



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 10:17 AM EDT

PDB ID : 5CKX
Title : Non-covalent complex of DAHP synthase and chorismate mutase from Mycobacterium tuberculosis with bound transition state analog and feedback effectors tyrosine and phenylalanine
Authors : Munack, S.; Okvist, M.; Krengel, U.
Deposited on : 2015-07-15
Resolution : 2.70 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

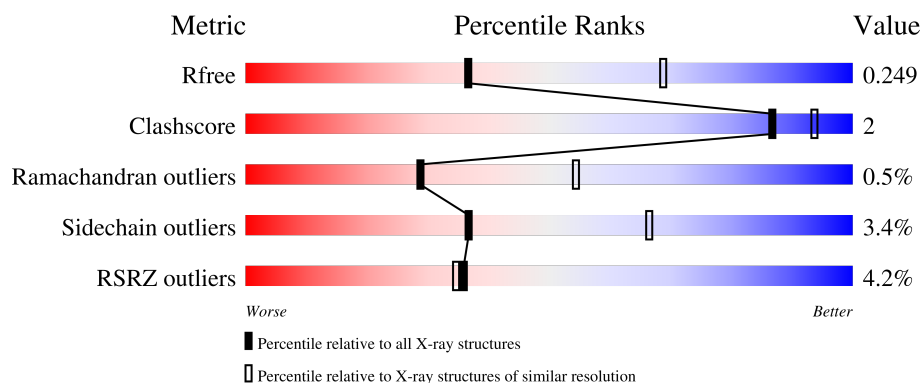
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	472	<div> <div>0%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	B	472	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>1%</div> </div>
2	C	90	<div> <div>12%</div> <div>83%</div> <div>13%</div> <div>2%</div> </div>
2	D	90	<div> <div>14%</div> <div>76%</div> <div>11%</div> <div>12%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16525 atoms, of which 8201 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 Phospho-2-dehydro-3-deoxyheptonate aldolase AroG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	0	0	0
			6832	2147	3392	624	652	17			
1	B	452	Total	C	H	N	O	S	0	0	0
			6896	2170	3422	630	656	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP O53512
A	-8	HIS	-	expression tag	UNP O53512
A	-7	HIS	-	expression tag	UNP O53512
A	-6	HIS	-	expression tag	UNP O53512
A	-5	HIS	-	expression tag	UNP O53512
A	-4	HIS	-	expression tag	UNP O53512
A	-3	HIS	-	expression tag	UNP O53512
A	-2	SER	-	expression tag	UNP O53512
A	-1	SER	-	expression tag	UNP O53512
A	0	GLY	-	expression tag	UNP O53512
B	-9	MET	-	initiating methionine	UNP O53512
B	-8	HIS	-	expression tag	UNP O53512
B	-7	HIS	-	expression tag	UNP O53512
B	-6	HIS	-	expression tag	UNP O53512
B	-5	HIS	-	expression tag	UNP O53512
B	-4	HIS	-	expression tag	UNP O53512
B	-3	HIS	-	expression tag	UNP O53512
B	-2	SER	-	expression tag	UNP O53512
B	-1	SER	-	expression tag	UNP O53512
B	0	GLY	-	expression tag	UNP O53512

