



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:19 AM UTC

PDB ID : 5O1O / pdb_00005o1o
Title : Crystal structure of human aminoadipate semialdehyde synthase, saccharopine dehydrogenase domain with proline bound.
Authors : Kopec, J.; Rembeza, E.; Pena, I.A.; Mathea, S.; Velupillai, S.; Strain-Damerell, C.; Goubin, S.; Kupinska, K.; Talon, R.; Collins, P.; Krojer, T.; Burgess-Brown, N.; Arrowsmith, C.; Edwards, A.; Bountra, C.; von Delft, F.; Arruda, P.; Yue, W.W.
Deposited on : 2017-05-18
Resolution : 2.48 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)

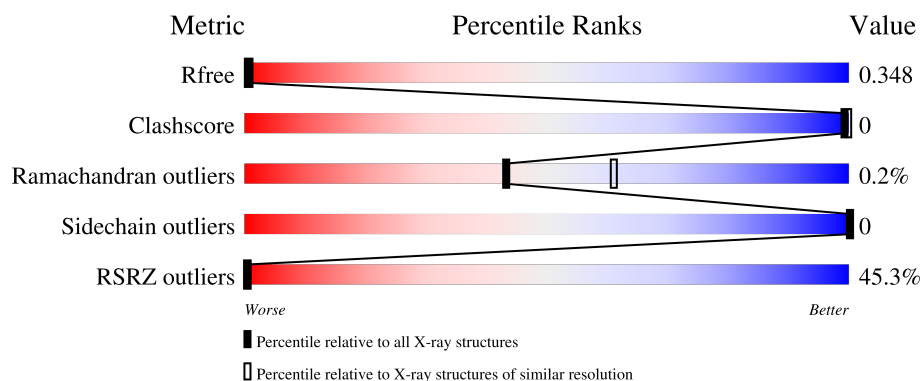
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	497	
1	B	497	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6529 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 Alpha-aminoadipic semialdehyde synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3262	2087	530	626	19			
1	B	435	Total	C	N	O	S	0	1	0
			3231	2068	523	620	20			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	MET	-	initiating methionine	UNP Q9UDR5
A	431	GLY	-	expression tag	UNP Q9UDR5
A	432	HIS	-	expression tag	UNP Q9UDR5
A	433	HIS	-	expression tag	UNP Q9UDR5
A	434	HIS	-	expression tag	UNP Q9UDR5
A	435	HIS	-	expression tag	UNP Q9UDR5
A	436	HIS	-	expression tag	UNP Q9UDR5
A	437	HIS	-	expression tag	UNP Q9UDR5
A	438	SER	-	expression tag	UNP Q9UDR5
A	439	SER	-	expression tag	UNP Q9UDR5
A	440	GLY	-	expression tag	UNP Q9UDR5
A	441	VAL	-	expression tag	UNP Q9UDR5
A	442	ASP	-	expression tag	UNP Q9UDR5
A	443	LEU	-	expression tag	UNP Q9UDR5
A	444	GLY	-	expression tag	UNP Q9UDR5
A	445	THR	-	expression tag	UNP Q9UDR5
A	446	GLU	-	expression tag	UNP Q9UDR5
A	447	ASN	-	expression tag	UNP Q9UDR5
A	448	LEU	-	expression tag	UNP Q9UDR5
A	449	TYR	-	expression tag	UNP Q9UDR5
A	450	PHE	-	expression tag	UNP Q9UDR5
A	451	GLN	-	expression tag	UNP Q9UDR5
A	452	SER	-	expression tag	UNP Q9UDR5
A	453	MET	-	expression tag	UNP Q9UDR5
A	454	ALA	-	expression tag	UNP Q9UDR5

