



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:44 PM UTC

PDB ID : 6S54 / pdb_00006s54
Title : Transaminase from Pseudomonas fluorescens
Authors : Smith, P.; Roura Padrosa, D.; Lopez-Gallego, F.; Paradisi, F.; Dreveny, I.
Deposited on : 2019-06-30
Resolution : 2.21 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

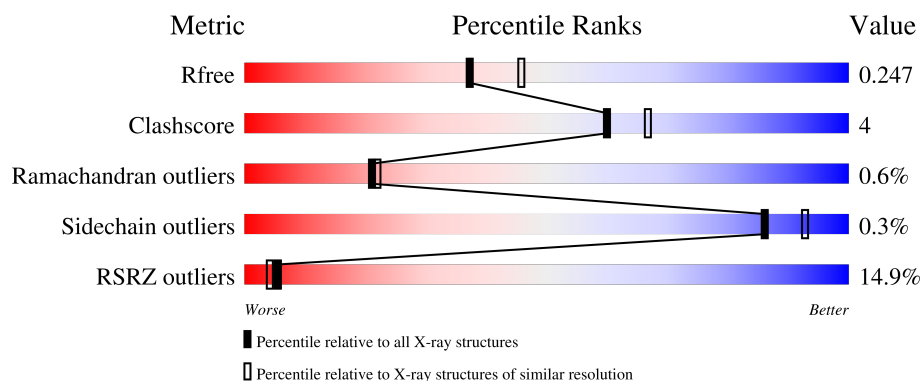
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	479	89% 5% 5%
1	B	479	85% 8% 6%
1	C	479	82% 11% 7%
1	D	479	84% 10% 6%

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	PLP	C	1001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14248 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
1	A	453	Total	C	N	O	S	0	0	0
			3489	2221	603	645	20			
1	B	450	Total	C	N	O	S	0	0	0
			3467	2210	598	639	20			
1	C	447	Total	C	N	O	S	0	0	0
			3432	2186	591	635	20			
1	D	449	Total	C	N	O	S	0	0	0
			3450	2198	595	637	20			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A2S8XV37
A	-18	GLY	-	expression tag	UNP A0A2S8XV37
A	-17	SER	-	expression tag	UNP A0A2S8XV37
A	-16	SER	-	expression tag	UNP A0A2S8XV37
A	-15	HIS	-	expression tag	UNP A0A2S8XV37
A	-14	HIS	-	expression tag	UNP A0A2S8XV37
A	-13	HIS	-	expression tag	UNP A0A2S8XV37
A	-12	HIS	-	expression tag	UNP A0A2S8XV37
A	-11	HIS	-	expression tag	UNP A0A2S8XV37
A	-10	HIS	-	expression tag	UNP A0A2S8XV37
A	-9	SER	-	expression tag	UNP A0A2S8XV37
A	-8	SER	-	expression tag	UNP A0A2S8XV37
A	-7	GLY	-	expression tag	UNP A0A2S8XV37
A	-6	LEU	-	expression tag	UNP A0A2S8XV37
A	-5	VAL	-	expression tag	UNP A0A2S8XV37
A	-4	PRO	-	expression tag	UNP A0A2S8XV37
A	-3	ARG	-	expression tag	UNP A0A2S8XV37
A	-2	GLY	-	expression tag	UNP A0A2S8XV37
A	-1	SER	-	expression tag	UNP A0A2S8XV37
A	0	HIS	-	expression tag	UNP A0A2S8XV37
A	1	MET	-	expression tag	UNP A0A2S8XV37

