



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:45 AM GMT

PDB ID : 2Y70
Title : CRYSTALLOGRAPHIC STRUCTURE OF GM23, MUTANT G89D, AN EXAMPLE OF CATALYTIC MIGRATION FROM TIM TO THIAMIN PHOSPHATE SYNTHASE.
Authors : Saab-Rincon, G.; Olvera, L.; Olvera, M.; Rudino-Pinera, E.; Soberon, X.; Morett, E.
Deposited on : 2011-01-27
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

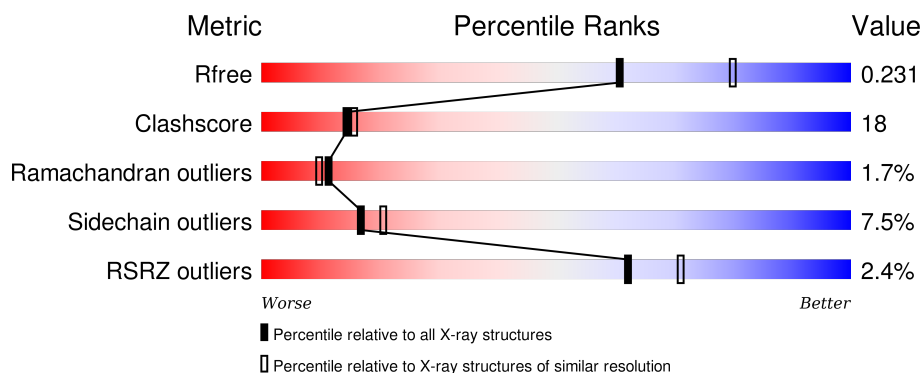
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	245	<div> <div>2%</div> <div>71% 24% 5%</div> </div>
1	B	245	<div> <div>2%</div> <div>73% 22% 5%</div> </div>
1	C	245	<div> <div>3%</div> <div>71% 23% 7%</div> </div>
1	D	245	<div> <div>2%</div> <div>69% 26% 5%</div> </div>

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
3	ACT	A	1267	-	-	X	-
3	ACT	A	1270	-	-	X	-
3	ACT	B	1267	-	-	X	-
3	ACT	B	1269	-	-	X	-
3	ACT	C	1268	-	-	X	-
3	ACT	D	1267	-	-	X	-
3	ACT	D	1268	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8064 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 TRIOSE-PHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1854	1172	327	348	7			
1	B	245	Total	C	N	O	S	0	1	0
			1859	1174	328	350	7			
1	C	245	Total	C	N	O	S	0	1	0
			1849	1166	325	351	7			
1	D	245	Total	C	N	O	S	0	0	0
			1853	1171	327	348	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	PRO	SER	ENGINEERED MUTATION	UNP P04789
A	64	SER	THR	ENGINEERED MUTATION	UNP P04789
A	65	TRP	PHE	ENGINEERED MUTATION	UNP P04789
A	66	TYR	VAL	ENGINEERED MUTATION	UNP P04789
A	67	MET	HIS	ENGINEERED MUTATION	UNP P04789
A	68	GLY	-	INSERTION	UNP P04789
A	69	ALA	-	INSERTION	UNP P04789
A	70	GLN	LEU	ENGINEERED MUTATION	UNP P04789
A	90	GLY	ILE	ENGINEERED MUTATION	UNP P04789
A	91	ASN	ALA	ENGINEERED MUTATION	UNP P04789
A	92	ALA	LYS	ENGINEERED MUTATION	UNP P04789
A	93	ASP	SER	ENGINEERED MUTATION	UNP P04789
A	.	-	GLY	DELETION	UNP P04789
A	.	-	ALA	DELETION	UNP P04789
A	.	-	PHE	DELETION	UNP P04789
A	.	-	THR	DELETION	UNP P04789
A	.	-	GLY	DELETION	UNP P04789
A	.	-	GLU	DELETION	UNP P04789
A	.	-	VAL	DELETION	UNP P04789
A	94	ALA	SER	ENGINEERED MUTATION	UNP P04789
A	96	ALA	PRO	ENGINEERED MUTATION	UNP P04789