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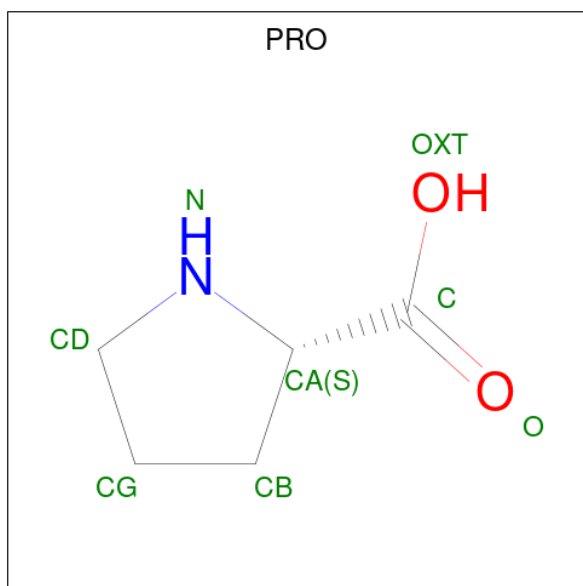
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	SER	THR	cloning artifact	UNP Q9UDR5
B	430	MET	-	initiating methionine	UNP Q9UDR5
B	431	GLY	-	expression tag	UNP Q9UDR5
B	432	HIS	-	expression tag	UNP Q9UDR5
B	433	HIS	-	expression tag	UNP Q9UDR5
B	434	HIS	-	expression tag	UNP Q9UDR5
B	435	HIS	-	expression tag	UNP Q9UDR5
B	436	HIS	-	expression tag	UNP Q9UDR5
B	437	HIS	-	expression tag	UNP Q9UDR5
B	438	SER	-	expression tag	UNP Q9UDR5
B	439	SER	-	expression tag	UNP Q9UDR5
B	440	GLY	-	expression tag	UNP Q9UDR5
B	441	VAL	-	expression tag	UNP Q9UDR5
B	442	ASP	-	expression tag	UNP Q9UDR5
B	443	LEU	-	expression tag	UNP Q9UDR5
B	444	GLY	-	expression tag	UNP Q9UDR5
B	445	THR	-	expression tag	UNP Q9UDR5
B	446	GLU	-	expression tag	UNP Q9UDR5
B	447	ASN	-	expression tag	UNP Q9UDR5
B	448	LEU	-	expression tag	UNP Q9UDR5
B	449	TYR	-	expression tag	UNP Q9UDR5
B	450	PHE	-	expression tag	UNP Q9UDR5
B	451	GLN	-	expression tag	UNP Q9UDR5
B	452	SER	-	expression tag	UNP Q9UDR5
B	453	MET	-	expression tag	UNP Q9UDR5
B	454	ALA	-	expression tag	UNP Q9UDR5
B	615	SER	THR	cloning artifact	UNP Q9UDR5

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: 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		

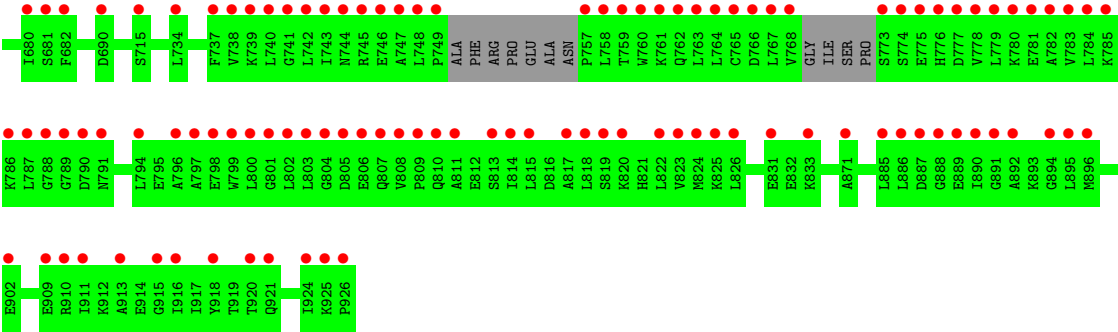
- Molecule 3 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	6	Total 6	O 6	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.37Å 102.41Å 142.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.08 – 2.48 83.08 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.8 (83.08-2.48) 93.0 (83.08-2.48)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.322 , 0.348 0.322 , 0.348	Depositor DCC
R_{free} test set	2331 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6529	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: 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	0.53	0/3322	0.74	0/4514
1	B	0.53	0/3290	0.74	0/4468
All	All	0.53	0/6612	0.74	0/8982

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

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	3262	0	3227	2	0
1	B	3231	0	3184	0	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
3	A	8	0	7	0	0
3	B	8	0	7	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
All	All	6529	0	6437	2	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 0.

