



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 06:44 AM EDT

PDB ID : 6SNU
Title : Crystal structure of the W60C mutant of the (S)-selective transaminase from *Chromobacterium violaceum*
Authors : Ruggieri, F.; Gustafsson, C.; Kimbung, R.Y.; Walse, B.; Logan, D.T.; Berglund, P.
Deposited on : 2019-08-27
Resolution : 2.00 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

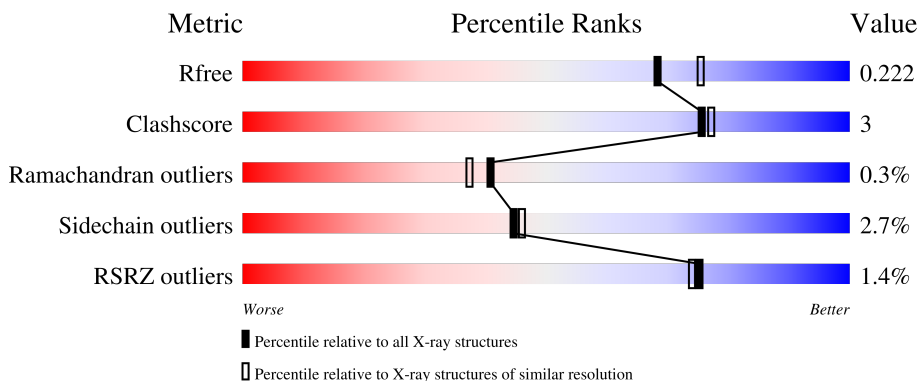
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	465	88% 8% ..
1	B	465	87% 9% ..
1	C	465	89% 8% ..
1	D	465	89% 8% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14564 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 Aspartate aminotransferase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	452	3551	2257	626	646	22	0	0	0
1	B	453	3555	2259	627	647	22	0	0	0
1	C	455	3579	2274	633	650	22	0	1	0
1	D	454	3574	2271	632	649	22	0	1	0

There are 28 discrepancies between the modelled and reference sequences:

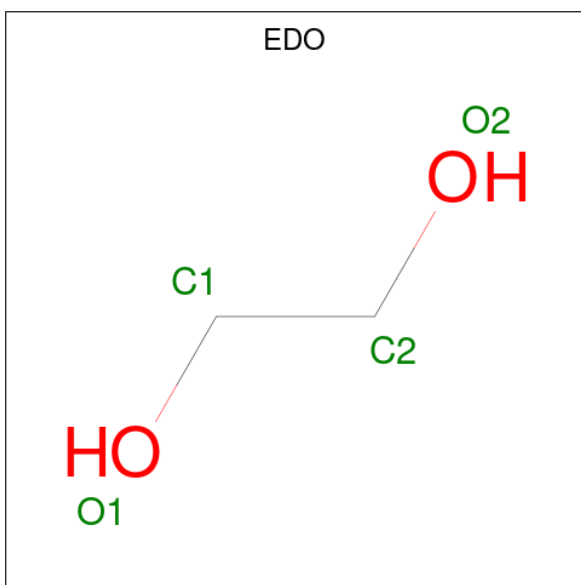
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0A1R0MXM9
A	-4	HIS	-	expression tag	UNP A0A1R0MXM9
A	-3	HIS	-	expression tag	UNP A0A1R0MXM9
A	-2	HIS	-	expression tag	UNP A0A1R0MXM9
A	-1	HIS	-	expression tag	UNP A0A1R0MXM9
A	0	HIS	-	expression tag	UNP A0A1R0MXM9
A	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9
B	-5	HIS	-	expression tag	UNP A0A1R0MXM9
B	-4	HIS	-	expression tag	UNP A0A1R0MXM9
B	-3	HIS	-	expression tag	UNP A0A1R0MXM9
B	-2	HIS	-	expression tag	UNP A0A1R0MXM9
B	-1	HIS	-	expression tag	UNP A0A1R0MXM9
B	0	HIS	-	expression tag	UNP A0A1R0MXM9
B	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9
C	-5	HIS	-	expression tag	UNP A0A1R0MXM9
C	-4	HIS	-	expression tag	UNP A0A1R0MXM9
C	-3	HIS	-	expression tag	UNP A0A1R0MXM9
C	-2	HIS	-	expression tag	UNP A0A1R0MXM9
C	-1	HIS	-	expression tag	UNP A0A1R0MXM9
C	0	HIS	-	expression tag	UNP A0A1R0MXM9
C	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP A0A1R0MXM9
D	-4	HIS	-	expression tag	UNP A0A1R0MXM9
D	-3	HIS	-	expression tag	UNP A0A1R0MXM9
D	-2	HIS	-	expression tag	UNP A0A1R0MXM9
D	-1	HIS	-	expression tag	UNP A0A1R0MXM9
D	0	HIS	-	expression tag	UNP A0A1R0MXM9
D	60	CYS	TRP	engineered mutation	UNP A0A1R0MXM9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