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	SER	ILE	ENGINEERED MUTATION	UNP P04789
A	103	ILE	VAL	ENGINEERED MUTATION	UNP P04789
A	104	SER	ASN	ENGINEERED MUTATION	UNP P04789
A	109	ASP	GLY	ENGINEERED MUTATION	UNP P04789
A	150	SER	GLU	ENGINEERED MUTATION	UNP P04789
A	163	THR	ALA	ENGINEERED MUTATION	UNP P04789
A	213	VAL	ILE	ENGINEERED MUTATION	UNP P04789
A	232	ARG	LYS	ENGINEERED MUTATION	UNP P04789
A	265	GLU	GLN	ENGINEERED MUTATION	UNP P04789
B	63	PRO	SER	ENGINEERED MUTATION	UNP P04789
B	64	SER	THR	ENGINEERED MUTATION	UNP P04789
B	65	TRP	PHE	ENGINEERED MUTATION	UNP P04789
B	66	TYR	VAL	ENGINEERED MUTATION	UNP P04789
B	67	MET	HIS	ENGINEERED MUTATION	UNP P04789
B	68	GLY	-	INSERTION	UNP P04789
B	69	ALA	-	INSERTION	UNP P04789
B	70	GLN	LEU	ENGINEERED MUTATION	UNP P04789
B	90	GLY	ILE	ENGINEERED MUTATION	UNP P04789
B	91	ASN	ALA	ENGINEERED MUTATION	UNP P04789
B	92	ALA	LYS	ENGINEERED MUTATION	UNP P04789
B	93	ASP	SER	ENGINEERED MUTATION	UNP P04789
B	.	-	GLY	DELETION	UNP P04789
B	.	-	ALA	DELETION	UNP P04789
B	.	-	PHE	DELETION	UNP P04789
B	.	-	THR	DELETION	UNP P04789
B	.	-	GLY	DELETION	UNP P04789
B	.	-	GLU	DELETION	UNP P04789
B	.	-	VAL	DELETION	UNP P04789
B	94	ALA	SER	ENGINEERED MUTATION	UNP P04789
B	96	ALA	PRO	ENGINEERED MUTATION	UNP P04789
B	97	SER	ILE	ENGINEERED MUTATION	UNP P04789
B	103	ILE	VAL	ENGINEERED MUTATION	UNP P04789
B	104	SER	ASN	ENGINEERED MUTATION	UNP P04789
B	109	ASP	GLY	ENGINEERED MUTATION	UNP P04789
B	150	SER	GLU	ENGINEERED MUTATION	UNP P04789
B	163	THR	ALA	ENGINEERED MUTATION	UNP P04789
B	213	VAL	ILE	ENGINEERED MUTATION	UNP P04789
B	232	ARG	LYS	ENGINEERED MUTATION	UNP P04789
B	265	GLU	GLN	ENGINEERED MUTATION	UNP P04789
C	63	PRO	SER	ENGINEERED MUTATION	UNP P04789
C	64	SER	THR	ENGINEERED MUTATION	UNP P04789
C	65	TRP	PHE	ENGINEERED MUTATION	UNP P04789

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	TYR	VAL	ENGINEERED MUTATION	UNP P04789
C	67	MET	HIS	ENGINEERED MUTATION	UNP P04789
C	68	GLY	-	INSERTION	UNP P04789
C	69	ALA	-	INSERTION	UNP P04789
C	70	GLN	LEU	ENGINEERED MUTATION	UNP P04789
C	90	GLY	ILE	ENGINEERED MUTATION	UNP P04789
C	91	ASN	ALA	ENGINEERED MUTATION	UNP P04789
C	92	ALA	LYS	ENGINEERED MUTATION	UNP P04789
C	93	ASP	SER	ENGINEERED MUTATION	UNP P04789
C	.	-	GLY	DELETION	UNP P04789
C	.	-	ALA	DELETION	UNP P04789
C	.	-	PHE	DELETION	UNP P04789
C	.	-	THR	DELETION	UNP P04789
C	.	-	GLY	DELETION	UNP P04789
C	.	-	GLU	DELETION	UNP P04789
C	.	-	VAL	DELETION	UNP P04789
C	94	ALA	SER	ENGINEERED MUTATION	UNP P04789
C	96	ALA	PRO	ENGINEERED MUTATION	UNP P04789
C	97	SER	ILE	ENGINEERED MUTATION	UNP P04789
C	103	ILE	VAL	ENGINEERED MUTATION	UNP P04789
C	104	SER	ASN	ENGINEERED MUTATION	UNP P04789
C	109	ASP	GLY	ENGINEERED MUTATION	UNP P04789
C	150	SER	GLU	ENGINEERED MUTATION	UNP P04789
C	163	THR	ALA	ENGINEERED MUTATION	UNP P04789
C	213	VAL	ILE	ENGINEERED MUTATION	UNP P04789
C	232	ARG	LYS	ENGINEERED MUTATION	UNP P04789
C	265	GLU	GLN	ENGINEERED MUTATION	UNP P04789
D	63	PRO	SER	ENGINEERED MUTATION	UNP P04789
D	64	SER	THR	ENGINEERED MUTATION	UNP P04789
D	65	TRP	PHE	ENGINEERED MUTATION	UNP P04789
D	66	TYR	VAL	ENGINEERED MUTATION	UNP P04789
D	67	MET	HIS	ENGINEERED MUTATION	UNP P04789
D	68	GLY	-	INSERTION	UNP P04789
D	69	ALA	-	INSERTION	UNP P04789
D	70	GLN	LEU	ENGINEERED MUTATION	UNP P04789
D	90	GLY	ILE	ENGINEERED MUTATION	UNP P04789
D	91	ASN	ALA	ENGINEERED MUTATION	UNP P04789
D	92	ALA	LYS	ENGINEERED MUTATION	UNP P04789
D	93	ASP	SER	ENGINEERED MUTATION	UNP P04789
D	.	-	GLY	DELETION	UNP P04789
D	.	-	ALA	DELETION	UNP P04789
D	.	-	PHE	DELETION	UNP P04789

