



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 01:58 PM UTC

PDB ID : 4EFK / pdb_00004efk
Title : Pantothenate synthetase in complex with N,N-DIMETHYLTHIOPHENE-3-SULFONAMIDE
Authors : Ciulli, A.; Silvestre, H.L.; Blundell, T.L.; Abell, C.
Deposited on : 2012-03-29
Resolution : 1.70 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	:	4-5-2 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

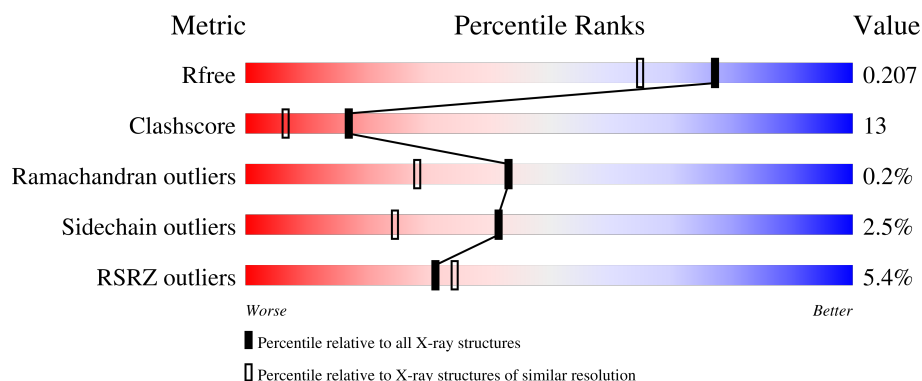
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

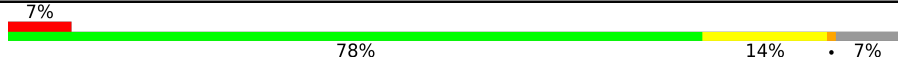
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	300	
1	B	300	

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
2	0OC	A	401	-	X	-	-
2	0OC	B	401	-	X	-	-
3	GOL	B	404	-	-	X	-
4	EOH	A	405	-	-	X	-
4	EOH	A	407	-	-	X	-
4	EOH	B	406	-	-	X	-
4	EOH	B	407	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4718 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.

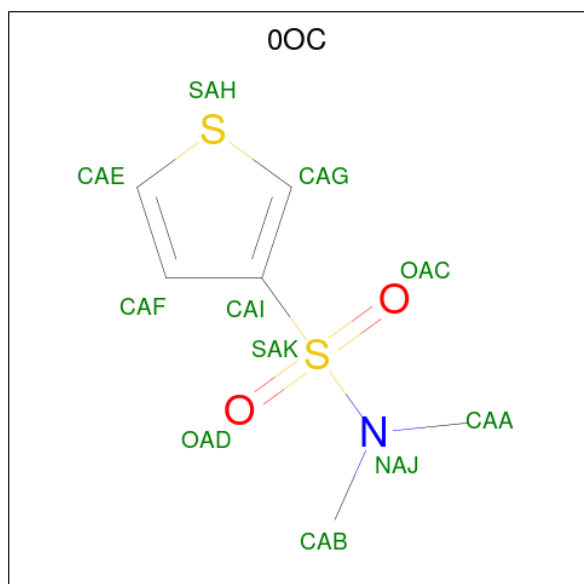
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	13	0
			2163	1367	395	395	6			
1	B	274	Total	C	N	O	S	0	8	0
			2082	1315	381	381	5			

There are 4 discrepancies between the modelled and reference sequences:

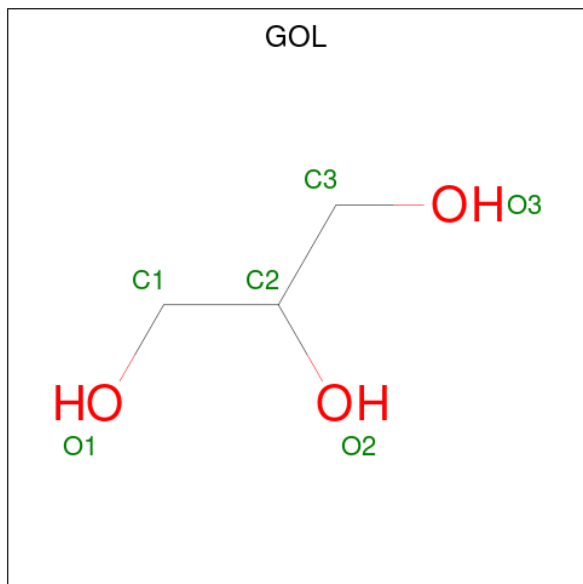
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P0A5R0
A	77	GLY	GLU	engineered mutation	UNP P0A5R0
B	2	ALA	THR	engineered mutation	UNP P0A5R0
B	77	GLY	GLU	engineered mutation	UNP P0A5R0

- Molecule 2 is N,N-dimethylthiophene-3-sulfonamide (CCD ID: 0OC) (formula: C₆H₉NO₂S₂).



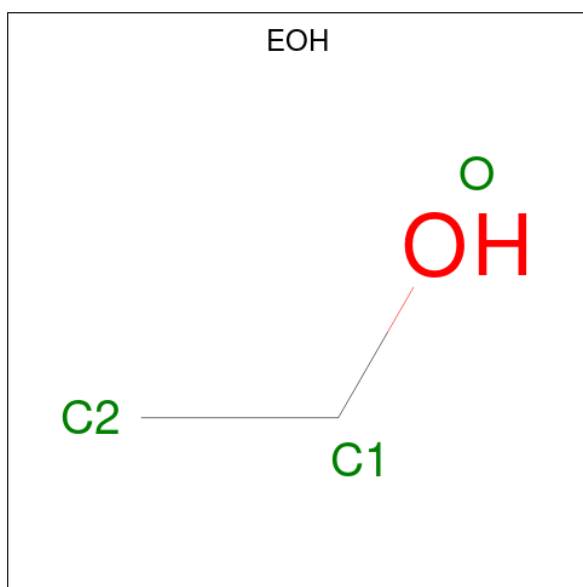
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
2	A	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
2	B	1	Total	C	N	O	S	0	0
			11	6	1	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



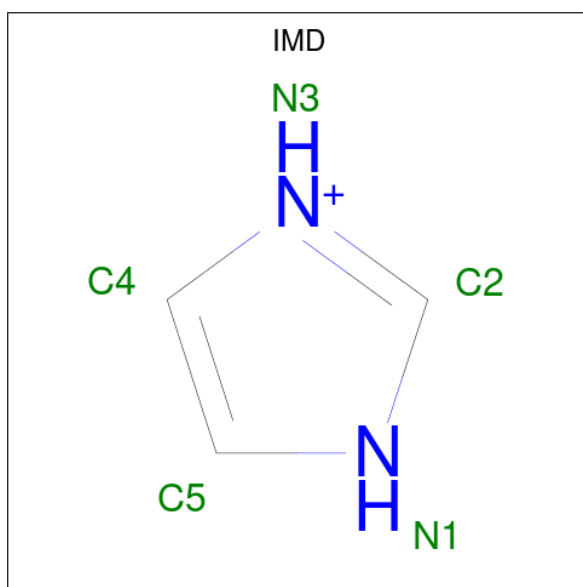
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



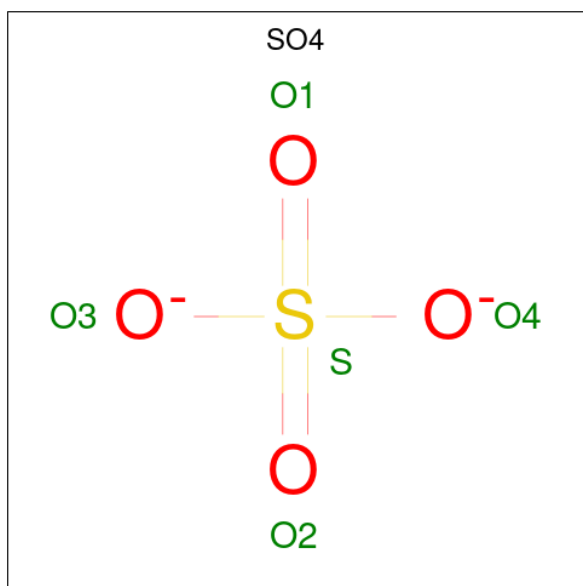
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	2	1		
4	A	1	Total	C	O	0	0
			3	2	1		
4	A	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