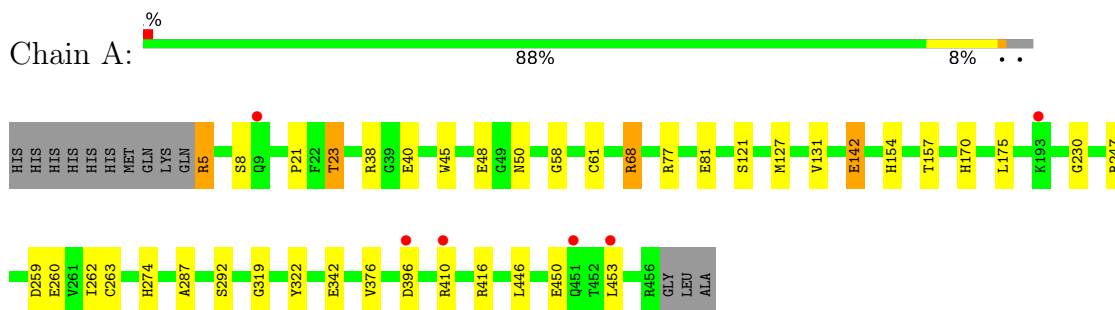
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	57	Total	O	0	0
			57	57		
4	C	78	Total	O	0	0
			78	78		
4	D	58	Total	O	0	0
			58	58		

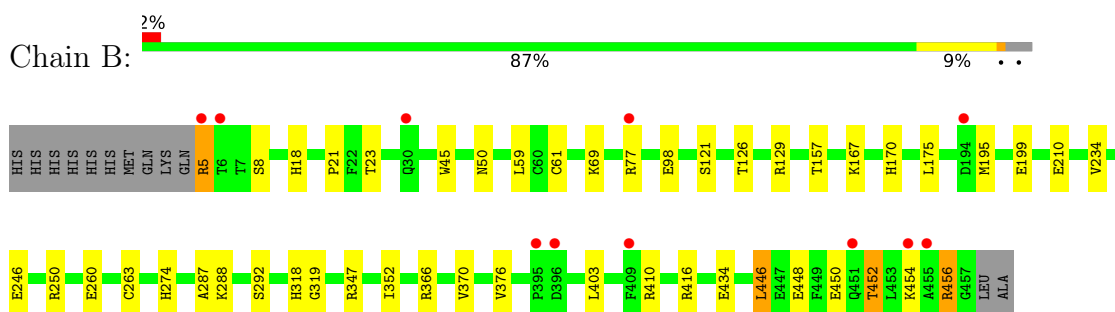
3 Residue-property plots [i](#)

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.