All (2) 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:695:LEU:HD23	1:A:697:LEU:HD11	1.93	0.50
1:A:700:TYR:CZ	1:A:731:MET:HE2	2.49	0.47

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	435/497 (88%)	412 (95%)	21 (5%)	2 (0%)	24	40
1	B	430/497 (86%)	407 (95%)	23 (5%)	0	100	100
All	All	865/994 (87%)	819 (95%)	44 (5%)	2 (0%)	43	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	703	ARG
1	A	898	PRO

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	343/418 (82%)	343 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	338/418 (81%)	338 (100%)	0	100	100
All	All	681/836 (82%)	681 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	547	GLN
1	A	756	ASN
1	B	516	GLN
1	B	547	GLN
1	B	865	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](#)

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](#)

4 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	1001	-	3,3,3	0.43	0	2,2,2	0.30	0
3	PRO	B	1002	-	8,8,8	0.91	1 (12%)	10,10,10	1.47	2 (20%)
3	PRO	A	1002	-	8,8,8	0.91	1 (12%)	10,10,10	1.42	2 (20%)
2	EDO	A	1001	-	3,3,3	0.43	0	2,2,2	0.32	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	EDO	B	1001	-	-	0/1/1/1	-
3	PRO	B	1002	-	-	2/4/11/11	0/1/1/1
3	PRO	A	1002	-	-	2/4/11/11	0/1/1/1
2	EDO	A	1001	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	PRO	OXT-C	-2.26	1.23	1.30
3	B	1002	PRO	OXT-C	-2.22	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	PRO	OXT-C-O	-2.84	117.64	124.08
3	A	1002	PRO	OXT-C-O	-2.73	117.89	124.08
3	B	1002	PRO	OXT-C-CA	2.40	121.63	113.51
3	A	1002	PRO	OXT-C-CA	2.19	120.91	113.51

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	PRO	O-C-CA-N
3	A	1002	PRO	OXT-C-CA-N
3	B	1002	PRO	OXT-C-CA-CB
3	B	1002	PRO	O-C-CA-CB
2	A	1001	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	439/497 (88%)	1.89	188 (42%) 0 0	36, 61, 88, 95	0
1	B	435/497 (87%)	2.00	208 (47%) 0 0	22, 64, 97, 105	1 (0%)
All	All	874/994 (87%)	1.95	396 (45%) 0 0	22, 62, 92, 105	1 (0%)