Continued on next page...

Continued from previous page...

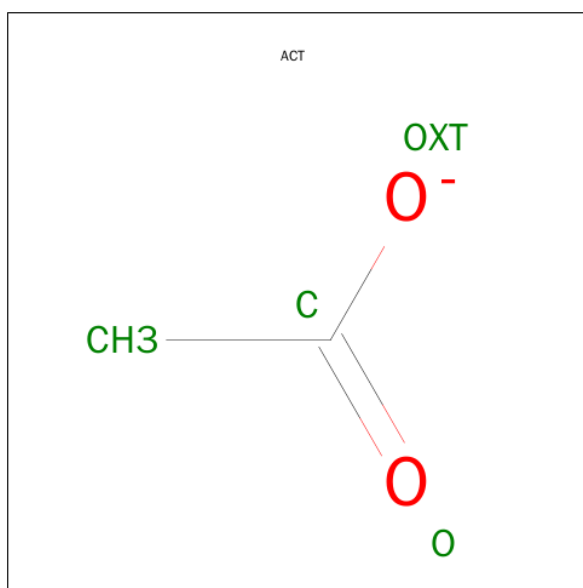
Chain	Residue	Modelled	Actual	Comment	Reference
D	.	-	THR	DELETION	UNP P04789
D	.	-	GLY	DELETION	UNP P04789
D	.	-	GLU	DELETION	UNP P04789
D	.	-	VAL	DELETION	UNP P04789
D	94	ALA	SER	ENGINEERED MUTATION	UNP P04789
D	96	ALA	PRO	ENGINEERED MUTATION	UNP P04789
D	97	SER	ILE	ENGINEERED MUTATION	UNP P04789
D	103	ILE	VAL	ENGINEERED MUTATION	UNP P04789
D	104	SER	ASN	ENGINEERED MUTATION	UNP P04789
D	109	ASP	GLY	ENGINEERED MUTATION	UNP P04789
D	150	SER	GLU	ENGINEERED MUTATION	UNP P04789
D	163	THR	ALA	ENGINEERED MUTATION	UNP P04789
D	213	VAL	ILE	ENGINEERED MUTATION	UNP P04789
D	232	ARG	LYS	ENGINEERED MUTATION	UNP P04789
D	265	GLU	GLN	ENGINEERED MUTATION	UNP P04789

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			3	1	2		

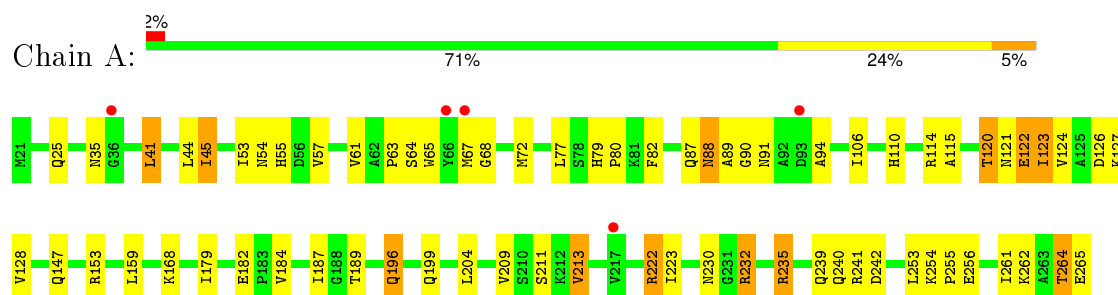
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		
4	B	151	Total	O	0	0
			151	151		
4	C	120	Total	O	0	0
			120	120		
4	D	122	Total	O	0	0
			122	122		