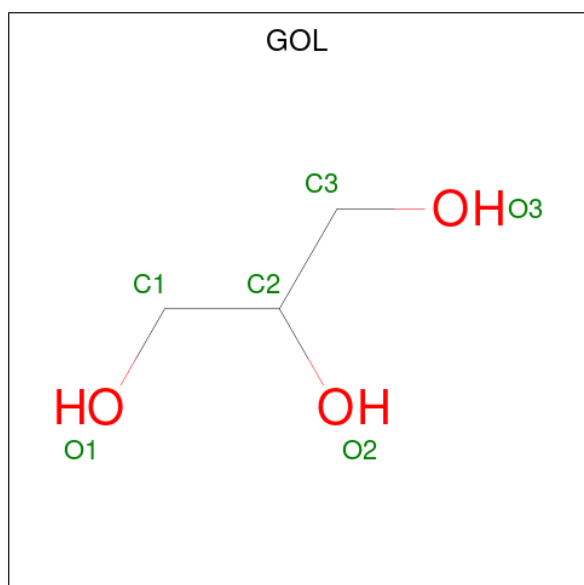
- Molecule 2 is a protein called Intracellular chorismate mutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	78	Total	C	H	N	O	S	0	0	0
			1261	377	650	120	112	2			
2	D	79	Total	C	H	N	O	S	0	0	0
			1269	380	653	121	113	2			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

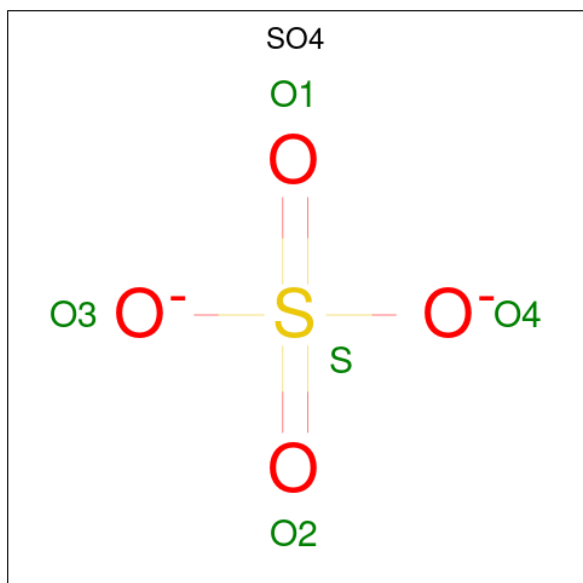


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

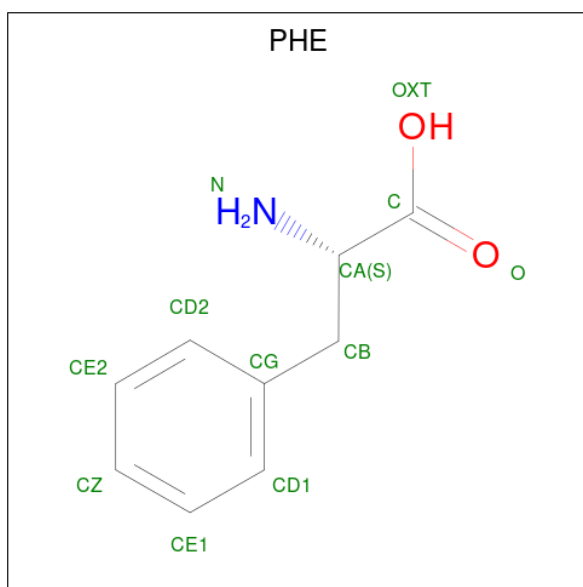
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



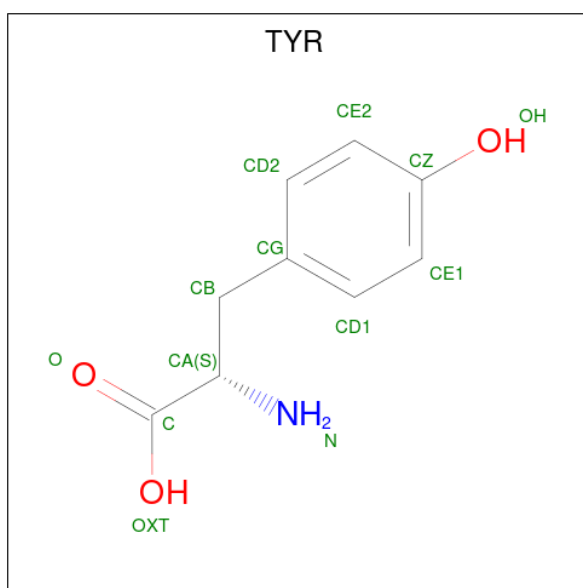
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			20	9	8	1	2		
7	B	1	Total	C	H	N	O	0	0
			20	9	8	1	2		

