



Full wwPDB X-ray Structure Validation Report

Sep 9, 2020 – 01:46 PM BST

PDB ID : 5KXJ
Title : Crystal Structure of L-Aspartate Oxidase from Salmonella typhimurium in the Complex with Substrate L-Aspartate
Authors : Kim, Y.; Osipiuk, J.; Mulligan, R.; Makowska-Grzyska, M.; Maltseva, N.; Shatsman, S.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2016-07-20
Resolution : 1.87 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 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 : 2.14.3.dev2
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) : 2.14.3.dev2

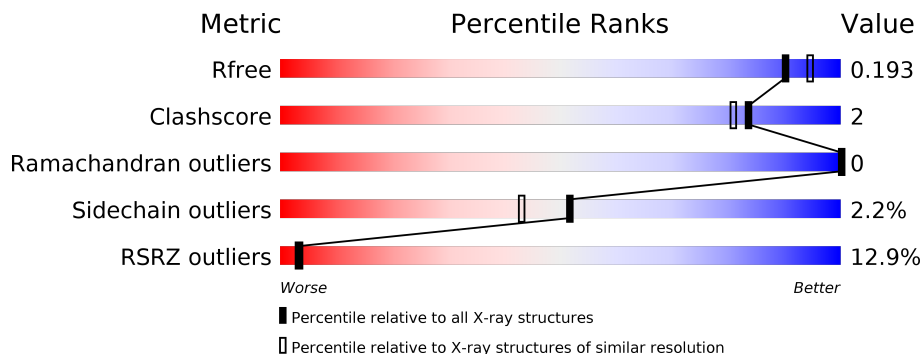
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	557	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4245 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 L-aspartate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3937	2465	707	738	27	0	22	0

There are 17 discrepancies between the modelled and reference sequences:

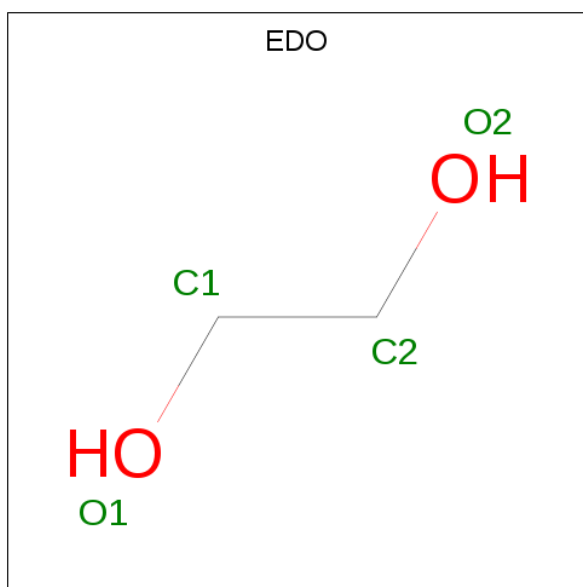
Chain	Residue	Modelled	Actual	Comment	Reference
A	541	ARG	-	expression tag	UNP Q8ZMX9
A	542	GLY	-	expression tag	UNP Q8ZMX9
A	543	GLU	-	expression tag	UNP Q8ZMX9
A	544	ASN	-	expression tag	UNP Q8ZMX9
A	545	LEU	-	expression tag	UNP Q8ZMX9
A	546	TYR	-	expression tag	UNP Q8ZMX9
A	547	PHE	-	expression tag	UNP Q8ZMX9
A	548	GLN	-	expression tag	UNP Q8ZMX9
A	549	SER	-	expression tag	UNP Q8ZMX9
A	550	ALA	-	expression tag	UNP Q8ZMX9
A	551	GLY	-	expression tag	UNP Q8ZMX9
A	552	HIS	-	expression tag	UNP Q8ZMX9
A	553	HIS	-	expression tag	UNP Q8ZMX9
A	554	HIS	-	expression tag	UNP Q8ZMX9
A	555	HIS	-	expression tag	UNP Q8ZMX9
A	556	HIS	-	expression tag	UNP Q8ZMX9
A	557	HIS	-	expression tag	UNP Q8ZMX9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



