THR:HG23	1.92	0.52
1:C:153:THR:HG22	1:C:153:THR:O	2.12	0.50
1:A:201:LEU:HD11	1:A:223:THR:HG23	1.94	0.50
1:A:217:LEU:HD11	1:A:232:MET:HE2	1.93	0.49
1:B:229:LEU:HD23	1:B:265:ILE:HB	1.94	0.49
1:B:335:ALA:HB1	1:B:336:PRO:HD2	1.94	0.49
1:C:140:ASP:OD1	1:C:143:ARG:NH1	2.38	0.48
1:C:229:LEU:HD23	1:C:265:ILE:HB	1.95	0.48
1:A:178:LEU:HG	1:A:195:LYS:HG2	1.96	0.48
1:B:178:LEU:HG	1:B:195:LYS:HG2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:HG2	1:C:169:TYR:OH	2.14	0.47
1:C:169:TYR:HH	1:C:173:ARG:NH1	2.11	0.47
1:B:148:TYR:CZ	1:B:347:GLY:HA2	2.50	0.46
1:A:247:THR:HG23	1:A:282:VAL:HG13	1.98	0.46
1:B:229:LEU:CD2	1:B:265:ILE:HB	2.47	0.45
1:C:327:ILE:HD12	1:C:343:MET:HE2	1.97	0.45
1:A:143:ARG:HG3	1:A:169:TYR:OH	2.17	0.44
1:A:279:VAL:O	1:A:282:VAL:HG22	2.18	0.44
1:A:126:ILE:HD12	1:A:154:PRO:HG3	2.00	0.43
1:B:126:ILE:HA	1:B:363:ILE:O	2.18	0.43
1:A:148:TYR:CZ	1:A:347:GLY:HA2	2.54	0.43
1:B:180[B]:PHE:CE2	1:B:220:ALA:HB2	2.53	0.43
1:C:258:LYS:HD3	1:C:286:PRO:HB3	2.01	0.43
1:B:217:LEU:HD11	1:B:232:MET:CE	2.48	0.42
1:C:215:ARG:HD2	1:C:235:HIS:O	2.19	0.42
1:B:247:THR:HG23	1:B:282:VAL:HG12	2.02	0.42
1:C:295:GLN:NE2	5:C:519:HOH:O	2.53	0.42
1:A:215:ARG:HD2	1:A:235:HIS:O	2.20	0.42
1:B:215:ARG:HD2	1:B:235:HIS:O	2.20	0.42
1:A:230[A]:TYR:CE2	1:A:261:PRO:HD2	2.55	0.41
1:C:157:VAL:HB	1:C:192:MET:HB2	2.03	0.41
1:A:145:LEU:HD23	1:A:166:TYR:HE1	1.86	0.41
1:A:202:GLU:HG3	3:A:403:EDO:H21	2.03	0.41
1:B:153:THR:HG22	1:B:153:THR:O	2.22	0.40
1:B:281:ASN:ND2	1:C:247:THR:HG21	2.34	0.40

All (8) 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)
5:A:591:HOH:O	5:C:634:HOH:O[3_555]	1.89	0.31
5:A:583:HOH:O	5:C:624:HOH:O[3_655]	1.96	0.24
5:B:624:HOH:O	5:C:559:HOH:O[4_545]	1.96	0.24
5:A:515:HOH:O	5:C:624:HOH:O[3_655]	2.12	0.08
5:A:622:HOH:O	5:C:627:HOH:O[3_655]	2.13	0.07
5:B:633:HOH:O	5:C:645:HOH:O[2_554]	2.14	0.06
5:A:610:HOH:O	5:A:638:HOH:O[4_455]	2.18	0.02
1:C:203:SER:OG	5:A:501:HOH:O[3_545]	2.19	0.01

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	243/250 (97%)	239 (98%)	4 (2%)	0	100	100
1	B	244/250 (98%)	243 (100%)	1 (0%)	0	100	100
1	C	227/250 (91%)	223 (98%)	4 (2%)	0	100	100
All	All	714/750 (95%)	705 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	217/218 (100%)	215 (99%)	2 (1%)	70	54
1	B	217/218 (100%)	216 (100%)	1 (0%)	81	70
1	C	203/218 (93%)	203 (100%)	0	100	100
All	All	637/654 (97%)	634 (100%)	3 (0%)	81	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	ARG
1	A	349	GLU
1	B	247	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	B	137	ASN
1	B	368	ASN
1	C	299	GLN
1	C	368	ASN