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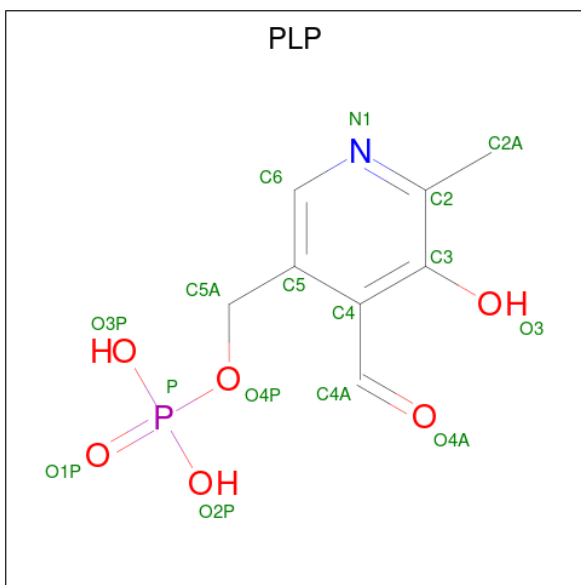
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP A0A2S8XV37
A	3	PHE	-	expression tag	UNP A0A2S8XV37
A	4	LYS	-	expression tag	UNP A0A2S8XV37
A	5	ARG	-	expression tag	UNP A0A2S8XV37
A	6	SER	-	expression tag	UNP A0A2S8XV37
B	-19	MET	-	initiating methionine	UNP A0A2S8XV37
B	-18	GLY	-	expression tag	UNP A0A2S8XV37
B	-17	SER	-	expression tag	UNP A0A2S8XV37
B	-16	SER	-	expression tag	UNP A0A2S8XV37
B	-15	HIS	-	expression tag	UNP A0A2S8XV37
B	-14	HIS	-	expression tag	UNP A0A2S8XV37
B	-13	HIS	-	expression tag	UNP A0A2S8XV37
B	-12	HIS	-	expression tag	UNP A0A2S8XV37
B	-11	HIS	-	expression tag	UNP A0A2S8XV37
B	-10	HIS	-	expression tag	UNP A0A2S8XV37
B	-9	SER	-	expression tag	UNP A0A2S8XV37
B	-8	SER	-	expression tag	UNP A0A2S8XV37
B	-7	GLY	-	expression tag	UNP A0A2S8XV37
B	-6	LEU	-	expression tag	UNP A0A2S8XV37
B	-5	VAL	-	expression tag	UNP A0A2S8XV37
B	-4	PRO	-	expression tag	UNP A0A2S8XV37
B	-3	ARG	-	expression tag	UNP A0A2S8XV37
B	-2	GLY	-	expression tag	UNP A0A2S8XV37
B	-1	SER	-	expression tag	UNP A0A2S8XV37
B	0	HIS	-	expression tag	UNP A0A2S8XV37
B	1	MET	-	expression tag	UNP A0A2S8XV37
B	2	GLU	-	expression tag	UNP A0A2S8XV37
B	3	PHE	-	expression tag	UNP A0A2S8XV37
B	4	LYS	-	expression tag	UNP A0A2S8XV37
B	5	ARG	-	expression tag	UNP A0A2S8XV37
B	6	SER	-	expression tag	UNP A0A2S8XV37
C	-19	MET	-	initiating methionine	UNP A0A2S8XV37
C	-18	GLY	-	expression tag	UNP A0A2S8XV37
C	-17	SER	-	expression tag	UNP A0A2S8XV37
C	-16	SER	-	expression tag	UNP A0A2S8XV37
C	-15	HIS	-	expression tag	UNP A0A2S8XV37
C	-14	HIS	-	expression tag	UNP A0A2S8XV37
C	-13	HIS	-	expression tag	UNP A0A2S8XV37
C	-12	HIS	-	expression tag	UNP A0A2S8XV37
C	-11	HIS	-	expression tag	UNP A0A2S8XV37
C	-10	HIS	-	expression tag	UNP A0A2S8XV37
C	-9	SER	-	expression tag	UNP A0A2S8XV37

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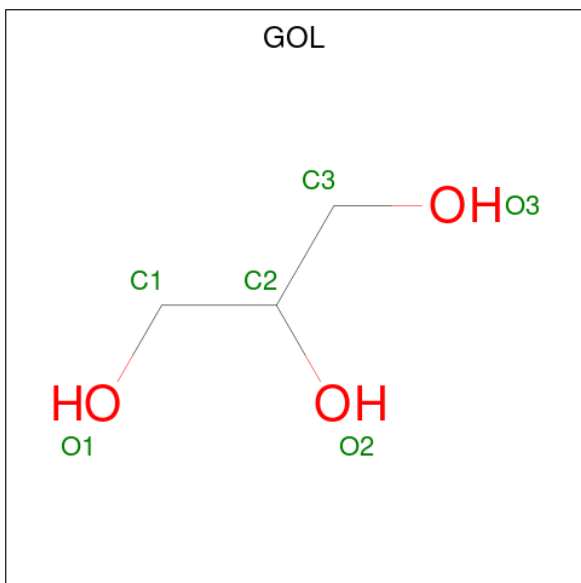
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP A0A2S8XV37
C	-7	GLY	-	expression tag	UNP A0A2S8XV37
C	-6	LEU	-	expression tag	UNP A0A2S8XV37
C	-5	VAL	-	expression tag	UNP A0A2S8XV37
C	-4	PRO	-	expression tag	UNP A0A2S8XV37
C	-3	ARG	-	expression tag	UNP A0A2S8XV37
C	-2	GLY	-	expression tag	UNP A0A2S8XV37
C	-1	SER	-	expression tag	UNP A0A2S8XV37
C	0	HIS	-	expression tag	UNP A0A2S8XV37
C	1	MET	-	expression tag	UNP A0A2S8XV37
C	2	GLU	-	expression tag	UNP A0A2S8XV37
C	3	PHE	-	expression tag	UNP A0A2S8XV37
C	4	LYS	-	expression tag	UNP A0A2S8XV37
C	5	ARG	-	expression tag	UNP A0A2S8XV37
C	6	SER	-	expression tag	UNP A0A2S8XV37
D	-19	MET	-	initiating methionine	UNP A0A2S8XV37
D	-18	GLY	-	expression tag	UNP A0A2S8XV37
D	-17	SER	-	expression tag	UNP A0A2S8XV37
D	-16	SER	-	expression tag	UNP A0A2S8XV37
D	-15	HIS	-	expression tag	UNP A0A2S8XV37
D	-14	HIS	-	expression tag	UNP A0A2S8XV37
D	-13	HIS	-	expression tag	UNP A0A2S8XV37
D	-12	HIS	-	expression tag	UNP A0A2S8XV37
D	-11	HIS	-	expression tag	UNP A0A2S8XV37
D	-10	HIS	-	expression tag	UNP A0A2S8XV37
D	-9	SER	-	expression tag	UNP A0A2S8XV37
D	-8	SER	-	expression tag	UNP A0A2S8XV37
D	-7	GLY	-	expression tag	UNP A0A2S8XV37
D	-6	LEU	-	expression tag	UNP A0A2S8XV37
D	-5	VAL	-	expression tag	UNP A0A2S8XV37
D	-4	PRO	-	expression tag	UNP A0A2S8XV37
D	-3	ARG	-	expression tag	UNP A0A2S8XV37
D	-2	GLY	-	expression tag	UNP A0A2S8XV37
D	-1	SER	-	expression tag	UNP A0A2S8XV37
D	0	HIS	-	expression tag	UNP A0A2S8XV37
D	1	MET	-	expression tag	UNP A0A2S8XV37
D	2	GLU	-	expression tag	UNP A0A2S8XV37
D	3	PHE	-	expression tag	UNP A0A2S8XV37
D	4	LYS	-	expression tag	UNP A0A2S8XV37
D	5	ARG	-	expression tag	UNP A0A2S8XV37
D	6	SER	-	expression tag	UNP A0A2S8XV37