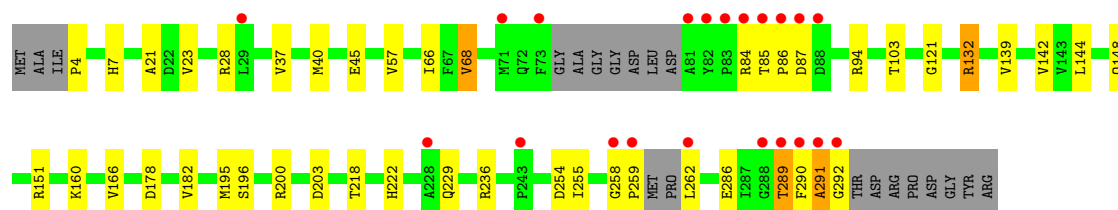
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	175	Total 175	O 175	0	0
7	B	216	Total 216	O 216	0	0

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.

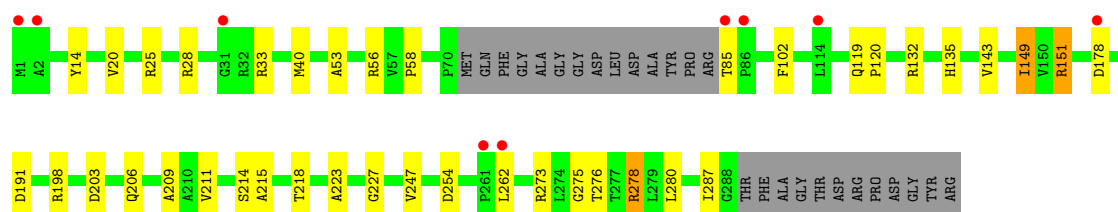
• Molecule 1: Pantothenate synthetase

Chain A: 



• Molecule 1: Pantothenate synthetase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.45Å 71.78Å 81.98Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	28.61 – 1.70 28.61 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.61-1.70) 98.8 (28.61-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.171 , 0.209 0.169 , 0.207	Depositor DCC
R_{free} test set	3087 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4718	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: GOL, IMD, EOH, OOC, SO4

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	1.42	7/2199 (0.3%)	1.26	11/2996 (0.4%)
1	B	1.41	7/2116 (0.3%)	1.22	6/2890 (0.2%)
All	All	1.42	14/4315 (0.3%)	1.24	17/5886 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLY	C-O	8.27	1.31	1.23
1	A	85	THR	CA-CB	6.05	1.60	1.53
1	B	53	ALA	CA-CB	5.76	1.62	1.53
1	A	68	VAL	CA-CB	5.71	1.61	1.54
1	A	166	VAL	CA-CB	-5.67	1.47	1.54
1	B	143	VAL	N-CA	5.65	1.53	1.46
1	B	247	VAL	CA-CB	5.57	1.60	1.54
1	A	66	ILE	N-CA	5.48	1.53	1.46
1	B	209	ALA	CA-CB	5.11	1.61	1.53
1	B	280	LEU	N-CA	5.11	1.52	1.45
1	B	120	PRO	C-O	5.07	1.29	1.23
1	A	37	VAL	N-CA	5.03	1.50	1.46
1	A	103	THR	CA-CB	5.02	1.59	1.53
1	A	182	VAL	CA-CB	-5.02	1.47	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ILE	N-CA-C	-7.43	103.61	110.82
1	A	132	ARG	CA-C-N	6.93	126.63	119.56
1	A	132	ARG	C-N-CA	6.93	126.63	119.56
1	A	21	ALA	N-CA-C	-6.60	104.16	111.36
1	A	121	GLY	CA-C-N	6.54	126.47	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	C-N-CA	6.54	126.47	119.28
1	A	87	ASP	CB-CA-C	-6.35	100.30	110.84
1	A	7	HIS	CA-C-N	-6.33	113.76	120.03
1	A	7	HIS	C-N-CA	-6.33	113.76	120.03
1	B	203	ASP	CA-C-N	-5.43	112.94	118.85
1	B	203	ASP	C-N-CA	-5.43	112.94	118.85
1	B	223	ALA	N-CA-C	-5.42	106.51	113.01
1	A	144	LEU	N-CA-C	-5.32	105.39	111.14
1	B	215	ALA	N-CA-C	-5.18	105.72	111.36
1	A	57	VAL	CA-C-N	-5.15	114.46	119.76
1	A	57	VAL	C-N-CA	-5.15	114.46	119.76
1	B	278	ARG	NE-CZ-NH2	-5.02	114.68	119.20