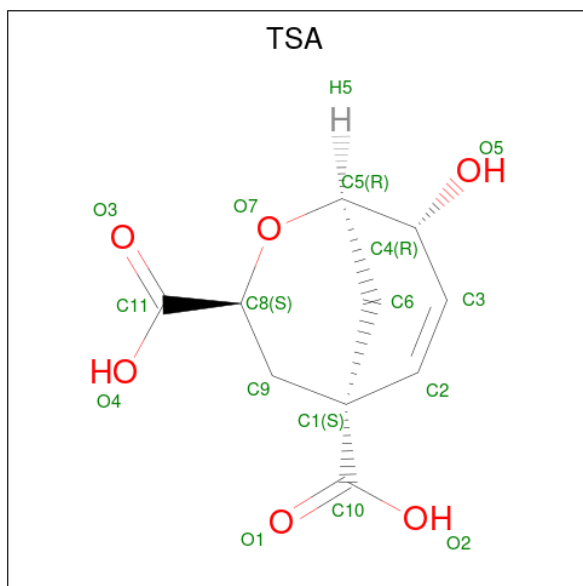
- Molecule 8 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			21	9	8	1	3		

- Molecule 9 is 8-HYDROXY-2-OXA-BICYCLO[3.3.1]NON-6-ENE-3,5-DICARBOXYLIC

ACID (three-letter code: TSA) (formula: C₁₀H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			26	10	10	6		
9	D	1	Total	C	H	O	0	0
			26	10	10	6		

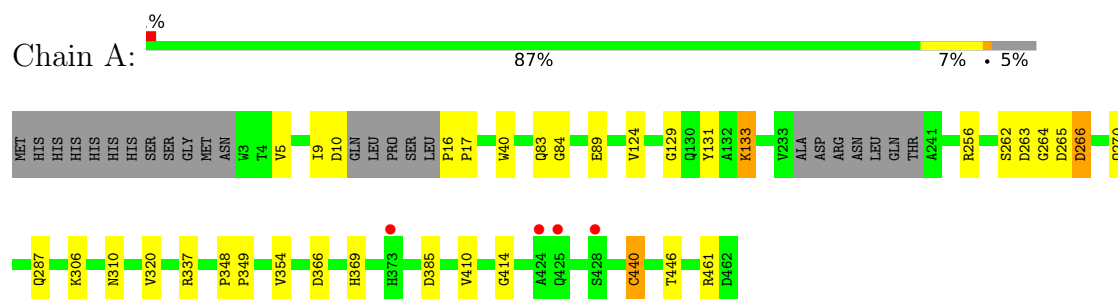
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	17	Total	O	0	0
			17	17		
10	B	22	Total	O	0	0
			22	22		