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	787	LEU	7.7
1	B	788	GLY	6.8
1	B	748	LEU	6.7
1	A	788	GLY	6.4
1	B	745	ARG	6.1
1	A	655	VAL	5.9
1	B	807	GLN	5.9
1	B	757	PRO	5.8
1	B	789	GLY	5.8
1	A	777	ASP	5.7
1	B	777	ASP	5.5
1	B	779	LEU	5.5
1	A	774	SER	5.4
1	B	542	PHE	5.4
1	B	783	VAL	5.3
1	B	808	VAL	5.2
1	B	760	TRP	5.1
1	B	657	VAL	5.1
1	A	490	TYR	5.0
1	B	749	PRO	4.8
1	A	776	HIS	4.8
1	B	784	LEU	4.6
1	A	656	GLY	4.5
1	B	778	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	595	ILE	4.5
1	A	575	THR	4.4
1	B	534	CYS	4.4
1	A	542	PHE	4.4
1	A	775	GLU	4.4
1	A	549	LEU	4.3
1	B	533	ILE	4.3
1	B	538	GLU	4.3
1	A	771	SER	4.3
1	A	487	GLY	4.2
1	B	768	VAL	4.2
1	B	602	GLY	4.2
1	B	763	LEU	4.1
1	A	657	VAL	4.1
1	B	515	ASN	4.1
1	B	758	LEU	4.1
1	B	767	LEU	4.1
1	B	926	PRO	4.1
1	B	761	LYS	4.0
1	A	510	GLY	4.0
1	A	578	TYR	4.0
1	B	811	ALA	4.0
1	A	529	VAL	3.9
1	A	544	VAL	3.9
1	B	531	MET	3.9
1	A	517	ILE	3.9
1	A	488	SER	3.9
1	B	578	TYR	3.9
1	B	576	ALA	3.9
1	B	514	LYS	3.9
1	B	887	ASP	3.9
1	A	779	LEU	3.8
1	B	787	LEU	3.8
1	B	815	LEU	3.8
1	B	762	GLN	3.8
1	A	765	CYS	3.8
1	A	485	VAL	3.8
1	A	576	ALA	3.8
1	B	782	ALA	3.8
1	A	601	LEU	3.8
1	A	805	ASP	3.8
1	A	602	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	533	ILE	3.7
1	B	658	LEU	3.7
1	A	804	GLY	3.7
1	A	543	LEU	3.7
1	B	528	PRO	3.7
1	A	540	LEU	3.7
1	A	483	VAL	3.7
1	B	574	VAL	3.7
1	B	653	SER	3.7
1	A	538	GLU	3.7
1	B	680	ILE	3.7
1	A	539	LYS	3.7
1	B	523	LYS	3.7
1	B	743	ILE	3.6
1	A	512	ASP	3.6
1	A	652	TRP	3.6
1	A	778	VAL	3.6
1	B	655	VAL	3.6
1	A	615	SER	3.6
1	A	784	LEU	3.6
1	B	776	HIS	3.6
1	B	592	ASP	3.6
1	B	780	LYS	3.5
1	B	652	TRP	3.5
1	A	561	LEU	3.5
1	A	888	GLY	3.5
1	B	747	ALA	3.5
1	A	597	ILE	3.5
1	B	597	ILE	3.5
1	B	810	GLN	3.5
1	B	561	LEU	3.5
1	A	535	LYS	3.5
1	B	481	ARG	3.5
1	B	571	VAL	3.5
1	A	582	ALA	3.5
1	A	505	ILE	3.5
1	B	781	GLU	3.4
1	A	513	MET	3.4
1	B	801	GLY	3.4
1	A	556	TYR	3.4
1	B	814	ILE	3.4
1	B	569	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	803	LEU	3.4
1	A	757	PRO	3.4
1	A	599	GLY	3.4
1	B	891	GLY	3.4
1	A	782	ALA	3.4
1	B	746	GLU	3.4
1	A	514	LYS	3.4
1	B	764	LEU	3.4
1	B	809	PRO	3.4
1	B	594	GLY	3.4
1	B	643[A]	ASN	3.3
1	B	539	LYS	3.3
1	A	756	ASN	3.3
1	A	810	GLN	3.3
1	A	509	VAL	3.3
1	A	673	VAL	3.3
1	A	708	TYR	3.3
1	A	520	LEU	3.3
1	A	531	MET	3.3
1	B	507	ILE	3.3
1	B	805	ASP	3.3
1	B	785	LYS	3.3
1	B	524	TYR	3.2
1	A	508	THR	3.2
1	B	659	MET	3.2
1	B	660	ASN	3.2
1	A	658	LEU	3.2