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	2163	0	2196	71	0
1	B	2082	0	2138	55	0
2	A	22	0	18	4	0
2	B	11	0	9	3	0
3	A	6	0	8	0	0
3	B	12	0	16	11	0
4	A	9	0	18	9	0
4	B	12	0	24	14	0
5	A	5	0	5	0	0
6	B	5	0	0	0	0
7	A	175	0	0	7	0
7	B	216	0	0	12	0
All	All	4718	0	4432	112	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 13.

All (112) 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:40[A]:MET:HE1	7:A:632:HOH:O	1.53	1.05
1:A:84[B]:ARG:HD2	1:A:84[B]:ARG:H	1.20	1.04
1:A:84[B]:ARG:CG	1:A:84[B]:ARG:HH11	1.73	1.01
4:B:407:EOH:H22	7:B:566:HOH:O	1.66	0.95
1:A:151[A]:ARG:NE	1:B:151[A]:ARG:HH12	1.62	0.95
1:B:40:MET:HE2	4:B:406:EOH:H22	1.49	0.95
1:A:151[A]:ARG:HE	1:B:151[A]:ARG:HH12	1.16	0.93
1:A:151[A]:ARG:CD	1:B:151[A]:ARG:HH12	1.85	0.89
1:A:84[B]:ARG:H	1:A:84[B]:ARG:CD	1.91	0.84
1:A:84[B]:ARG:HH11	1:A:84[B]:ARG:HG3	1.43	0.83
1:A:142[A]:VAL:HG11	2:A:401:0OC:CAF	2.10	0.82
1:A:151[A]:ARG:HE	1:B:151[A]:ARG:NH1	1.77	0.81
1:A:40[A]:MET:HE3	2:A:401:0OC:SAH	2.21	0.81
1:B:262:LEU:O	7:B:676:HOH:O	1.97	0.80
1:A:218[B]:THR:HG21	4:A:405:EOH:O	1.83	0.78
1:A:148:GLN:HE22	1:B:151[B]:ARG:HH12	1.31	0.78
1:A:84[B]:ARG:HH11	1:A:84[B]:ARG:HG2	1.49	0.76
2:B:401:0OC:H3	4:B:406:EOH:H11	1.67	0.76
2:B:401:0OC:CAA	4:B:406:EOH:H11	2.16	0.76
1:B:40:MET:HE2	4:B:406:EOH:C2	2.15	0.75
1:B:33[B]:ARG:CZ	7:B:623:HOH:O	2.33	0.75
1:A:84[B]:ARG:CG	1:A:84[B]:ARG:NH1	2.44	0.74
1:B:151[A]:ARG:HG3	3:B:404:GOL:H31	1.68	0.74
1:A:28:ARG:CB	4:A:407:EOH:H12	2.17	0.74
1:A:151[A]:ARG:NE	1:B:151[A]:ARG:NH1	2.36	0.73
1:A:28:ARG:HB3	4:A:407:EOH:H12	1.69	0.73
4:A:404:EOH:H22	7:B:675:HOH:O	1.89	0.73
1:A:151[A]:ARG:NE	1:B:151[A]:ARG:HH22	1.90	0.70
1:A:229:GLN:OE1	7:A:566:HOH:O	2.10	0.69
1:A:151[A]:ARG:HD3	1:B:151[A]:ARG:HH12	1.57	0.69
1:A:151[A]:ARG:HD3	1:B:151[A]:ARG:NH1	2.08	0.68
1:A:84[B]:ARG:HG3	1:A:84[B]:ARG:NH1	2.03	0.67
1:A:151[A]:ARG:O	4:A:407:EOH:H22	1.94	0.67