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



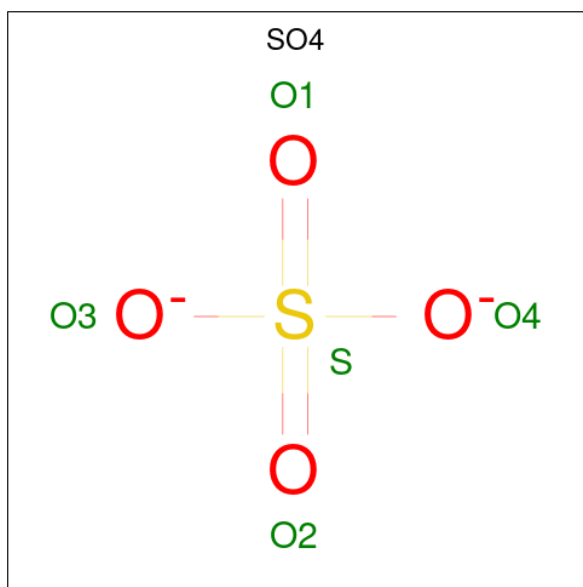
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- 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		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

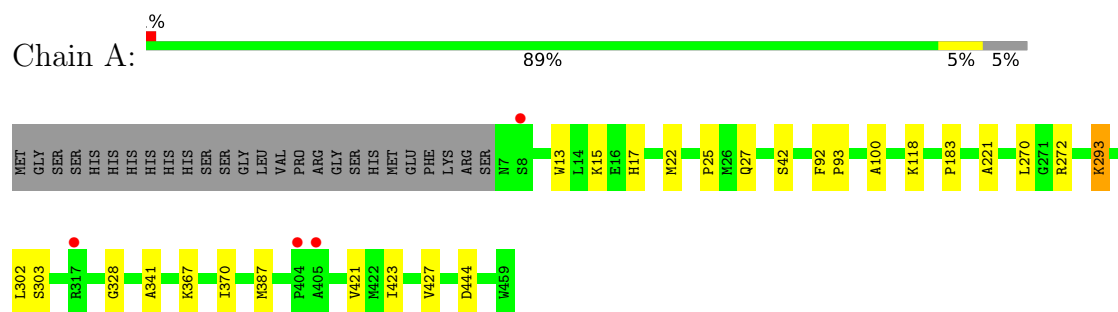
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total	O	0	0
			158	158		
5	B	126	Total	O	0	0
			126	126		
5	C	26	Total	O	0	0
			26	26		
5	D	18	Total	O	0	0
			18	18		

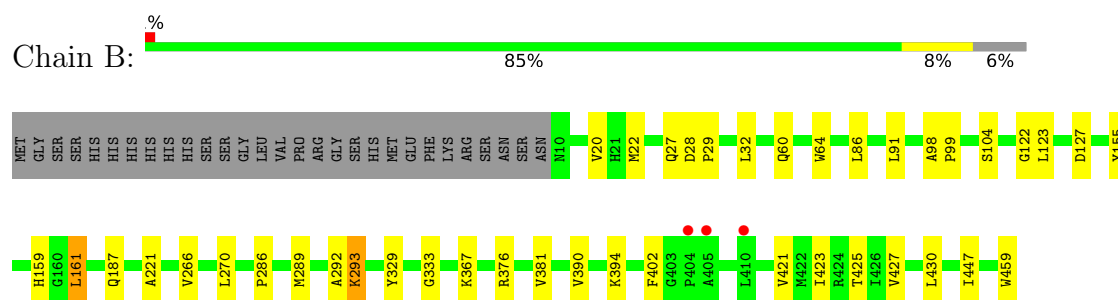
3 Residue-property plots [i](#)