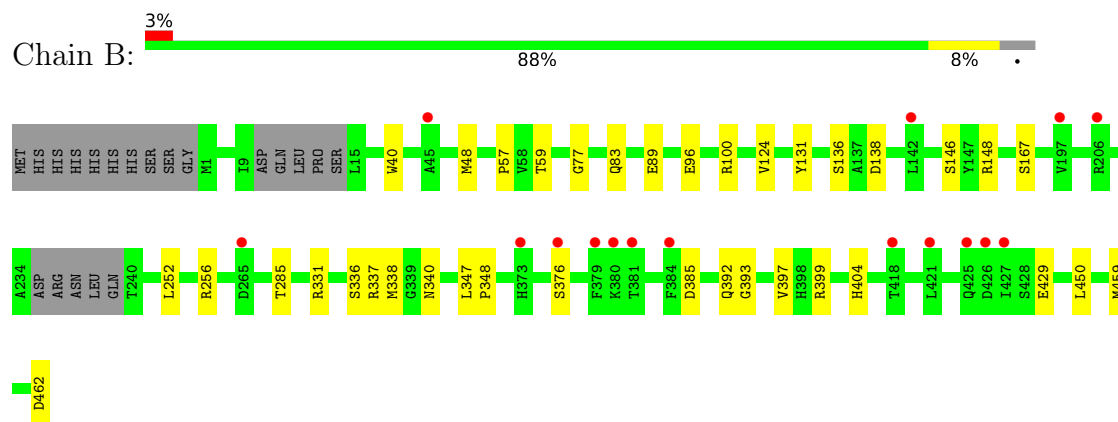
3 Residue-property plots

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.

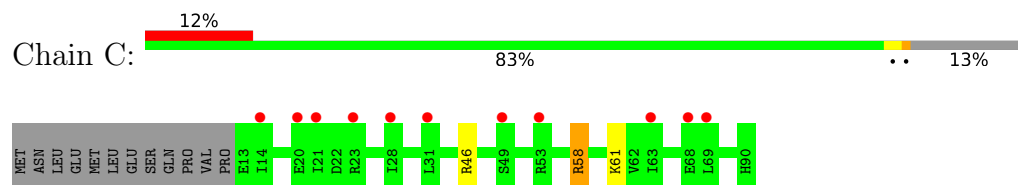
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase AroG



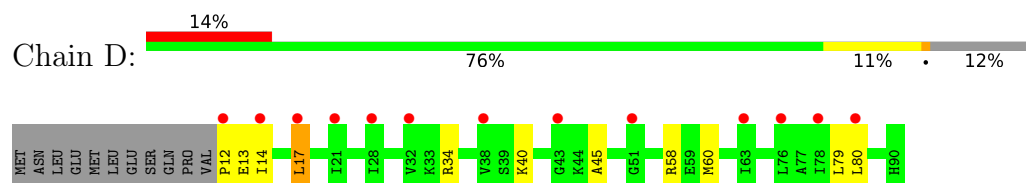
- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase AroG



- Molecule 2: Intracellular chorismate mutase



- Molecule 2: Intracellular chorismate mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.40Å 203.40Å 67.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.72 – 2.70 88.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (58.72-2.70) 98.3 (88.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.200 , 0.248 0.200 , 0.249	Depositor DCC
R_{free} test set	2173 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16525	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: TSA, MN, SO4, CL, GOL

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	0.28	0/3509	0.47	0/4770
1	B	0.30	0/3545	0.48	0/4821
2	C	0.24	0/614	0.43	0/816
2	D	0.26	0/619	0.48	0/823
All	All	0.29	0/8287	0.48	0/11230

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	3440	3392	3388	16	0
1	B	3474	3422	3423	16	0
2	C	611	650	650	2	0
2	D	616	653	652	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	6	8	8	0	0
4	B	18	24	24	0	0
4	D	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	20	0	0	1	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	A	12	8	8	0	0
7	B	12	8	8	0	0
8	B	13	8	8	0	0
9	C	16	10	10	1	0
9	D	16	10	10	0	0
10	A	17	0	0	0	0
10	B	22	0	0	0	0
All	All	8324	8201	8197	35	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 2.