1:A:151[A]:ARG:NH2	1:B:151[A]:ARG:HH22	1.94	0.65
1:A:151[A]:ARG:CZ	1:B:151[A]:ARG:HH22	2.08	0.65
1:A:151[A]:ARG:NH1	1:B:178:ASP:HB2	2.12	0.65
1:A:148:GLN:O	1:A:151[A]:ARG:NH1	2.33	0.62
1:A:151[A]:ARG:CD	1:B:151[A]:ARG:NH1	2.60	0.60
1:A:178[A]:ASP:HB2	3:B:404:GOL:H32	1.84	0.60
1:A:151[A]:ARG:HE	1:B:151[A]:ARG:NH2	2.01	0.59
1:A:84[B]:ARG:HD2	1:A:84[B]:ARG:N	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218[B]:THR:HG21	4:A:405:EOH:C1	2.33	0.59
1:A:151[A]:ARG:HE	1:B:151[A]:ARG:CZ	2.16	0.58
1:B:20[B]:VAL:HG21	1:B:102:PHE:CD1	2.39	0.58
1:A:151[A]:ARG:HE	1:B:151[A]:ARG:HH22	1.49	0.58
1:A:45:GLU:HB3	1:A:195[A]:MET:SD	2.44	0.57
1:A:84[B]:ARG:CD	1:A:84[B]:ARG:N	2.61	0.57
1:A:148:GLN:NE2	1:B:151[B]:ARG:HH12	2.01	0.57
1:A:142[A]:VAL:CG1	2:A:401:OOC:CAF	2.83	0.57
1:B:275:GLY:HA3	4:B:407:EOH:H11	1.87	0.56
1:A:254[A]:ASP:OD1	1:A:254[A]:ASP:C	2.47	0.56
1:B:151[A]:ARG:HG3	3:B:404:GOL:H2	1.87	0.56
1:A:178[B]:ASP:HB3	3:B:404:GOL:H32	1.88	0.56
1:A:291:ALA:HB1	1:A:292:GLY:C	2.30	0.56
1:A:178[B]:ASP:OD1	3:B:404:GOL:H32	2.08	0.54
1:B:151[A]:ARG:HG3	3:B:404:GOL:C3	2.37	0.54
1:B:278:ARG:HG2	1:B:278:ARG:NH2	2.23	0.54
1:B:276:THR:H	4:B:407:EOH:H21	1.74	0.53
1:B:33[B]:ARG:NH1	7:B:623:HOH:O	2.41	0.53
1:B:25:ARG:NH1	3:B:404:GOL:O2	2.40	0.53
1:B:191:ASP:OD2	1:B:211[B]:VAL:HG22	2.09	0.51
1:B:273:ARG:O	3:B:402:GOL:H12	2.10	0.51
1:B:276:THR:H	4:B:407:EOH:C2	2.23	0.51
1:B:214:SER:O	1:B:218[B]:THR:HG22	2.10	0.51
1:B:14:TYR:HB2	1:B:20[B]:VAL:HG23	1.92	0.51
1:B:40:MET:CE	4:B:406:EOH:H22	2.31	0.51
1:B:56:ARG:NH1	7:B:637:HOH:O	2.36	0.51
1:B:149:ILE:O	3:B:404:GOL:H12	2.11	0.50
1:A:200:ARG:NH1	7:A:659:HOH:O	2.45	0.50
1:A:4:PRO:HG2	1:A:23:VAL:HG23	1.93	0.49
4:B:407:EOH:C2	7:B:566:HOH:O	2.40	0.49
1:A:94[A]:ARG:NH2	7:A:654:HOH:O	2.36	0.48
1:A:151[A]:ARG:HH21	1:B:151[A]:ARG:HH22	1.59	0.48
1:A:151[A]:ARG:NE	1:B:151[A]:ARG:NH2	2.56	0.48
1:A:151[A]:ARG:NH2	1:B:178:ASP:H	2.11	0.48