1	B	765	CYS	3.2
1	A	588	LYS	3.2
1	B	671	GLY	3.2
1	B	786	LYS	3.2
1	B	545	ALA	3.2
1	B	483	VAL	3.2
1	B	557	VAL	3.2
1	B	517	ILE	3.2
1	A	654	PRO	3.1
1	B	513	MET	3.1
1	A	783	VAL	3.1
1	B	894	GLY	3.1
1	A	507	ILE	3.1
1	B	819	SER	3.1
1	A	886	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	770	ILE	3.1
1	A	864	ILE	3.1
1	A	889	GLU	3.1
1	B	530	SER	3.1
1	B	487	GLY	3.1
1	B	590	VAL	3.1
1	A	763	LEU	3.1
1	B	540	LEU	3.1
1	A	526	ILE	3.1
1	A	551	ILE	3.1
1	A	574	VAL	3.1
1	B	529	VAL	3.1
1	A	892	ALA	3.0
1	A	534	CYS	3.0
1	A	548	ASP	3.0
1	A	786	LYS	3.0
1	A	571	VAL	3.0
1	A	768	VAL	3.0
1	A	882	ALA	3.0
1	B	593	ALA	3.0
1	B	549	LEU	3.0
1	A	577	SER	3.0
1	A	759	THR	3.0
1	B	824	MET	3.0
1	B	802	LEU	3.0
1	A	532	ASP	3.0
1	A	848	SER	3.0
1	A	900	SER	3.0
1	B	482	LYS	3.0
1	B	662	MET	3.0
1	A	486	LEU	3.0
1	A	885	LEU	3.0
1	B	774	SER	3.0
1	B	503	GLY	3.0
1	A	590	VAL	2.9
1	B	890	ILE	2.9
1	B	591	GLU	2.9
1	A	596	THR	2.9
1	A	481	ARG	2.9
1	B	588	LYS	2.9
1	B	740	LEU	2.9
1	B	925	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	532	ASP	2.9
1	B	550	VAL	2.9
1	A	545	ALA	2.9
1	A	536	GLN	2.9
1	A	568	THR	2.9
1	A	749	PRO	2.9
1	B	535	LYS	2.9
1	B	520	LEU	2.9
1	B	583	LEU	2.9
1	B	818	LEU	2.9
1	B	512	ASP	2.9
1	B	505	ILE	2.9
1	A	710	GLU	2.9
1	A	789	GLY	2.9
1	A	891	GLY	2.9
1	B	599	GLY	2.9
1	B	924	ILE	2.8
1	B	800	LEU	2.8
1	A	803	LEU	2.8
1	B	896	MET	2.8
1	A	537	GLU	2.8
1	A	761	LYS	2.8
1	B	656	GLY	2.8
1	A	595	ILE	2.8
1	A	598	ILE	2.8
1	A	680	ILE	2.8
1	A	758	LEU	2.8
1	A	569	ASN	2.8
1	B	690	ASP	2.8
1	A	567	ILE	2.7
1	B	911	ILE	2.7
1	B	525	ASN	2.7
1	A	500	SER	2.7
1	A	716	SER	2.7
1	A	895	LEU	2.7
1	A	564	LYS	2.7
1	B	567	ILE	2.7
1	B	543	LEU	2.7
1	B	820	LYS	2.7
1	B	871	ALA	2.7
1	B	921	GLN	2.7
1	B	661	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	583	LEU	2.7
1	A	720	LEU	2.7
1	B	547	GLN	2.7
1	A	711	ILE	2.7
1	B	654	PRO	2.7
1	B	742	LEU	2.7
1	A	593	ALA	2.7
1	B	766	ASP	2.6
1	B	560	PRO	2.6
1	A	562	VAL	2.6
1	B	544	VAL	2.6
1	B	902	GLU	2.6
1	A	547	GLN	2.6
1	A	625	THR	2.6
1	B	582	ALA	2.6
1	B	759	THR	2.6
1	B	913	ALA	2.6
1	B	804	GLY	2.6
1	B	806	GLU	2.6
1	A	816	ASP	2.6
1	A	579	ILE	2.6
1	A	516	GLN	2.6
1	B	575	THR	2.6
1	A	674	VAL	2.6
1	B	675	ASN	2.6
1	A	511	SER	2.6
1	B	488	SER	2.6
1	B	511	SER	2.6
1	A	707	LYS	2.6
1	A	659	MET	2.5
1	B	506	GLU	2.5
1	A	484	LEU	2.5
1	B	826	LEU	2.5
1	A	557	VAL	2.5
1	B	485	VAL	2.5
1	B	823	VAL	2.5
1	A	530	SER	2.5
1	B	584	LYS	2.5
1	B	628	SER	2.5
1	B	541	GLY	2.5