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 [i](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\# Z > 2$
3	EDO	C	403	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	409	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	B	403	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	404	-	3,3,3	0.42	0	2,2,2	0.36	0
3	EDO	B	402	-	3,3,3	0.41	0	2,2,2	0.38	0
3	EDO	A	403	-	3,3,3	0.39	0	2,2,2	0.53	0
3	EDO	A	408	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	C	402	-	3,3,3	0.42	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	402	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	A	407	-	3,3,3	0.44	0	2,2,2	0.35	0
4	MLI	B	404	-	6,6,6	1.40	0	7,7,7	1.18	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
3	EDO	C	403	-	-	0/1/1/1	-
3	EDO	A	409	-	-	0/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	A	404	-	-	0/1/1/1	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	408	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	A	405	-	-	0/1/1/1	-
3	EDO	A	406	-	-	0/1/1/1	-
3	EDO	A	407	-	-	0/1/1/1	-
4	MLI	B	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	MLI	C2-C1-C3-O8
4	B	404	MLI	C2-C1-C3-O9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	1	0

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, 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	243/250 (97%)	0.12	13 (5%) 32 34	12, 31, 68, 93	2 (0%)
1	B	244/250 (97%)	0.26	13 (5%) 32 34	13, 37, 78, 100	2 (0%)
1	C	229/250 (91%)	0.23	15 (6%) 24 26	19, 34, 67, 111	1 (0%)
All	All	716/750 (95%)	0.20	41 (5%) 29 31	12, 34, 70, 111	5 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	CYS	4.8
1	A	319	ALA	4.8
1	C	322	LEU	4.4
1	C	348	MET	3.8
1	C	146	CYS	3.7
1	C	353	CYS	3.7
1	B	320	CYS	3.5
1	A	311	ASN	3.5
1	B	319	ALA	3.4
1	B	318	ALA	3.3
1	B	353	CYS	3.3
1	C	121	SER	3.3
1	A	369	THR	3.1
1	A	120	SER	3.0
1	A	320	CYS	2.9
1	A	348	MET	2.9
1	B	348	MET	2.8
1	B	310	ALA	2.7
1	C	120	SER	2.7
1	A	232	MET	2.7
1	B	335	ALA	2.7
1	B	120	SER	2.7
1	A	230[A]	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	321	LYS	2.6
1	C	369	THR	2.6
1	C	336	PRO	2.6
1	B	336	PRO	2.5
1	B	369	THR	2.5
1	C	232	MET	2.4
1	B	334	THR	2.3
1	A	277	ALA	2.3
1	A	353	CYS	2.3
1	A	310	ALA	2.2
1	C	335	ALA	2.2
1	C	337	PRO	2.2
1	B	342	HIS	2.2
1	C	281	ASN	2.2
1	C	298	LYS	2.1
1	A	121	SER	2.0
1	C	135	THR	2.0
1	B	207[A]	CYS	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 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
3	EDO	C	403	4/4	0.80	0.26	71,87,104,104	0
3	EDO	A	404	4/4	0.82	0.20	54,74,88,88	0
3	EDO	A	403	4/4	0.82	0.21	43,55,63,70	0
3	EDO	A	402	4/4	0.84	0.22	48,67,80,80	0
3	EDO	A	409	4/4	0.87	0.20	59,83,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	408	4/4	0.87	0.20	56,71,83,85	0
3	EDO	A	407	4/4	0.89	0.20	55,73,87,87	0
3	EDO	B	403	4/4	0.90	0.13	38,48,63,63	0
3	EDO	B	402	4/4	0.90	0.14	33,52,62,62	0
2	MG	B	401	1/1	0.91	0.09	32,32,32,32	0
3	EDO	A	405	4/4	0.91	0.13	28,47,59,59	0
2	MG	C	401	1/1	0.92	0.18	34,34,34,34	0
3	EDO	A	406	4/4	0.94	0.13	41,62,75,75	0
4	MLI	B	404	7/7	0.94	0.08	32,41,53,53	0
3	EDO	C	402	4/4	0.95	0.08	35,42,47,47	0
2	MG	A	401	1/1	0.96	0.09	38,38,38,38	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.