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

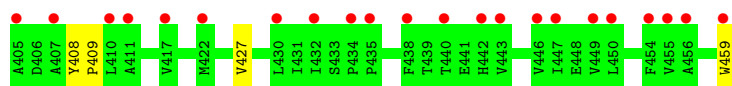


- Molecule 1: Aspartate aminotransferase family protein

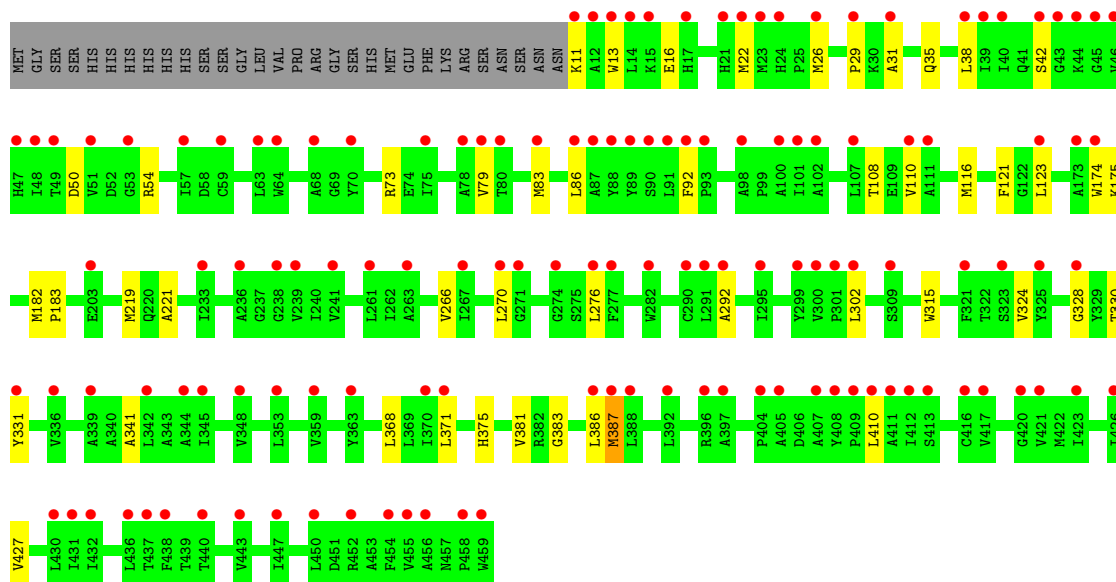
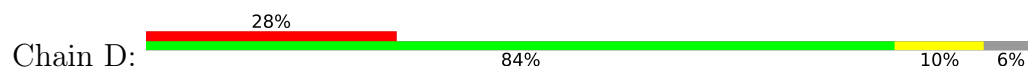


- Molecule 1: Aspartate aminotransferase family protein





- Molecule 1: Aspartate aminotransferase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 94.54Å 242.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.07 – 2.21 88.07 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.07-2.21) 99.9 (88.07-2.21)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.244 0.216 , 0.247	Depositor DCC
R_{free} test set	5329 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	1.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14248	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, GOL, 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	0.50	0/3570	0.67	0/4846
1	B	0.58	6/3548 (0.2%)	0.70	0/4816
1	C	0.32	0/3511	0.58	0/4767
1	D	0.32	1/3529 (0.0%)	0.57	0/4789
All	All	0.44	7/14158 (0.0%)	0.64	0/19218