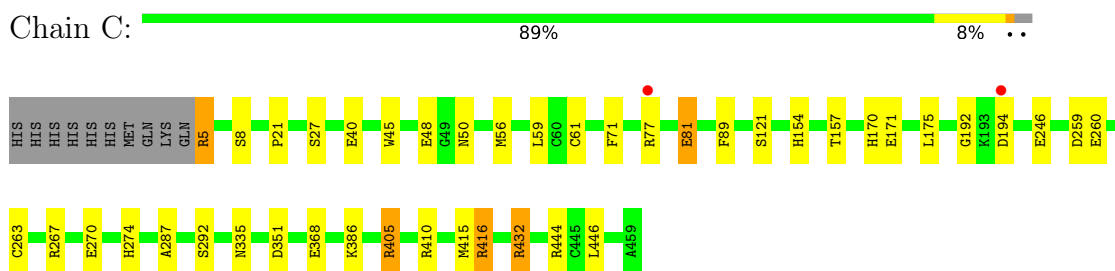
- Molecule 1: Aspartate aminotransferase family protein



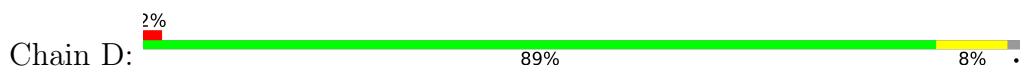
- Molecule 1: Aspartate aminotransferase family protein

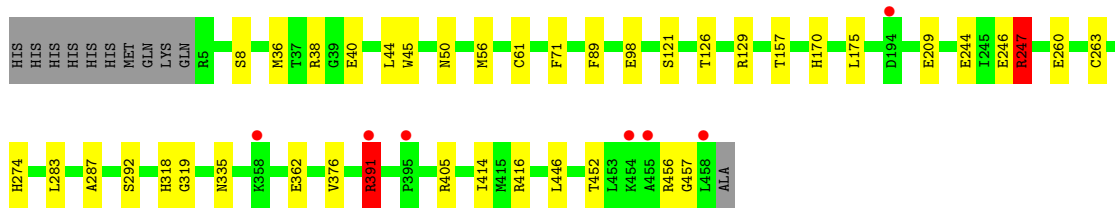


- Molecule 1: Aspartate aminotransferase family protein



- Molecule 1: Aspartate aminotransferase family protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.22Å 62.20Å 118.42Å 75.03° 81.31° 75.30°	Depositor
Resolution (Å)	48.28 – 2.00 48.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.28-2.00) 96.2 (48.23-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.181 , 0.215 0.190 , 0.222	Depositor DCC
R_{free} test set	5299 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14564	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% 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: OCS, PLP, EDO

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	0.87	2/3633 (0.1%)	0.95	5/4915 (0.1%)
1	B	0.88	4/3637 (0.1%)	0.97	6/4920 (0.1%)
1	C	0.90	6/3661 (0.2%)	1.00	7/4952 (0.1%)
1	D	0.85	3/3656 (0.1%)	0.97	5/4945 (0.1%)
All	All	0.88	15/14587 (0.1%)	0.97	23/19732 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	GLU	CD-OE2	11.08	1.37	1.25
1	A	142	GLU	CD-OE1	9.45	1.36	1.25
1	D	246	GLU	CD-OE2	-6.95	1.18	1.25
1	C	81	GLU	CD-OE1	6.42	1.32	1.25
1	B	246	GLU	CD-OE2	-6.38	1.18	1.25
1	D	209	GLU	CD-OE1	-5.80	1.19	1.25
1	A	48	GLU	CD-OE2	5.70	1.31	1.25
1	C	171	GLU	CD-OE1	5.42	1.31	1.25
1	B	434	GLU	CD-OE2	-5.35	1.19	1.25
1	C	246	GLU	CD-OE2	-5.30	1.19	1.25
1	B	210	GLU	CD-OE1	5.23	1.31	1.25
1	D	362	GLU	CD-OE1	5.18	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	270	GLU	CD-OE1	5.15	1.31	1.25
1	C	48	GLU	CD-OE2	5.09	1.31	1.25
1	C	368	GLU	CD-OE2	5.08	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	247	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	D	247	ARG	CG-CD-NE	-7.10	96.89	111.80
1	B	129	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	38	ARG	CG-CD-NE	6.54	125.54	111.80
1	D	247	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	250	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	410	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	129	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	415	MET	CG-SD-CE	-5.67	91.12	100.20
1	D	391	ARG	CG-CD-NE	5.62	123.60	111.80
1	C	416[A]	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	416[B]	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	366	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	68	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	405	ARG	CG-CD-NE	-5.53	100.18	111.80
1	A	68	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	416	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	416	ARG	CB-CG-CD	5.23	125.21	111.60
1	B	347	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	432	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	267	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	247	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	77	ARG	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	192	GLY	Peptide
1	D	457	GLY	Peptide