All (35) 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:133:LYS:NZ	1:A:440:CYS:SG	2.57	0.76
1:A:306:LYS:NZ	1:A:366:ASP:OD2	2.22	0.72
1:B:399:ARG:NH2	1:B:459:MET:O	2.27	0.68
2:C:46:ARG:NH1	9:C:102:TSA:O4	2.31	0.63
1:B:376:SER:OG	1:B:429:GLU:OE1	2.23	0.57
2:C:58:ARG:O	2:C:61:LYS:N	2.37	0.56
1:A:5:VAL:HG21	1:B:48:MET:HE1	1.87	0.56
1:A:262:SER:O	1:A:270:GLN:N	2.39	0.55
1:A:337:ARG:NH2	1:A:369:HIS:O	2.38	0.54
1:A:266:ASP:OD2	1:A:270:GLN:NE2	2.41	0.53
1:B:138:ASP:OD1	1:B:148:ARG:NH2	2.42	0.53
1:B:96:GLU:OE2	1:B:100:ARG:NH1	2.42	0.51
1:B:83:GLN:HA	1:B:124:VAL:O	2.14	0.48
1:B:252:LEU:O	1:B:256:ARG:HG3	2.14	0.47
1:B:393:GLY:O	1:B:397:VAL:HG12	2.15	0.46
1:B:347:LEU:N	1:B:348:PRO:CD	2.79	0.46
1:A:84:GLY:HA2	1:A:410:VAL:O	2.15	0.46
1:A:264:GLY:O	1:A:266:ASP:N	2.48	0.46
1:A:320:VAL:HG21	1:A:354:VAL:HG13	1.99	0.45
1:A:414:GLY:O	1:A:446:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:HB3	1:A:131:TYR:CE1	2.52	0.45
1:A:16:PRO:N	1:A:17:PRO:CD	2.81	0.43
1:B:48:MET:SD	1:B:167:SER:HA	2.57	0.43
6:A:508:SO4:O4	1:B:100:ARG:NH2	2.52	0.43
1:B:89:GLU:HB3	1:B:131:TYR:CE1	2.53	0.43
1:B:340:ASN:OD1	1:B:340:ASN:N	2.51	0.43
1:B:347:LEU:HD23	1:B:397:VAL:HG11	2.01	0.43
2:D:12:PRO:O	2:D:13:GLU:HB3	2.19	0.43
1:A:83:GLN:HA	1:A:124:VAL:O	2.19	0.42
1:B:57:PRO:HB2	1:B:59:THR:O	2.20	0.41
1:A:16:PRO:N	1:A:17:PRO:HD3	2.35	0.41
1:B:77:GLY:HA2	1:B:404:HIS:CD2	2.55	0.41
1:A:348:PRO:N	1:A:349:PRO:HD2	2.34	0.41
2:D:17:LEU:H	2:D:17:LEU:HD12	1.85	0.41
1:A:9:ILE:HG22	1:A:10:ASP:N	2.37	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	442/472 (94%)	413 (93%)	25 (6%)	4 (1%)	17	40
1	B	446/472 (94%)	425 (95%)	21 (5%)	0	100	100
2	C	76/90 (84%)	66 (87%)	10 (13%)	0	100	100
2	D	77/90 (86%)	71 (92%)	5 (6%)	1 (1%)	12	30
All	All	1041/1124 (93%)	975 (94%)	61 (6%)	5 (0%)	29	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	CYS
2	D	45	ALA
1	A	265	ASP
1	A	266	ASP
1	A	129	GLY

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	362/385 (94%)	354 (98%)	8 (2%)	52	79
1	B	365/385 (95%)	353 (97%)	12 (3%)	38	67
2	C	63/75 (84%)	62 (98%)	1 (2%)	62	85
2	D	63/75 (84%)	55 (87%)	8 (13%)	4	10
All	All	853/920 (93%)	824 (97%)	29 (3%)	37	66

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	TRP
1	A	133	LYS
1	A	256	ARG
1	A	263	ASP
1	A	287	GLN
1	A	310	ASN
1	A	385	ASP
1	A	461	ARG
1	B	40	TRP
1	B	136	SER
1	B	146	SER
1	B	285	THR
1	B	331	ARG
1	B	336	SER
1	B	337	ARG
1	B	338	MET
1	B	385	ASP