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	ASP	C-O	-6.28	1.16	1.24
1	B	29	PRO	C-O	-5.92	1.16	1.24
1	B	161	LEU	C-N	5.82	1.41	1.33
1	D	42	SER	C-N	5.65	1.39	1.33
1	B	159	HIS	CE1-NE2	-5.62	1.26	1.32
1	B	159	HIS	CG-ND1	-5.21	1.32	1.38
1	B	159	HIS	CD2-NE2	-5.14	1.32	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	LEU	Peptide
1	B	270	LEU	Peptide
1	C	270	LEU	Peptide
1	D	270	LEU	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	3489	0	3469	20	0
1	B	3467	0	3452	28	0
1	C	3432	0	3409	56	0
1	D	3450	0	3435	39	0
2	A	15	0	6	3	0
2	B	15	0	6	4	0
2	C	15	0	6	14	0
2	D	15	0	6	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	158	0	0	2	0
5	B	126	0	0	1	0
5	C	26	0	0	0	0
5	D	18	0	0	1	0
All	All	14248	0	13805	120	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 4.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LYS:NZ	2:C:1001:PLP:C4A	1.77	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LYS:HZ1	2:C:1001:PLP:C4A	1.29	1.42
1:A:293:LYS:NZ	2:A:501:PLP:C4A	2.07	1.18
1:A:293:LYS:HZ1	2:A:501:PLP:C4A	1.57	1.18
1:B:293:LYS:HZ1	2:B:501:PLP:C4A	1.70	1.04
1:B:293:LYS:NZ	2:B:501:PLP:C4A	2.21	1.03
1:C:293:LYS:HZ3	2:C:1001:PLP:C4A	1.68	0.95
1:A:293:LYS:HZ2	2:A:501:PLP:C4A	1.87	0.86
1:C:293:LYS:HZ1	2:C:1001:PLP:C4	1.90	0.84
1:C:293:LYS:CE	2:C:1001:PLP:C4A	2.62	0.77
1:C:50:ASP:OD2	1:C:54:ARG:NE	2.20	0.75
1:C:375:HIS:O	1:C:396:ARG:NH2	2.24	0.70
1:D:26:MET:HE1	1:D:174:TRP:HE1	1.56	0.70
1:B:293:LYS:HZ2	2:B:501:PLP:C4A	2.02	0.70
1:B:376:ARG:NH1	1:B:459:TRP:O	2.25	0.70
1:C:119:ALA:HB3	1:D:22:MET:HE1	1.75	0.68
1:C:16:GLU:HG3	1:C:17:HIS:CD2	2.30	0.65
1:B:293:LYS:NZ	2:B:501:PLP:O3	2.32	0.63
1:C:264:ASP:CG	2:C:1001:PLP:H2A3	2.25	0.62
1:C:119:ALA:HB3	1:D:22:MET:CE	2.31	0.61
1:D:31:ALA:O	1:D:35:GLN:HG2	2.01	0.61
1:C:125:GLY:C	2:C:1001:PLP:H5A2	2.27	0.60
1:C:83:MET:HE1	1:D:79:VAL:HG11	1.85	0.59
1:A:272:ARG:HG2	1:A:387:MET:HE2	1.85	0.58
1:D:38:LEU:HD22	1:D:54:ARG:HH22	1.69	0.58
1:C:126:SER:N	2:C:1001:PLP:H5A2	2.17	0.58
1:C:38:LEU:HD22	1:C:54:ARG:HH22	1.68	0.58
1:B:64:TRP:HB2	1:B:293:LYS:HD3	1.85	0.58
1:B:266:VAL:HG13	1:B:292:ALA:HB3	1.87	0.57
1:C:346:ASP:O	1:C:350:GLN:HG2	2.05	0.57
1:C:22:MET:HE1	1:D:121:PHE:HE2	1.71	0.56
1:A:183:PRO:HG3	1:D:183:PRO:HG3	1.89	0.55
1:C:264:ASP:OD2	2:C:1001:PLP:H2A3	2.08	0.54
1:C:123:LEU:N	1:C:127:ASP:OD2	2.27	0.52
1:C:192:HIS:HD1	1:C:195:ARG:HB2	1.74	0.52
1:D:368:LEU:HB3	1:D:381:VAL:HG11	1.91	0.51
1:D:31:ALA:HB1	1:D:35:GLN:NE2	2.26	0.51
1:C:266:VAL:HG12	1:C:293:LYS:HD2	1.91	0.51
1:B:122:GLY:C	1:B:123:LEU:HD22	2.35	0.51
1:C:268:THR:HG22	1:C:387:MET:HE1	1.93	0.51
2:C:1001:PLP:O1P	1:D:330:THR:HB	2.11	0.50
1:B:155:TYR:CE1	1:C:219:MET:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:HE2	1:B:20:VAL:O	2.11	0.50
1:C:363:TYR:CZ	1:C:367:LYS:HE2	2.45	0.49
1:C:38:LEU:HD22	1:C:54:ARG:NH2	2.27	0.49
1:B:91:LEU:HD11	1:B:333:GLY:HA3	1.93	0.49
1:C:84:GLU:OE1	1:D:73:ARG:NH1	2.45	0.49
1:B:60:GLN:HG2	5:B:675:HOH:O	2.12	0.49
1:A:100:ALA:HB1	1:B:22:MET:HE1	1.93	0.49
1:C:104:SER:OG	1:C:105:GLN:N	2.44	0.49
1:C:25:PRO:HB3	1:D:328:GLY:HA3	1.94	0.49
1:C:79:VAL:HG11	1:D:83:MET:HE1	1.95	0.49
1:D:13:TRP:O	1:D:16:GLU:HG2	2.12	0.48
1:A:302:LEU:HD22	1:A:341:ALA:HB2	1.95	0.48
1:C:384:LYS:O	1:C:387:MET:HG2	2.13	0.48