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	3551	0	3446	18	1
1	B	3555	0	3449	29	0
1	C	3579	0	3478	22	0
1	D	3574	0	3472	24	0
2	A	4	0	6	0	0
2	B	12	0	18	0	0
3	A	15	0	6	1	0
3	B	15	0	6	0	0
3	C	15	0	6	1	0
3	D	15	0	6	1	0
4	A	36	0	0	2	0
4	B	57	0	0	1	0
4	C	78	0	0	4	0
4	D	58	0	0	1	0
All	All	14564	0	13893	87	1

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 3.

All (87) 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:B:21:PRO:O	1:B:23:THR:HG23	1.63	0.99
1:A:21:PRO:O	1:A:23:THR:HG23	1.66	0.95
1:D:391:ARG:O	1:D:391:ARG:HG2	1.79	0.81
1:C:416[B]:ARG:CZ	4:C:601:HOH:O	2.31	0.78
3:C:501:PLP:P	4:C:603:HOH:O	2.42	0.77
1:C:77:ARG:NH1	1:C:81:GLU:OE1	2.23	0.72
1:B:21:PRO:O	1:B:23:THR:CG2	2.41	0.67
1:C:154:HIS:HD2	1:C:259:ASP:OD2	1.78	0.66
1:C:416[B]:ARG:NH2	4:C:601:HOH:O	2.29	0.66
1:A:154:HIS:HD2	1:A:259:ASP:OD2	1.79	0.65
1:D:129:ARG:HH11	1:D:318:HIS:HD2	1.44	0.64
1:A:21:PRO:O	1:A:23:THR:CG2	2.43	0.62
1:B:5:ARG:N	1:B:5:ARG:HE	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:MET:HG3	1:C:416[A]:ARG:HG2	1.81	0.62
1:B:448:GLU:O	1:B:452:THR:HG23	2.00	0.62
1:D:126:THR:OG1	1:D:318:HIS:HE1	1.84	0.61
1:B:195:MET:HE2	1:B:199:GLU:HB3	1.82	0.60
1:A:21:PRO:HB3	1:B:319:GLY:HA3	1.84	0.59
1:B:403:LEU:C	1:B:403:LEU:HD23	2.24	0.58
1:D:405:ARG:HD2	1:D:416[A]:ARG:CZ	2.36	0.56
1:B:126:THR:OG1	1:B:318:HIS:HE1	1.88	0.56
1:B:121:SER:HB3	1:B:157:THR:HG23	1.87	0.55
1:C:194:ASP:OD1	1:C:194:ASP:N	2.36	0.55
1:A:5:ARG:NH1	1:B:98:GLU:OE1	2.40	0.54
1:D:244:GLU:OE2	1:D:247:ARG:NH1	2.41	0.54
1:D:260:GLU:OE2	1:D:274:HIS:HD2	1.91	0.54
1:B:403:LEU:HD23	1:B:403:LEU:O	2.07	0.54
1:B:260:GLU:OE2	1:B:274:HIS:HD2	1.91	0.54
1:C:260:GLU:OE2	1:C:274:HIS:HD2	1.90	0.54
1:A:170:HIS:HA	1:A:175:LEU:HB2	1.90	0.53
1:C:416[A]:ARG:HG3	1:D:89:PHE:CZ	2.44	0.53
1:A:68:ARG:NH2	1:A:342:GLU:OE1	2.33	0.53
1:B:5:ARG:N	1:B:5:ARG:NE	2.57	0.52
1:D:61:CYS:O	1:D:292:SER:HA	2.11	0.51
1:D:391:ARG:HH11	1:D:391:ARG:HG3	1.76	0.51
4:A:631:HOH:O	1:B:18:HIS:HE1	1.93	0.51
1:A:121:SER:HB3	1:A:157:THR:HG23	1.93	0.50
1:A:260:GLU:OE2	1:A:274:HIS:HD2	1.94	0.50
1:B:61:CYS:O	1:B:292:SER:HA	2.11	0.50