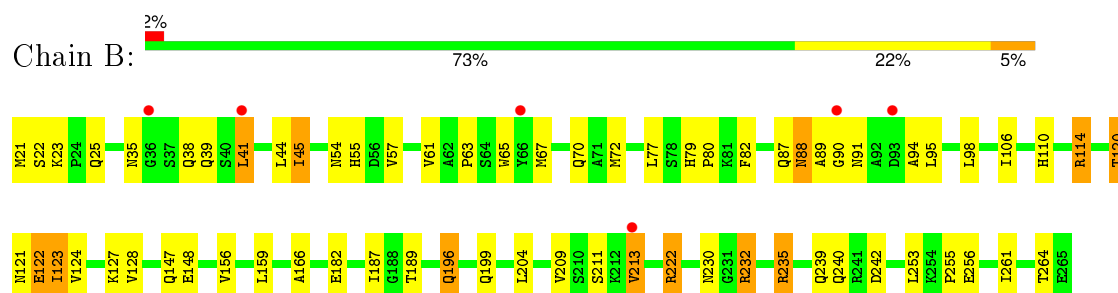
3 Residue-property plots

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.

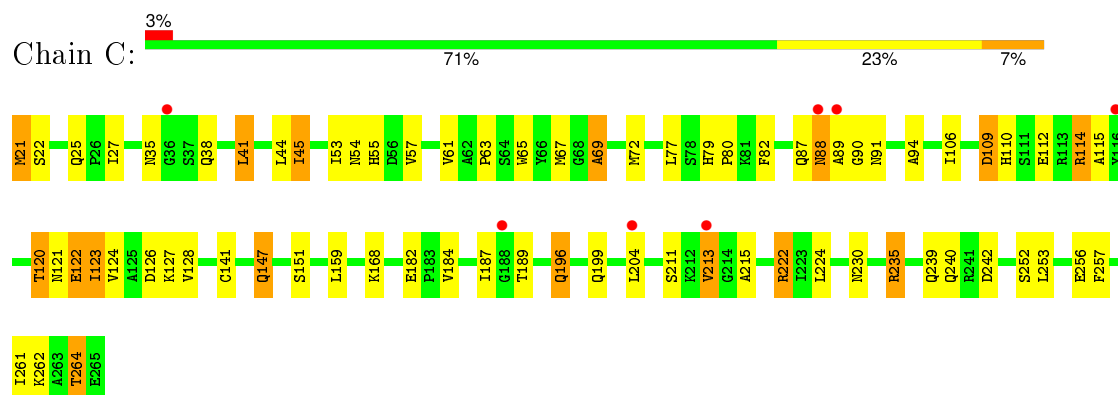
• Molecule 1: TRIOSE-PHOSPHATE ISOMERASE



• Molecule 1: TRIOSE-PHOSPHATE ISOMERASE

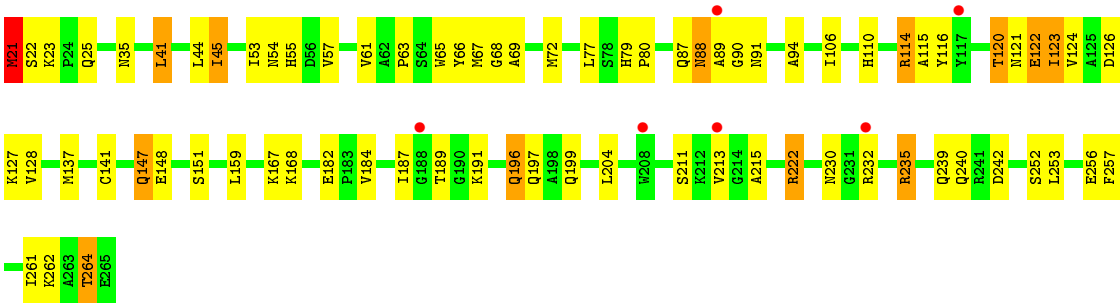


• Molecule 1: TRIOSE-PHOSPHATE ISOMERASE



• Molecule 1: TRIOSE-PHOSPHATE ISOMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	109.44Å 109.44Å 95.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.45 – 2.30 67.18 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.45-2.30) 98.5 (67.18-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.199 , 0.230 0.188 , 0.231	Depositor DCC
R_{free} test set	2824 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.4	EDS
Estimated twinning fraction	0.017 for -h,-k,l 0.477 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 55847 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8064	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, ACT