1:D:50:ASP:OD2	1:D:54:ARG:NE	2.43	0.48
1:A:13:TRP:CE2	1:A:17:HIS:CD2	3.02	0.47
1:D:38:LEU:HD22	1:D:54:ARG:NH2	2.28	0.47
1:B:421:VAL:HG12	1:B:423:ILE:HG13	1.97	0.47
1:C:16:GLU:HG3	1:C:17:HIS:HD2	1.77	0.47
1:C:125:GLY:HA3	2:C:1001:PLP:C5A	2.45	0.47
1:C:42:SER:HA	1:D:86:LEU:HB2	1.96	0.47
1:D:108:THR:HG23	1:D:116:MET:O	2.15	0.47
1:D:371:LEU:HD11	1:D:375:HIS:HD2	1.80	0.47
1:A:421:VAL:HG12	1:A:423:ILE:HG13	1.96	0.46
1:C:125:GLY:CA	2:C:1001:PLP:H5A2	2.44	0.46
1:D:175:LYS:NZ	5:D:901:HOH:O	2.45	0.46
1:C:127:ASP:OD1	1:C:128:ALA:N	2.49	0.46
1:A:370:ILE:HD11	5:A:742:HOH:O	2.15	0.46
1:C:125:GLY:HA3	2:C:1001:PLP:H5A2	1.98	0.45
1:A:328:GLY:O	1:B:161:LEU:CD1	2.65	0.45
1:D:371:LEU:CD1	1:D:375:HIS:HD2	2.30	0.45
1:B:155:TYR:CD1	1:C:219:MET:HG3	2.52	0.45
1:C:27:GLN:OE1	1:C:32:LEU:HD21	2.17	0.45
1:D:110:VAL:HG13	1:D:276:LEU:HD21	1.99	0.45
1:B:123:LEU:HD22	1:B:123:LEU:N	2.33	0.44
1:C:40:ILE:HA	1:C:50:ASP:HA	1.98	0.44
1:C:110:VAL:HG13	1:C:276:LEU:HD21	1.98	0.44
1:D:410:LEU:HD22	1:D:410:LEU:H	1.81	0.44
1:C:192:HIS:ND1	1:C:195:ARG:HB2	2.32	0.44
1:D:26:MET:HE1	1:D:174:TRP:NE1	2.27	0.44
1:A:15:LYS:NZ	5:A:619:HOH:O	2.50	0.43
1:B:394:LYS:HG2	1:B:402:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:O	1:A:27:GLN:HG3	2.19	0.43
1:D:368:LEU:CB	1:D:381:VAL:HG11	2.49	0.43
1:C:408:TYR:CE2	1:C:459:TRP:HB2	2.53	0.43
1:B:187:GLN:OE1	1:C:219:MET:HE1	2.19	0.43
1:C:219:MET:HB3	1:C:219:MET:HE3	1.50	0.43
1:B:367:LYS:HD3	1:B:447:ILE:HG13	2.00	0.42
1:D:266:VAL:HG13	1:D:292:ALA:HB3	2.01	0.42
1:B:27:GLN:NE2	1:B:32:LEU:HD21	2.34	0.42
1:C:28:ASP:HB2	1:D:324:VAL:HG22	2.00	0.42
1:B:381:VAL:HG22	1:B:390:VAL:HG22	2.00	0.42
1:C:103:LEU:HD21	1:C:302:LEU:HD21	2.01	0.42
1:A:22:MET:HE2	1:B:104:SER:HB3	2.01	0.42
1:C:29:PRO:CG	1:D:315:TRP:HB3	2.50	0.42
1:A:272:ARG:CG	1:A:387:MET:HE2	2.49	0.41
1:B:286:PRO:HG2	1:B:289:MET:HG2	2.01	0.41
1:C:408:TYR:HB3	1:C:409:PRO:HD3	2.02	0.41
1:A:42:SER:HA	1:B:86:LEU:HB2	2.03	0.41
1:B:98:ALA:HB3	1:B:99:PRO:HD3	2.03	0.41
1:D:123:LEU:HD11	1:D:331:TYR:HB2	2.02	0.41
1:B:127:ASP:HB2	1:B:329:TYR:CZ	2.55	0.41
1:C:26:MET:HG3	1:D:92:PHE:CE2	2.56	0.41
1:C:127:ASP:HB2	1:C:329:TYR:CZ	2.56	0.41
1:D:302:LEU:HD23	1:D:341:ALA:HB2	2.02	0.41
1:A:302:LEU:HG	1:A:303:SER:N	2.35	0.41
1:A:367:LYS:NZ	1:A:444:ASP:OD1	2.32	0.41
1:C:29:PRO:HG3	1:D:315:TRP:HB3	2.02	0.41
1:C:182:MET:SD	1:D:182:MET:HG2	2.60	0.41
1:C:264:ASP:CG	2:C:1001:PLP:C2A	2.93	0.41
1:A:92:PHE:O	1:A:93:PRO:C	2.64	0.41
1:B:425:THR:HG22	1:B:430:LEU:HD23	2.03	0.41
1:D:13:TRP:HA	1:D:16:GLU:HG2	2.01	0.40
1:C:123:LEU:HD11	1:C:331:TYR:HB2	2.04	0.40
1:D:383:GLY:HA2	1:D:387:MET:O	2.21	0.40
3:B:502:GOL:O3	1:C:188:VAL:HA	2.22	0.40
1:C:315:TRP:HB3	1:D:29:PRO:HG2	2.02	0.40
1:D:35:GLN:HG3	1:D:35:GLN:O	2.22	0.40
1:D:386:LEU:HD23	1:D:386:LEU:HA	1.98	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	451/479 (94%)	434 (96%)	14 (3%)	3 (1%)	18	18
1	B	448/479 (94%)	431 (96%)	14 (3%)	3 (1%)	18	18
1	C	445/479 (93%)	427 (96%)	16 (4%)	2 (0%)	30	33
1	D	447/479 (93%)	430 (96%)	15 (3%)	2 (0%)	30	33
All	All	1791/1916 (94%)	1722 (96%)	59 (3%)	10 (1%)	21	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ALA
1	A	427	VAL
1	B	221	ALA
1	B	293	LYS
1	B	427	VAL
1	C	221	ALA
1	C	427	VAL
1	D	221	ALA
1	D	427	VAL
1	A	293	LYS