1:C:21:PRO:HB3	1:D:319:GLY:HA3	1.93	0.50
1:B:170:HIS:HA	1:B:175:LEU:HB2	1.94	0.49
1:C:61:CYS:O	1:C:292:SER:HA	2.13	0.49
1:B:260:GLU:OE2	1:B:274:HIS:CD2	2.67	0.48
1:A:61:CYS:O	1:A:292:SER:HA	2.13	0.48
1:C:170:HIS:HA	1:C:175:LEU:HB2	1.95	0.47
1:B:370:VAL:HG21	1:B:446:LEU:HD21	1.95	0.47
1:B:450:GLU:OE1	4:B:601:HOH:O	2.20	0.47
1:C:89:PHE:CZ	1:D:416[A]:ARG:HG3	2.49	0.47
1:D:36:MET:CE	1:D:44:LEU:HB3	2.45	0.47
3:D:501:PLP:P	4:D:604:HOH:O	2.73	0.47
1:D:260:GLU:OE2	1:D:274:HIS:CD2	2.68	0.46
1:A:260:GLU:OE2	1:A:274:HIS:CD2	2.68	0.46
1:C:260:GLU:OE2	1:C:274:HIS:CD2	2.68	0.46
1:D:170:HIS:HA	1:D:175:LEU:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:SER:HB3	1:D:157:THR:HG23	1.97	0.46
1:D:391:ARG:O	1:D:391:ARG:CG	2.59	0.46
1:D:126:THR:OG1	1:D:318:HIS:CE1	2.66	0.46
1:D:56:MET:HG3	1:D:416[A]:ARG:HG2	1.98	0.45
1:C:351:ASP:OD1	1:C:432:ARG:NH2	2.49	0.45
1:D:129:ARG:HD3	1:D:318:HIS:CD2	2.52	0.44
4:A:631:HOH:O	1:B:18:HIS:CE1	2.70	0.44
1:A:262:ILE:HG13	3:A:502:PLP:O3	2.18	0.44
1:B:352:ILE:HD12	1:B:352:ILE:HA	1.87	0.44
1:A:230:GLY:HA3	1:A:262:ILE:HD12	1.99	0.43
1:B:126:THR:OG1	1:B:318:HIS:CE1	2.69	0.43
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.86	0.43
1:C:40:GLU:O	1:C:40:GLU:HG3	2.19	0.42
1:C:121:SER:HB3	1:C:157:THR:HG23	2.02	0.42
1:A:45:TRP:HA	1:A:50:ASN:O	2.19	0.42
1:B:45:TRP:HA	1:B:50:ASN:O	2.19	0.42
1:C:45:TRP:HA	1:C:50:ASN:O	2.20	0.42
1:D:416[A]:ARG:HA	1:D:416[A]:ARG:HD2	1.86	0.42
1:A:319:GLY:HA3	1:B:21:PRO:HB3	2.02	0.41
1:C:5:ARG:NH1	1:D:98:GLU:OE1	2.52	0.41
1:D:129:ARG:HH11	1:D:318:HIS:CD2	2.32	0.41
1:B:195:MET:HE2	1:B:199:GLU:CB	2.50	0.41
1:B:403:LEU:C	1:B:403:LEU:CD2	2.88	0.41
1:B:456:ARG:HB3	1:B:456:ARG:HH11	1.86	0.41
1:C:71:PHE:CZ	1:C:335:ASN:HA	2.55	0.41
1:A:322:TYR:OH	1:B:288:LYS:HA	2.21	0.41
1:D:71:PHE:CZ	1:D:335:ASN:HA	2.56	0.41
1:C:416[B]:ARG:NH1	4:C:601:HOH:O	2.51	0.41
1:D:45:TRP:HA	1:D:50:ASN:O	2.20	0.41
1:A:453:LEU:C	1:A:453:LEU:HD23	2.41	0.40
1:C:416[B]:ARG:HH11	1:C:416[B]:ARG:HD3	1.65	0.40
1:B:234:VAL:O	1:B:234:VAL:HG12	2.20	0.40
1:A:127:MET:O	1:A:131:VAL:HG13	2.22	0.40