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	0.44	0/1888	0.80	6/2562 (0.2%)
1	B	0.43	0/1893	0.72	5/2570 (0.2%)
1	C	0.42	0/1883	0.65	2/2559 (0.1%)
1	D	0.42	0/1887	0.73	3/2560 (0.1%)
All	All	0.43	0/7551	0.72	16/10251 (0.2%)

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	D	0	1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	ARG	NE-CZ-NH2	-15.34	112.63	120.30
1	A	232	ARG	NE-CZ-NH2	-15.26	112.67	120.30
1	B	114	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	A	232	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	D	114	ARG	NE-CZ-NH1	13.38	126.99	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	21	MET	Peptide

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	1854	0	1866	70	0
1	B	1859	0	1862	61	0
1	C	1849	0	1832	68	0
1	D	1853	0	1862	70	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	24	0	18	12	0
3	B	20	0	15	8	0
3	C	8	0	6	8	0
3	D	15	0	9	7	0
4	A	169	0	0	7	0
4	B	151	0	0	8	0
4	C	120	0	0	5	0
4	D	122	0	0	7	0
All	All	8064	0	7470	270	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 18.

The worst 5 of 270 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:232:ARG:HH12	3:B:1267:ACT:H2	1.12	1.05
1:D:120:THR:HG22	1:D:123:ILE:H	1.24	1.02
1:A:54:ASN:H	3:A:1270:ACT:H1	1.24	1.02
1:C:120:THR:HG22	1:C:123:ILE:H	1.24	1.01
1:B:25:GLN:HE21	1:B:222:ARG:HH21	1.04	1.01

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	243/245 (99%)	235 (97%)	5 (2%)	3 (1%)	16	16
1	B	244/245 (100%)	236 (97%)	4 (2%)	4 (2%)	12	11
1	C	244/245 (100%)	235 (96%)	4 (2%)	5 (2%)	9	7
1	D	243/245 (99%)	234 (96%)	4 (2%)	5 (2%)	9	7
All	All	974/980 (99%)	940 (96%)	17 (2%)	17 (2%)	11	10

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	B	22	SER
1	B	91	ASN
1	C	91	ASN
1	D	22	SER

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	192/192 (100%)	179 (93%)	13 (7%)	20	25
1	B	192/192 (100%)	178 (93%)	14 (7%)	17	22
1	C	190/192 (99%)	173 (91%)	17 (9%)	12	14
1	D	192/192 (100%)	177 (92%)	15 (8%)	16	19
All	All	766/768 (100%)	707 (92%)	59 (8%)	17	20

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	235	ARG
1	C	120	THR
1	D	211	SER
1	C	21	MET
1	C	45	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	C	25	GLN
1	D	197	GLN
1	B	88	ASN
1	B	199	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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	SO4	A	1266	-	4,4,4	0.32	0	6,6,6	0.19	0
3	ACT	A	1267	-	1,3,3	2.47	1 (100%)	0,3,3	0.00	-
3	ACT	A	1268	-	1,3,3	3.29	1 (100%)	0,3,3	0.00	-
3	ACT	A	1269	-	1,3,3	3.17	1 (100%)	0,3,3	0.00	-
3	ACT	A	1270	-	1,3,3	3.45	1 (100%)	0,3,3	0.00	-
3	ACT	A	1271	-	1,3,3	3.04	1 (100%)	0,3,3	0.00	-
3	ACT	A	1272	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
2	SO4	B	1266	-	4,4,4	0.30	0	6,6,6	0.36	0
3	ACT	B	1267	-	1,3,3	3.11	1 (100%)	0,3,3	0.00	-
3	ACT	B	1268	-	1,3,3	3.37	1 (100%)	0,3,3	0.00	-
3	ACT	B	1269	-	1,3,3	3.56	1 (100%)	0,3,3	0.00	-
3	ACT	B	1270	-	1,3,3	3.16	1 (100%)	0,3,3	0.00	-
3	ACT	B	1271	-	1,3,3	3.36	1 (100%)	0,3,3	0.00	-
2	SO4	C	1266	-	4,4,4	0.16	0	6,6,6	0.88	1 (16%)
3	ACT	C	1267	-	1,3,3	3.23	1 (100%)	0,3,3	0.00	-
3	ACT	C	1268	-	1,3,3	2.63	1 (100%)	0,3,3	0.00	-
2	SO4	D	1266	-	4,4,4	0.37	0	6,6,6	0.68	0
3	ACT	D	1267	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
3	ACT	D	1268	-	1,3,3	3.08	1 (100%)	0,3,3	0.00	-
3	ACT	D	1269	-	1,3,3	3.26	1 (100%)	0,3,3	0.00	-
3	ACT	D	1270	-	0,2,3	0.00	-	0,1,3	0.00	-