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	366/389 (94%)	366 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	363/389 (93%)	363 (100%)	0	100	100
1	C	359/389 (92%)	357 (99%)	2 (1%)	78	88
1	D	361/389 (93%)	358 (99%)	3 (1%)	73	84
All	All	1449/1556 (93%)	1444 (100%)	5 (0%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	73	ARG
1	C	219	MET
1	D	11	LYS
1	D	219	MET
1	D	387	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	138	GLN
1	A	192	HIS
1	A	356	ASN
1	B	27	GLN
1	B	138	GLN
1	B	356	ASN
1	C	138	GLN
1	C	162	ASN
1	C	192	HIS
1	D	35	GLN
1	D	60	GLN
1	D	138	GLN
1	D	162	ASN
1	D	192	HIS
1	D	375	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	PLP	A	501	-	15,15,16	0.77	1 (6%)	21,22,23	0.59	0
2	PLP	D	801	1	15,15,16	0.76	1 (6%)	21,22,23	0.60	0
2	PLP	B	501	-	15,15,16	0.76	1 (6%)	21,22,23	0.61	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.31	0
3	GOL	A	502	-	5,5,5	0.09	0	5,5,5	0.31	0
2	PLP	C	1001	-	15,15,16	0.77	1 (6%)	21,22,23	0.60	0
4	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.41	0
4	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.15	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	PLP	A	501	-	-	0/6/6/8	0/1/1/1
2	PLP	D	801	1	-	5/6/6/8	0/1/1/1
2	PLP	B	501	-	-	2/6/6/8	0/1/1/1
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	1001	-	-	2/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	PLP	C4A-C4	-2.40	1.46	1.51
2	A	501	PLP	C4A-C4	-2.40	1.46	1.51
2	B	501	PLP	C4A-C4	-2.39	1.46	1.51
2	D	801	PLP	C4A-C4	-2.36	1.46	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PLP	C4-C5-C5A-O4P
2	B	501	PLP	C6-C5-C5A-O4P
2	C	1001	PLP	C4-C5-C5A-O4P
2	C	1001	PLP	C6-C5-C5A-O4P
3	A	502	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-O2
2	D	801	PLP	C5A-O4P-P-O3P
2	D	801	PLP	C4-C5-C5A-O4P
2	D	801	PLP	C5A-O4P-P-O1P
2	D	801	PLP	C6-C5-C5A-O4P
2	D	801	PLP	C5A-O4P-P-O2P