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Mol	Chain	Res	Type
1	B	392	GLN
1	B	450	LEU
1	B	462	ASP
2	C	58	ARG
2	D	14	ILE
2	D	17	LEU
2	D	34	ARG
2	D	40	LYS
2	D	58	ARG
2	D	60	MET
2	D	79	LEU
2	D	80	LEU

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

Mol	Chain	Res	Type
1	B	404	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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	$\# Z > 2$
4	GOL	B	502	-	5,5,5	0.46	0	5,5,5	0.31	0
6	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.10	0
6	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.07	0
4	GOL	D	101	-	5,5,5	0.39	0	5,5,5	0.19	0
7	PHE	A	509	-	11,12,12	0.69	1 (9%)	14,15,15	1.04	2 (14%)
8	TYR	B	509	-	12,13,13	0.73	1 (8%)	16,17,17	0.96	2 (12%)
4	GOL	B	504	-	5,5,5	0.36	0	5,5,5	0.30	0
9	TSA	C	102	-	16,17,17	1.08	1 (6%)	16,26,26	1.53	4 (25%)
4	GOL	A	502	-	5,5,5	0.33	0	5,5,5	0.48	0
9	TSA	D	103	-	16,17,17	1.07	1 (6%)	16,26,26	1.33	2 (12%)
6	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.09	0
6	SO4	D	102	-	4,4,4	0.12	0	6,6,6	0.11	0
6	SO4	B	506	-	4,4,4	0.12	0	6,6,6	0.13	0
6	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.09	0
7	PHE	B	508	-	11,12,12	0.67	0	14,15,15	0.84	2 (14%)
6	SO4	C	101	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.10	0
4	GOL	B	503	-	5,5,5	0.45	0	5,5,5	0.43	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
4	GOL	B	502	-	-	2/4/4/4	-
7	PHE	A	509	-	-	0/8/8/8	0/1/1/1
8	TYR	B	509	-	-	0/8/8/8	0/1/1/1
4	GOL	D	101	-	-	0/4/4/4	-
9	TSA	C	102	-	-	1/10/34/34	1/3/2/2
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
9	TSA	D	103	-	-	2/10/34/34	1/3/2/2
7	PHE	B	508	-	-	0/8/8/8	0/1/1/1
4	GOL	B	503	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	509	PHE	OXT-C	-2.12	1.23	1.30
9	C	102	TSA	C6-C1	-2.12	1.52	1.55
9	D	103	TSA	C6-C1	-2.10	1.52	1.55
8	B	509	TYR	OXT-C	-2.07	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	102	TSA	C5-C4-C3	3.27	113.71	109.05
7	A	509	PHE	OXT-C-O	-2.93	117.44	124.09
8	B	509	TYR	OXT-C-O	-2.92	117.46	124.09
9	D	103	TSA	C5-C4-C3	2.85	113.11	109.05
7	A	509	PHE	OXT-C-CA	2.42	121.63	113.38
9	C	102	TSA	O7-C8-C9	2.39	113.45	109.92
8	B	509	TYR	OXT-C-CA	2.32	121.27	113.38
7	B	508	PHE	OXT-C-O	-2.21	119.07	124.09
9	C	102	TSA	O4-C11-C8	2.20	119.31	113.03
9	C	102	TSA	O7-C8-C11	2.20	112.00	107.70
9	D	103	TSA	O4-C11-C8	2.18	119.26	113.03
7	B	508	PHE	OXT-C-CA	2.10	120.53	113.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	B	504	GOL	O1-C1-C2-O2
4	B	504	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
4	A	502	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
9	D	103	TSA	O3-C11-C8-O7
9	D	103	TSA	C9-C1-C10-O1
9	C	102	TSA	O3-C11-C8-O7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	103	TSA	C1-C2-C3-C4-C5-C8-C9-O7
9	C	102	TSA	C1-C2-C3-C4-C5-C8-C9-O7