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	SO4	A	1266	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1267	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1268	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1269	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1270	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1271	-	-	0/0/0/0	0/0/0/0
3	ACT	A	1272	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1266	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1267	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1268	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1269	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	B	1270	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1271	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1266	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1267	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1268	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1266	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1267	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1268	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1269	-	-	0/0/0/0	0/0/0/0
3	ACT	D	1270	-	-	0/0/0/0	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1267	ACT	CH3-C	2.47	1.52	1.48
3	C	1268	ACT	CH3-C	2.63	1.52	1.48
3	A	1272	ACT	CH3-C	2.68	1.52	1.48
3	D	1267	ACT	CH3-C	2.78	1.52	1.48
3	A	1271	ACT	CH3-C	3.04	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1266	SO4	O2-S-O1	2.03	115.93	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1267	ACT	5	0
3	A	1270	ACT	6	0
3	A	1271	ACT	1	0
3	B	1267	ACT	5	0
3	B	1269	ACT	3	0
3	C	1267	ACT	1	0
3	C	1268	ACT	7	0
3	D	1267	ACT	2	0
3	D	1268	ACT	4	0
3	D	1269	ACT	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 [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	245/245 (100%)	-0.10	5 (2%) 68 75	25, 43, 90, 139	0
1	B	245/245 (100%)	-0.11	6 (2%) 62 71	26, 43, 87, 118	0
1	C	245/245 (100%)	0.01	7 (2%) 55 64	26, 46, 91, 124	0
1	D	245/245 (100%)	0.01	6 (2%) 62 71	27, 46, 88, 124	0
All	All	980/980 (100%)	-0.05	24 (2%) 62 71	25, 45, 92, 139	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLY	4.3
1	A	36	GLY	3.8
1	C	188	GLY	3.6
1	C	88	ASN	3.3
1	A	66	TYR	3.1

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
3	ACT	A	1270	4/4	0.97	0.14	0.56	34,49,51,73	0
2	SO4	C	1266	5/5	0.98	0.14	0.14	30,37,68,70	0
2	SO4	A	1266	5/5	0.99	0.11	0.02	44,45,49,56	0
2	SO4	B	1266	5/5	0.99	0.11	-0.18	40,42,52,54	0
2	SO4	D	1266	5/5	0.98	0.10	-0.41	27,40,67,69	0
3	ACT	B	1267	4/4	0.97	0.12	-0.73	45,52,63,81	0
3	ACT	B	1271	4/4	0.91	0.13	-0.88	33,65,68,70	0
3	ACT	D	1268	4/4	0.97	0.11	-1.22	35,41,51,57	0
3	ACT	A	1271	4/4	0.96	0.08	-1.63	48,53,56,69	0
3	ACT	A	1272	4/4	0.97	0.11	-1.63	47,55,58,71	0
3	ACT	C	1268	4/4	0.97	0.10	-1.71	27,45,46,52	0
3	ACT	D	1267	4/4	0.98	0.13	-	39,44,51,58	0
3	ACT	B	1269	4/4	0.91	0.13	-	45,64,66,68	0
3	ACT	A	1267	4/4	0.96	0.17	-	29,43,60,61	0
3	ACT	D	1270	3/4	0.77	0.12	-	55,55,70,75	0
3	ACT	B	1268	4/4	0.95	0.13	-	47,52,56,58	0
3	ACT	C	1267	4/4	0.97	0.14	-	46,48,50,61	0
3	ACT	B	1270	4/4	0.96	0.10	-	41,51,58,70	0
3	ACT	D	1269	4/4	0.95	0.10	-	54,62,73,87	0
3	ACT	A	1268	4/4	0.95	0.13	-	52,53,59,66	0
3	ACT	A	1269	4/4	0.97	0.10	-	36,50,52,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.