1	B	537	GLU	2.5
1	B	798	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	519	GLN	2.5
1	B	536	GLN	2.5
1	A	925	LYS	2.5
1	B	546	LYS	2.5
1	A	565	ALA	2.5
1	A	624	ALA	2.5
1	B	813	SER	2.5
1	A	524	TYR	2.5
1	A	594	GLY	2.5
1	A	764	LEU	2.5
1	B	559	HIS	2.5
1	A	653	SER	2.5
1	B	568	THR	2.5
1	B	566	CYS	2.5
1	A	502	ASP	2.5
1	B	556	TYR	2.5
1	B	526	ILE	2.5
1	B	916	ILE	2.5
1	A	554	LEU	2.5
1	B	833	LYS	2.5
1	B	886	LEU	2.5
1	A	528	PRO	2.4
1	A	772	PRO	2.4
1	A	809	PRO	2.4
1	B	889	GLU	2.4
1	A	903	ILE	2.4
1	A	924	ILE	2.4
1	B	918	TYR	2.4
1	B	794	LEU	2.4
1	A	563	ALA	2.4
1	A	847	PRO	2.4
1	A	586	LEU	2.4
1	B	885	LEU	2.4
1	B	744	ASN	2.4
1	A	581	PRO	2.4
1	B	910	ARG	2.4
1	A	667	TYR	2.4
1	B	796	ALA	2.4
1	A	482	LYS	2.4
1	B	825	LYS	2.4
1	A	681	SER	2.4
1	A	519	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	826	LEU	2.4
1	B	548	ASP	2.4
1	B	601	LEU	2.4
1	B	920	THR	2.3
1	B	888	GLY	2.3
1	A	802	LEU	2.3
1	B	682	PHE	2.3
1	B	737	PHE	2.3
1	A	523	LYS	2.3
1	A	808	VAL	2.3
1	B	587	GLU	2.3
1	A	830	PRO	2.3
1	A	760	TRP	2.3
1	A	559	HIS	2.3
1	A	807	GLN	2.3
1	A	506	GLU	2.3
1	A	831	GLU	2.3
1	B	831	GLU	2.3
1	B	565	ALA	2.3
1	A	715	SER	2.3
1	B	681	SER	2.3
1	B	895	LEU	2.3
1	A	546	LYS	2.3
1	A	912	LYS	2.3
1	B	775	GLU	2.3
1	B	817	ALA	2.3
1	B	741	GLY	2.3
1	B	553	LEU	2.3
1	B	603	LEU	2.3
1	A	780	LYS	2.3
1	A	709	ALA	2.2
1	A	801	GLY	2.2
1	A	553	LEU	2.2
1	B	551	ILE	2.2
1	B	715	SER	2.2
1	B	739	LYS	2.2
1	B	738	VAL	2.2
1	B	791	ASN	2.2
1	B	892	ALA	2.2
1	A	838	MET	2.2
1	A	896	MET	2.2
1	B	734	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	591	GLU	2.2
1	B	564	LYS	2.2
1	A	890	ILE	2.2
1	B	579	ILE	2.2
1	A	552	SER	2.2
1	B	909	GLU	2.2
1	B	669	LEU	2.2
1	A	527	ASN	2.1
1	A	501	ARG	2.1
1	B	518	GLU	2.1
1	B	673	VAL	2.1
1	A	811	ALA	2.1
1	B	822	LEU	2.1
1	B	598	ILE	2.1
1	A	518	GLU	2.1
1	A	745	ARG	2.1
1	B	490	TYR	2.1
1	A	651	SER	2.1
1	B	577	SER	2.1
1	B	790	ASP	2.1
1	A	612	ALA	2.1
1	B	915	GLY	2.1
1	B	585	GLU	2.1
1	A	712	TYR	2.1
1	A	850	HIS	2.1
1	A	865	ASN	2.1
1	A	584	LYS	2.1
1	A	589	SER	2.1
1	A	824	MET	2.1
1	A	499	LEU	2.0
1	A	515	ASN	2.0
1	B	799	TRP	2.0
1	B	773	SER	2.0
1	B	797	ALA	2.0
1	A	503	GLY	2.0
1	A	592	ASP	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	EDO	B	1001	4/4	0.51	0.26	60,60,60,60	0
2	EDO	A	1001	4/4	0.79	0.27	61,62,62,62	0
3	PRO	A	1002	8/8	0.88	0.17	56,58,58,58	0
3	PRO	B	1002	8/8	0.92	0.10	46,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.