All (1) 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)
1:A:38:ARG:NH1	1:A:142:GLU:OE2[1_565]	2.18	0.02

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	449/465 (97%)	435 (97%)	12 (3%)	2 (0%)	34	30
1	B	450/465 (97%)	433 (96%)	16 (4%)	1 (0%)	47	44
1	C	453/465 (97%)	438 (97%)	14 (3%)	1 (0%)	47	44
1	D	452/465 (97%)	435 (96%)	16 (4%)	1 (0%)	47	44
All	All	1804/1860 (97%)	1741 (96%)	58 (3%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	ALA
1	A	287	ALA
1	C	287	ALA
1	D	287	ALA
1	A	58	GLY

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	362/373 (97%)	352 (97%)	10 (3%)	43	44
1	B	362/373 (97%)	350 (97%)	12 (3%)	38	37
1	C	364/373 (98%)	357 (98%)	7 (2%)	57	61
1	D	364/373 (98%)	354 (97%)	10 (3%)	44	46
All	All	1452/1492 (97%)	1413 (97%)	39 (3%)	44	46

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	8	SER
1	A	23	THR
1	A	40	GLU
1	A	81	GLU
1	A	376	VAL
1	A	396	ASP
1	A	410	ARG
1	A	446	LEU
1	A	450	GLU
1	B	5	ARG
1	B	8	SER
1	B	59	LEU
1	B	69	LYS
1	B	77	ARG
1	B	167	LYS
1	B	376	VAL
1	B	410	ARG
1	B	446	LEU
1	B	452	THR
1	B	454	LYS
1	B	456	ARG
1	C	5	ARG
1	C	8	SER
1	C	27	SER
1	C	386	LYS
1	C	405	ARG
1	C	444	ARG
1	C	446	LEU
1	D	8	SER
1	D	40	GLU
1	D	247	ARG
1	D	283	LEU
1	D	376	VAL
1	D	391	ARG
1	D	414	ILE
1	D	446	LEU
1	D	452	THR
1	D	456	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	274	HIS
1	A	451	GLN
1	B	18	HIS
1	B	274	HIS
1	B	318	HIS
1	C	154	HIS
1	C	274	HIS
1	C	369	HIS
1	D	274	HIS
1	D	318	HIS
1	D	411	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](#)

4 non-standard protein/DNA/RNA residues 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
1	OCS	D	263	1	7,8,9	1.09	1 (14%)	6,11,13	3.90	2 (33%)
1	OCS	A	263	1	7,8,9	1.18	1 (14%)	6,11,13	1.57	1 (16%)
1	OCS	B	263	1	7,8,9	0.63	0	6,11,13	2.31	2 (33%)
1	OCS	C	263	1	7,8,9	0.96	0	6,11,13	2.19	3 (50%)