1:B:278:ARG:HG2	1:B:278:ARG:HH21	1.79	0.47
1:A:178[B]:ASP:CB	3:B:404:GOL:H32	2.44	0.47
1:B:151[A]:ARG:HG3	3:B:404:GOL:C2	2.45	0.47
1:A:28:ARG:HB2	4:A:407:EOH:H12	1.97	0.47
1:A:195[B]:MET:CE	7:A:607:HOH:O	2.62	0.47
1:B:278:ARG:HH21	1:B:278:ARG:CG	2.28	0.47
1:A:28:ARG:CB	4:A:407:EOH:C1	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLY:CA	4:B:407:EOH:H11	2.45	0.46
1:B:276:THR:OG1	4:B:407:EOH:H21	2.15	0.46
1:A:148:GLN:HE22	1:B:151[B]:ARG:NH1	2.07	0.46
1:B:206:GLN:HG2	7:B:618:HOH:O	2.16	0.46
1:A:139:VAL:O	1:A:142[A]:VAL:HG12	2.16	0.46
1:B:151[B]:ARG:HD3	7:B:642:HOH:O	2.16	0.46
1:A:142[A]:VAL:HG11	2:A:401:OOC:CAE	2.45	0.46
1:A:289:THR:HG23	1:A:290:PHE:CD1	2.51	0.46
1:A:286:GLU:HB2	1:A:291:ALA:HB3	1.97	0.45
1:A:218[A]:THR:O	1:A:222:HIS:HD2	1.99	0.45
1:B:287:ILE:HA	1:B:287:ILE:HD13	1.58	0.45
1:A:40[B]:MET:HB3	1:A:68:VAL:HG22	1.98	0.45
4:B:406:EOH:H12	7:B:687:HOH:O	2.16	0.45
1:A:289:THR:HA	1:A:290:PHE:HA	1.59	0.44
1:A:178[B]:ASP:OD2	1:A:178[B]:ASP:O	2.36	0.43
1:A:195[B]:MET:HE3	7:A:607:HOH:O	2.18	0.43
1:A:258[A]:GLY:O	1:A:259[A]:PRO:O	2.36	0.43
1:A:195[B]:MET:HE2	7:A:579:HOH:O	2.19	0.43
1:B:198:ARG:HD2	7:B:617:HOH:O	2.18	0.43
1:B:214:SER:O	1:B:218[A]:THR:HG23	2.19	0.43
1:A:84[A]:ARG:O	1:A:86:PRO:HD3	2.19	0.42
1:B:278:ARG:NH2	1:B:278:ARG:CG	2.80	0.42
1:A:203:ASP:OD1	1:A:203:ASP:C	2.63	0.41
1:A:236:ARG:HH21	1:A:236:ARG:HG3	1.85	0.41
1:B:211[B]:VAL:HG21	7:B:615:HOH:O	2.20	0.41
1:B:132:ARG:HB3	1:B:135:HIS:HB2	2.01	0.41
1:A:84[A]:ARG:C	1:A:86:PRO:HD3	2.46	0.41
1:A:218[B]:THR:HG21	4:A:405:EOH:H12	2.01	0.41
2:B:401:OOC:H3	4:B:406:EOH:C1	2.42	0.41
1:A:160:LYS:HE3	1:A:196:SER:HB2	2.03	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	286/300 (95%)	277 (97%)	8 (3%)	1 (0%)	36	22
1	B	278/300 (93%)	274 (99%)	4 (1%)	0	100	100
All	All	564/600 (94%)	551 (98%)	12 (2%)	1 (0%)	43	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ALA