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PLP	3	0
2	B	501	PLP	4	0
3	B	502	GOL	1	0
2	C	1001	PLP	14	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	453/479 (94%)	-0.24	4 (0%) 81 79	21, 34, 54, 94	0
1	B	450/479 (93%)	-0.14	3 (0%) 84 83	23, 37, 60, 94	0
1	C	447/479 (93%)	1.42	129 (28%) 1 1	36, 94, 132, 149	0
1	D	449/479 (93%)	1.46	132 (29%) 1 1	36, 97, 131, 150	0
All	All	1799/1916 (93%)	0.62	268 (14%) 5 4	21, 53, 126, 150	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	13	TRP	5.6
1	D	12	ALA	5.4
1	A	317	ARG	4.8
1	C	87	ALA	4.5
1	D	22	MET	4.5
1	C	302	LEU	4.5
1	C	40	ILE	4.3
1	D	14	LEU	4.3
1	D	13	TRP	4.2
1	C	339	ALA	4.1
1	C	270	LEU	4.1
1	C	368	LEU	4.0
1	C	51	VAL	4.0
1	C	119	ALA	4.0
1	D	38	LEU	3.9
1	D	51	VAL	3.8
1	D	17	HIS	3.8
1	D	68	ALA	3.8
1	C	102	ALA	3.7
1	C	57	ILE	3.7
1	C	49	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	407	ALA	3.7
1	C	299	TYR	3.7
1	D	57	ILE	3.6
1	D	423	ILE	3.6
1	C	14	LEU	3.6
1	D	40	ILE	3.6
1	C	340	ALA	3.5
1	C	405	ALA	3.5
1	D	87	ALA	3.5
1	C	410	LEU	3.5
1	D	405	ALA	3.4
1	D	64	TRP	3.4
1	C	56	PHE	3.4
1	C	343	ALA	3.4
1	C	344	ALA	3.4
1	D	410	LEU	3.3
1	D	421	VAL	3.3
1	C	238	GLY	3.3
1	C	237	GLY	3.3
1	D	91	LEU	3.3
1	D	328	GLY	3.2
1	C	447	ILE	3.2
1	C	121	PHE	3.2
1	C	46	VAL	3.2
1	C	174	TRP	3.2
1	D	102	ALA	3.2
1	C	76	ILE	3.2
1	D	345	ILE	3.2
1	D	59	CYS	3.2
1	C	68	ALA	3.2
1	D	295	ILE	3.2
1	D	43	GLY	3.2
1	D	447	ILE	3.2
1	C	438	PHE	3.1
1	D	89	TYR	3.1
1	C	39	ILE	3.1
1	C	365	LEU	3.1
1	C	404	PRO	3.1
1	C	331	TYR	3.1
1	C	53	GLY	3.1
1	B	405	ALA	3.1
1	C	301	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	299	TYR	3.0
1	D	331	TYR	3.0
1	C	459	TRP	3.0
1	D	174	TRP	3.0
1	D	93	PRO	3.0
1	C	369	LEU	3.0
1	C	370	ILE	3.0
1	D	45	GLY	3.0
1	C	29	PRO	3.0
1	D	432	ILE	3.0
1	D	459	TRP	3.0
1	D	23	MET	3.0
1	D	404	PRO	3.0
1	C	31	ALA	3.0
1	C	78	ALA	3.0
1	C	98	ALA	3.0
1	D	86	LEU	3.0
1	D	359	VAL	3.0
1	D	44	LYS	3.0
1	D	440	THR	3.0
1	D	292	ALA	2.9
1	D	353	LEU	2.9
1	D	300	VAL	2.9
1	D	271	GLY	2.9
1	D	291	LEU	2.9
1	C	417	VAL	2.9
1	C	295	ILE	2.9
1	C	454	PHE	2.9
1	D	450	LEU	2.9
1	D	11	LYS	2.9
1	D	409	PRO	2.9
1	D	412	ILE	2.9
1	D	458	PRO	2.8
1	C	91	LEU	2.8
1	D	436	LEU	2.8
1	C	390	VAL	2.8
1	D	39	ILE	2.8
1	C	32	LEU	2.8
1	C	450	LEU	2.8
1	D	302	LEU	2.8
1	C	321	PHE	2.8
1	D	407	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	48	ILE	2.8
1	D	42	SER	2.8
1	D	274	GLY	2.8
1	C	332	SER	2.8
1	C	20	VAL	2.8
1	C	300	VAL	2.8
1	C	348	VAL	2.7
1	C	440	THR	2.7
1	A	8	SER	2.7
1	A	405	ALA	2.7
1	D	454	PHE	2.7
1	C	446	VAL	2.7
1	D	336	VAL	2.7
1	D	417	VAL	2.7
1	D	49	THR	2.7
1	D	431	ILE	2.7
1	D	301	PRO	2.7
1	D	339	ALA	2.7
1	D	79	VAL	2.7
1	C	30	LYS	2.7
1	D	90	SER	2.7
1	D	342	LEU	2.7
1	D	371	LEU	2.7
1	D	363	TYR	2.6
1	C	239	VAL	2.6
1	D	426	ILE	2.6
1	C	376	ARG	2.6
1	C	271	GLY	2.6
1	C	449	VAL	2.6
1	C	276	LEU	2.6
1	C	430	LEU	2.6
1	D	386	LEU	2.6
1	D	98	ALA	2.6
1	C	45	GLY	2.5
1	C	435	PRO	2.5
1	C	110	VAL	2.5
1	C	75	ILE	2.5
1	D	323	SER	2.5
1	D	123	LEU	2.5
1	D	236	ALA	2.5
1	C	361	GLY	2.5
1	D	416	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	370	ILE	2.5
1	D	452	ARG	2.5
1	C	388	LEU	2.5
1	D	21	HIS	2.5
1	D	397	ALA	2.5
1	C	455	VAL	2.4
1	C	89	TYR	2.4
1	C	71	GLY	2.4
1	C	233	ILE	2.4
1	D	408	TYR	2.4
1	D	78	ALA	2.4
1	D	456	ALA	2.4
1	C	267	ILE	2.4
1	C	336	VAL	2.4
1	D	75	ILE	2.4
1	D	233	ILE	2.4
1	D	88	TYR	2.4
1	D	420	GLY	2.4
1	C	330	THR	2.4
1	C	123	LEU	2.4
1	D	430	LEU	2.4
1	C	94	GLY	2.3
1	C	236	ALA	2.3
1	C	387	MET	2.3
1	C	381	VAL	2.3
1	D	290	CYS	2.3
1	D	270	LEU	2.3
1	D	276	LEU	2.3
1	C	315	TRP	2.3
1	D	83	MET	2.3
1	C	364	PHE	2.3
1	D	277	PHE	2.3
1	C	86	LEU	2.3
1	C	282	TRP	2.3
1	C	22	MET	2.3
1	C	314	ALA	2.3
1	C	319	ALA	2.3
1	D	387	MET	2.3
1	D	411	ALA	2.3
1	C	80	THR	2.3
1	D	437	THR	2.3
1	C	79	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	46	VAL	2.3
1	D	63	LEU	2.3
1	D	111	ALA	2.3
1	C	366	GLU	2.3
1	C	63	LEU	2.2
1	C	349	LEU	2.2
1	D	92	PHE	2.2
1	D	388	LEU	2.2
1	C	289	MET	2.2
1	C	396	ARG	2.2
1	C	291	LEU	2.2
1	C	342	LEU	2.2
1	D	348	VAL	2.2
1	C	59	CYS	2.2
1	D	29	PRO	2.2
1	D	53	GLY	2.2
1	C	21	HIS	2.2
1	D	413	SER	2.2
1	D	267	ILE	2.2
1	C	83	MET	2.2
1	C	333	GLY	2.2
1	C	442	HIS	2.2
1	D	325	TYR	2.2
1	C	371	LEU	2.2
1	D	107	LEU	2.2
1	C	24	HIS	2.2
1	D	47	HIS	2.2
1	D	80	THR	2.2
1	D	344	ALA	2.2
1	D	70	TYR	2.1
1	C	353	LEU	2.1
1	D	48	ILE	2.1
1	D	455	VAL	2.1
1	D	321	PHE	2.1
1	C	456	ALA	2.1
1	D	173	ALA	2.1
1	D	396	ARG	2.1
1	C	386	LEU	2.1
1	D	26	MET	2.1
1	D	15	LYS	2.1
1	D	392	LEU	2.1
1	B	404	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	17	HIS	2.1
1	C	64	TRP	2.1
1	C	443	VAL	2.1
1	D	238	GLY	2.1
1	B	410	LEU	2.1
1	C	38	LEU	2.1
1	C	392	LEU	2.1
1	D	101	ILE	2.1
1	A	404	PRO	2.1
1	C	66	VAL	2.1
1	D	239	VAL	2.1
1	D	309	SER	2.1
1	C	15	LYS	2.1
1	C	411	ALA	2.1
1	D	100	ALA	2.1
1	C	422	MET	2.1
1	C	107	LEU	2.1
1	C	200	ASN	2.1
1	C	347	ILE	2.1
1	C	360	VAL	2.1
1	D	110	VAL	2.1
1	C	92	PHE	2.1
1	D	438	PHE	2.1
1	D	282	TRP	2.1
1	C	19	THR	2.0
1	D	31	ALA	2.0
1	D	203	GLU	2.0
1	C	327	HIS	2.0
1	D	24	HIS	2.0
1	C	103	LEU	2.0
1	D	261	LEU	2.0
1	D	241	VAL	2.0
1	D	443	VAL	2.0
1	C	26	MET	2.0
1	D	263	ALA	2.0
1	C	432	ILE	2.0
1	C	434	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
2	PLP	D	801	15/16	0.85	0.17	79,97,106,109	0
2	PLP	C	1001	15/16	0.86	0.13	57,69,89,95	0
3	GOL	A	502	6/6	0.93	0.12	49,54,57,59	0
3	GOL	B	502	6/6	0.93	0.13	39,58,61,62	0
2	PLP	B	501	15/16	0.94	0.08	18,26,33,34	0
4	SO4	A	503	5/5	0.95	0.09	55,58,61,66	0
2	PLP	A	501	15/16	0.96	0.08	15,26,31,40	0
4	SO4	B	503	5/5	0.96	0.08	49,55,57,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.