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
1	OCS	D	263	1	-	3/4/7/9	-
1	OCS	A	263	1	-	3/4/7/9	-
1	OCS	B	263	1	-	3/4/7/9	-
1	OCS	C	263	1	-	3/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	OCS	OD3-SG	2.59	1.52	1.45
1	D	263	OCS	OD3-SG	2.42	1.52	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	OCS	OD3-SG-CB	-8.31	97.07	106.94
1	B	263	OCS	OD3-SG-CB	-5.00	101.00	106.94
1	D	263	OCS	OD2-SG-OD1	4.31	121.80	111.27
1	C	263	OCS	OD1-SG-CB	3.40	110.98	106.94
1	A	263	OCS	OD3-SG-CB	-3.10	103.25	106.94
1	C	263	OCS	OD2-SG-CB	-2.90	101.12	105.74
1	C	263	OCS	OD2-SG-OD1	2.32	116.94	111.27
1	B	263	OCS	OD2-SG-CB	2.13	109.13	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	263	OCS	CA-CB-SG-OD1
1	B	263	OCS	CA-CB-SG-OD1
1	B	263	OCS	CA-CB-SG-OD2
1	B	263	OCS	CA-CB-SG-OD3
1	C	263	OCS	CA-CB-SG-OD1
1	C	263	OCS	CA-CB-SG-OD3
1	D	263	OCS	CA-CB-SG-OD2
1	D	263	OCS	CA-CB-SG-OD3
1	A	263	OCS	CA-CB-SG-OD3
1	D	263	OCS	CA-CB-SG-OD1
1	A	263	OCS	CA-CB-SG-OD2
1	C	263	OCS	CA-CB-SG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	EDO	B	503	-	3,3,3	0.17	0	2,2,2	0.26	0
2	EDO	A	501	-	3,3,3	0.26	0	2,2,2	0.49	0
3	PLP	A	502	1	15,15,16	1.40	1 (6%)	20,22,23	2.54	6 (30%)
3	PLP	C	501	1	15,15,16	1.59	1 (6%)	20,22,23	2.94	8 (40%)
2	EDO	B	502	-	3,3,3	0.35	0	2,2,2	0.56	0
3	PLP	B	504	1	15,15,16	1.15	1 (6%)	20,22,23	2.47	6 (30%)
2	EDO	B	501	-	3,3,3	0.53	0	2,2,2	0.47	0
3	PLP	D	501	1	15,15,16	1.48	1 (6%)	20,22,23	2.86	8 (40%)

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	EDO	B	503	-	-	1/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
3	PLP	A	502	1	-	0/6/6/8	0/1/1/1
3	PLP	C	501	1	-	0/6/6/8	0/1/1/1
2	EDO	B	502	-	-	1/1/1/1	-
3	PLP	B	504	1	-	0/6/6/8	0/1/1/1
2	EDO	B	501	-	-	1/1/1/1	-
3	PLP	D	501	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	PLP	P-O4P	5.25	1.77	1.60
3	D	501	PLP	P-O4P	4.42	1.74	1.60
3	A	502	PLP	P-O4P	4.40	1.74	1.60
3	B	504	PLP	P-O4P	2.32	1.67	1.60