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	217/223 (97%)	213 (98%)	4 (2%)	51	36
1	B	211/223 (95%)	204 (97%)	7 (3%)	33	17
All	All	428/446 (96%)	417 (97%)	11 (3%)	42	23

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ARG
1	A	255	ILE
1	A	262	LEU
1	A	289	THR
1	B	28	ARG
1	B	58	PRO
1	B	85	THR
1	B	119	GLN
1	B	151[A]	ARG
1	B	151[B]	ARG
1	B	254	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	222	HIS
1	B	170	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	OOC	A	402	-	10,11,11	4.77	5 (50%)	11,16,16	2.27	3 (27%)
4	EOH	A	407	-	2,2,2	0.66	0	1,1,1	0.60	0
4	EOH	B	406	-	2,2,2	0.50	0	1,1,1	0.13	0
4	EOH	A	405	-	2,2,2	0.52	0	1,1,1	0.76	0
4	EOH	A	404	-	2,2,2	0.55	0	1,1,1	0.15	0
4	EOH	B	408	-	2,2,2	0.51	0	1,1,1	0.20	0
6	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.12	0
3	GOL	B	402	-	5,5,5	0.21	0	5,5,5	0.95	0
3	GOL	A	403	-	5,5,5	0.87	0	5,5,5	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0OC	A	401	-	10,11,11	6.54	4 (40%)	11,16,16	2.58	4 (36%)
4	EOH	B	405	-	2,2,2	0.44	0	1,1,1	0.30	0
2	0OC	B	401	-	10,11,11	4.22	4 (40%)	11,16,16	2.91	5 (45%)
4	EOH	B	407	-	2,2,2	0.40	0	1,1,1	0.44	0
3	GOL	B	404	-	5,5,5	0.52	0	5,5,5	1.21	1 (20%)
5	IMD	A	406	-	5,5,5	0.64	0	5,5,5	0.88	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
2	0OC	A	402	-	-	0/10/12/12	0/1/1/1
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
2	0OC	A	401	-	-	8/10/12/12	0/1/1/1
2	0OC	B	401	-	-	7/10/12/12	0/1/1/1
3	GOL	B	404	-	-	4/4/4/4	-
5	IMD	A	406	-	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	0OC	OAC-SAK	13.29	1.56	1.43
2	A	401	0OC	SAK-NAJ	12.03	1.81	1.63
2	A	401	0OC	OAD-SAK	9.41	1.52	1.43
2	A	402	0OC	OAD-SAK	9.36	1.52	1.43
2	A	402	0OC	OAC-SAK	8.49	1.51	1.43
2	B	401	0OC	SAK-NAJ	8.31	1.75	1.63
2	B	401	0OC	OAD-SAK	7.39	1.50	1.43
2	B	401	0OC	OAC-SAK	6.06	1.49	1.43
2	A	402	0OC	SAK-NAJ	5.03	1.70	1.63
2	A	402	0OC	CAG-SAH	-4.54	1.56	1.70
2	A	402	0OC	CAF-CAI	-4.08	1.37	1.42
2	A	401	0OC	CAF-CAI	-3.91	1.37	1.42
2	B	401	0OC	CAF-CAI	-3.25	1.38	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	0OC	OAD-SAK-OAC	-6.09	110.95	119.69
2	A	401	0OC	CAE-CAF-CAI	6.08	116.92	110.84
2	B	401	0OC	OAD-SAK-OAC	-5.67	111.55	119.69
2	B	401	0OC	CAE-CAF-CAI	4.28	115.12	110.84
2	B	401	0OC	OAD-SAK-NAJ	4.21	115.23	106.87
2	B	401	0OC	OAC-SAK-NAJ	3.76	114.34	106.87
2	A	401	0OC	CAB-NAJ-CAA	3.73	122.15	114.75
2	A	401	0OC	OAD-SAK-NAJ	2.75	112.32	106.87
2	A	401	0OC	OAC-SAK-NAJ	2.63	112.10	106.87
3	B	404	GOL	C3-C2-C1	-2.41	102.95	111.80
2	B	401	0OC	CAA-NAJ-SAK	2.32	121.52	116.53
3	A	403	GOL	O1-C1-C2	2.20	120.29	110.38
2	A	402	0OC	CAA-NAJ-SAK	-2.17	111.85	116.53
2	A	402	0OC	CAE-CAF-CAI	2.12	112.96	110.84