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	102	TSA	1	0
6	A	508	SO4	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	448/472 (94%)	0.33	4 (0%) 84 85	32, 59, 99, 174	0
1	B	452/472 (95%)	0.35	16 (3%) 44 44	29, 52, 106, 137	0
2	C	78/90 (86%)	1.31	11 (14%) 2 1	68, 93, 113, 120	0
2	D	79/90 (87%)	1.00	13 (16%) 1 1	56, 80, 105, 122	0
All	All	1057/1124 (94%)	0.46	44 (4%) 36 35	29, 60, 107, 174	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	ASP	5.7
2	C	14	ILE	5.0
2	C	69	LEU	4.5
2	C	21	ILE	3.8
2	D	12	PRO	3.7
1	B	381	THR	3.6
2	C	31	LEU	3.5
2	D	14	ILE	3.4
1	B	376	SER	3.3
1	B	418	THR	3.2
1	B	197	VAL	3.1
2	C	23	ARG	3.1
1	A	428	SER	3.0
2	D	43	GLY	3.0
1	B	206	ARG	2.9
1	B	421	LEU	2.9
2	D	17	LEU	2.8
1	B	373	HIS	2.7
2	C	28	ILE	2.7
1	B	380	LYS	2.6
2	D	28	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	80	LEU	2.6
1	A	373	HIS	2.5
2	C	68	GLU	2.5
1	B	427	ILE	2.5
2	C	63	ILE	2.5
1	B	379	PHE	2.5
1	B	142	LEU	2.5
2	D	38	VAL	2.4
1	A	425	GLN	2.4
1	B	265	ASP	2.3
2	D	78	ILE	2.3
2	D	51	GLY	2.2
2	D	76	LEU	2.2
1	B	425	GLN	2.2
2	C	20	GLU	2.2
2	D	32	VAL	2.2
2	D	63	ILE	2.2
2	C	53	ARG	2.2
2	D	21	ILE	2.2
2	C	49	SER	2.1
1	B	45	ALA	2.1
1	B	384	PHE	2.0
1	A	424	ALA	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	B	501	1/1	0.73	0.19	92,92,92,92	0
4	GOL	D	101	6/6	0.75	0.38	74,90,113,113	0
6	SO4	A	506	5/5	0.76	0.20	79,87,106,111	0
6	SO4	C	101	5/5	0.83	0.26	78,101,105,119	5
6	SO4	B	507	5/5	0.85	0.14	89,104,116,121	0
9	TSA	C	102	16/16	0.86	0.29	83,98,117,118	0
6	SO4	A	507	5/5	0.89	0.14	85,87,99,103	5
4	GOL	B	504	6/6	0.91	0.25	38,50,60,62	0
9	TSA	D	103	16/16	0.91	0.23	70,82,99,101	0
6	SO4	D	102	5/5	0.92	0.17	73,74,81,88	5
5	CL	A	503	1/1	0.93	0.29	71,71,71,71	0
3	MN	A	501	1/1	0.94	0.13	79,79,79,79	0
8	TYR	B	509	13/13	0.95	0.20	42,47,55,66	0
5	CL	A	504	1/1	0.95	0.08	73,73,73,73	0
7	PHE	B	508	12/12	0.95	0.21	35,47,56,61	0
5	CL	B	505	1/1	0.96	0.24	53,53,53,53	0
4	GOL	B	503	6/6	0.96	0.22	33,45,56,59	0
6	SO4	A	508	5/5	0.97	0.19	42,58,66,73	5
6	SO4	A	505	5/5	0.97	0.18	71,74,87,87	0
4	GOL	A	502	6/6	0.97	0.19	41,53,64,64	0
4	GOL	B	502	6/6	0.97	0.14	33,48,58,58	0
6	SO4	B	506	5/5	0.98	0.17	37,51,68,78	0
7	PHE	A	509	12/12	0.98	0.20	37,45,56,56	0

6.5 Other polymers

There are no such residues in this entry.