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	PLP	O4P-C5A-C5	7.36	123.39	109.35
3	D	501	PLP	O4P-C5A-C5	6.95	122.60	109.35
3	B	504	PLP	O4P-C5A-C5	6.51	121.76	109.35
3	D	501	PLP	O4P-P-O1P	-6.50	88.25	106.47
3	C	501	PLP	O3P-P-O4P	-6.37	89.79	106.73
3	A	502	PLP	O4P-C5A-C5	6.18	121.12	109.35
3	B	504	PLP	O4P-P-O1P	-4.80	93.01	106.47
3	B	504	PLP	C4A-C4-C5	4.59	125.67	120.94
3	A	502	PLP	C4A-C4-C5	4.58	125.65	120.94
3	D	501	PLP	C4A-C4-C5	4.57	125.65	120.94
3	C	501	PLP	O2P-P-O4P	-4.52	94.71	106.73
3	A	502	PLP	O3P-P-O2P	4.37	124.35	107.64
3	C	501	PLP	O3P-P-O2P	4.22	123.78	107.64
3	A	502	PLP	O3P-P-O4P	-4.20	95.55	106.73
3	D	501	PLP	O2P-P-O4P	-4.19	95.58	106.73
3	A	502	PLP	O2P-P-O4P	-3.82	96.56	106.73
3	C	501	PLP	C4A-C4-C5	3.72	124.77	120.94
3	B	504	PLP	O2P-P-O4P	-2.97	98.83	106.73
3	D	501	PLP	C4A-C4-C3	-2.75	115.83	120.50
3	D	501	PLP	O2P-P-O1P	2.71	121.29	110.68
3	A	502	PLP	C4A-C4-C3	-2.57	116.14	120.50
3	B	504	PLP	C4A-C4-C3	-2.49	116.28	120.50
3	C	501	PLP	C4A-C4-C3	-2.41	116.41	120.50
3	C	501	PLP	O3P-P-O1P	2.36	119.90	110.68
3	C	501	PLP	C6-C5-C4	-2.25	116.39	118.16
3	B	504	PLP	O2P-P-O1P	2.18	119.22	110.68
3	D	501	PLP	O3P-P-O1P	2.17	119.16	110.68
3	D	501	PLP	O3P-P-O2P	2.15	115.86	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
2	B	503	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PLP	1	0
3	C	501	PLP	1	0
3	D	501	PLP	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	451/465 (96%)	0.03	6 (1%) 77 76	12, 25, 44, 67	0
1	B	452/465 (97%)	-0.12	11 (2%) 59 57	10, 21, 40, 62	0
1	C	454/465 (97%)	-0.33	2 (0%) 92 92	9, 15, 28, 50	0
1	D	453/465 (97%)	-0.20	7 (1%) 73 72	10, 19, 38, 63	0
All	All	1810/1860 (97%)	-0.16	26 (1%) 75 74	9, 19, 40, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	LEU	4.8
1	A	396	ASP	4.1
1	B	451	GLN	3.5
1	C	194	ASP	3.2
1	D	454	LYS	3.2
1	D	194	ASP	3.1
1	D	395	PRO	3.0
1	B	6	THR	2.9
1	A	9	GLN	2.8
1	B	455	ALA	2.7
1	B	5	ARG	2.7
1	B	194	ASP	2.6
1	A	193	LYS	2.6
1	D	455	ALA	2.6
1	A	451	GLN	2.6
1	B	395	PRO	2.5
1	B	30	GLN	2.5
1	B	454	LYS	2.4
1	B	396	ASP	2.3
1	D	391	ARG	2.2
1	B	409	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	358	LYS	2.2
1	C	77	ARG	2.2
1	A	410	ARG	2.1
1	B	77	ARG	2.1
1	A	453	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	D	263	9/10	0.95	0.13	19,21,30,31	0
1	OCS	A	263	9/10	0.96	0.10	23,25,31,32	0
1	OCS	C	263	9/10	0.97	0.09	14,15,23,23	0
1	OCS	B	263	9/10	0.98	0.09	17,19,21,23	0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	503	4/4	0.86	0.14	41,42,43,43	0
2	EDO	B	502	4/4	0.88	0.14	39,39,40,41	0
2	EDO	B	501	4/4	0.90	0.13	37,37,39,39	0
3	PLP	B	504	15/16	0.92	0.14	27,29,34,35	0
2	EDO	A	501	4/4	0.93	0.18	36,36,37,38	0
3	PLP	A	502	15/16	0.95	0.12	20,22,26,26	0
3	PLP	C	501	15/16	0.95	0.12	12,15,19,22	0
3	PLP	D	501	15/16	0.95	0.13	16,18,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.