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	0OC	CAF-CAI-SAK-OAC
2	A	401	0OC	CAF-CAI-SAK-OAD
2	B	401	0OC	CAA-NAJ-SAK-OAC
2	B	401	0OC	CAA-NAJ-SAK-OAD
2	B	401	0OC	CAA-NAJ-SAK-CAI
2	B	401	0OC	CAF-CAI-SAK-OAD
3	B	404	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
2	A	401	0OC	CAA-NAJ-SAK-OAC
2	A	401	0OC	CAB-NAJ-SAK-OAD
3	A	403	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3
2	A	401	0OC	CAA-NAJ-SAK-OAD
2	A	401	0OC	CAB-NAJ-SAK-OAC
3	A	403	GOL	O1-C1-C2-O2
2	A	401	0OC	CAB-NAJ-SAK-CAI
2	B	401	0OC	CAB-NAJ-SAK-OAC
2	B	401	0OC	CAB-NAJ-SAK-OAD
2	A	401	0OC	CAA-NAJ-SAK-CAI
2	B	401	0OC	CAB-NAJ-SAK-CAI
3	B	402	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	EOH	5	0
4	B	406	EOH	7	0
4	A	405	EOH	3	0
4	A	404	EOH	1	0
3	B	402	GOL	1	0
2	A	401	0OC	4	0
2	B	401	0OC	3	0
4	B	407	EOH	7	0
3	B	404	GOL	10	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	280/300 (93%)	0.19	21 (7%)	20 22	9, 27, 49, 70	13 (4%)
1	B	274/300 (91%)	-0.16	9 (3%)	49 53	9, 24, 43, 65	8 (2%)
All	All	554/600 (92%)	0.02	30 (5%)	31 34	9, 25, 47, 70	21 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	7.2
1	A	259[A]	PRO	6.6
1	A	292	GLY	5.9
1	A	291	ALA	5.2
1	A	290	PHE	4.9
1	A	258[A]	GLY	4.0
1	A	82	TYR	3.2
1	A	84[A]	ARG	3.0
1	B	1	MET	3.0
1	A	243	PRO	2.9
1	B	85	THR	2.8
1	B	2	ALA	2.8
1	B	262	LEU	2.7
1	A	71	MET	2.6
1	A	228	ALA	2.6
1	B	86	PRO	2.5
1	B	178	ASP	2.5
1	A	87	ASP	2.4
1	A	288	GLY	2.4
1	B	31	GLY	2.3
1	A	73	PHE	2.3
1	A	289	THR	2.3
1	A	88	ASP	2.3
1	A	85	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	86	PRO	2.2
1	A	29	LEU	2.2
1	B	261	PRO	2.2
1	A	262	LEU	2.2
1	A	83	PRO	2.2
1	B	114	LEU	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 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($\text{\AA}^2$)	Q<0.9
4	EOH	B	408	3/3	0.73	0.15	53,53,53,54	0
6	SO4	B	403	5/5	0.77	0.15	98,98,98,98	0
5	IMD	A	406	5/5	0.79	0.12	42,48,49,49	0
4	EOH	B	407	3/3	0.81	0.14	41,41,42,43	0
4	EOH	A	404	3/3	0.81	0.22	46,46,46,47	0
4	EOH	A	407	3/3	0.82	0.18	36,36,41,42	0
4	EOH	A	405	3/3	0.83	0.13	35,35,36,40	0
3	GOL	B	402	6/6	0.85	0.13	37,46,49,53	0
4	EOH	B	405	3/3	0.85	0.17	50,50,50,51	0
3	GOL	B	404	6/6	0.87	0.09	46,47,50,51	0
2	0OC	A	402	11/11	0.90	0.12	28,34,41,43	11
2	0OC	A	401	11/11	0.95	0.10	26,31,33,34	0
4	EOH	B	406	3/3	0.95	0.09	37,37,38,39	0
3	GOL	A	403	6/6	0.96	0.07	22,25,27,28	0
2	0OC	B	401	11/11	0.96	0.07	28,33,36,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.