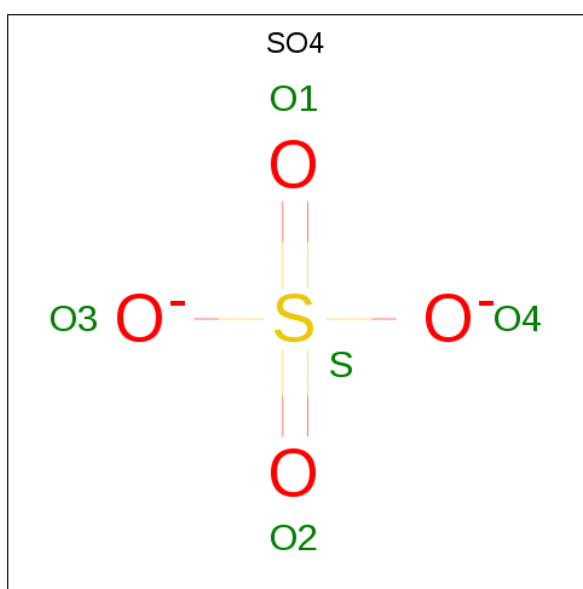
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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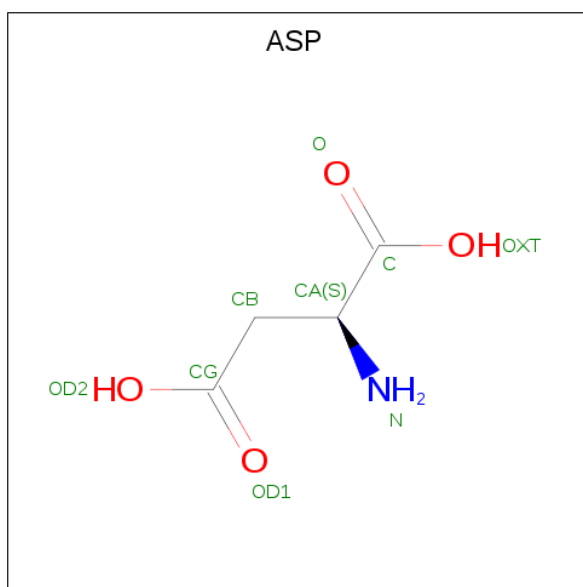
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	18	8	2	8	0	1

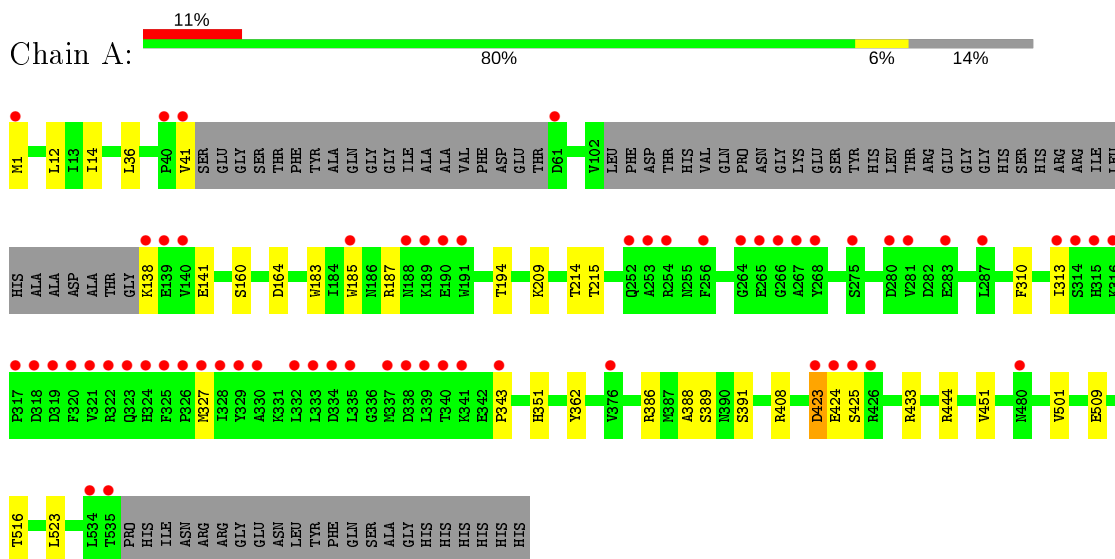
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	247	Total	O	0	0
			247	247		

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: L-aspartate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	290.94Å 290.94Å 290.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.88 – 1.87 38.88 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.2 (38.88-1.87) 97.1 (38.88-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.87Å)	Xtrriage
Refinement program	PHENIX (dev_2411: ???)	Depositor
R, R_{free}	0.174 , 0.193 0.174 , 0.193	Depositor DCC
R_{free} test set	4315 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4245	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, SO4, 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	0.38	0/4015	0.53	0/5448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3937	0	3879	18	0
2	A	18	0	24	1	0
3	A	20	0	30	0	0
4	A	5	0	0	0	0
5	A	18	0	6	1	0
6	A	247	0	0	1	0
All	All	4245	0	3939	19	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (19) 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:451:VAL:HG21	1:A:501[B]:VAL:HG22	1.64	0.79
1:A:14:ILE:HG23	1:A:36[B]:LEU:HD23	1.80	0.64
1:A:444:ARG:HH22	2:A:603:GOL:H11	1.68	0.59
1:A:310:PHE:HB3	1:A:343:PRO:HB2	1.89	0.55
1:A:185[A]:TRP:CZ3	1:A:187:ARG:HG2	2.43	0.54
1:A:423:ASP:N	1:A:423:ASP:OD1	2.41	0.54
5:A:610[B]:ASP:N	6:A:710:HOH:O	2.41	0.53
1:A:209:LYS:HA	1:A:214[A]:THR:HG21	1.92	0.52
1:A:215:THR:OG1	1:A:351:HIS:HD2	1.92	0.51
1:A:138:LYS:HE2	1:A:141:GLU:HG3	1.93	0.49
1:A:388[B]:ALA:O	1:A:389[B]:SER:OG	2.28	0.47
1:A:183:TRP:CD1	1:A:194[B]:THR:HG22	2.50	0.47
1:A:451:VAL:CG2	1:A:501[B]:VAL:HG22	2.42	0.46
1:A:424:GLU:HG3	1:A:425:SER:N	2.34	0.42
1:A:362:TYR:CE2	1:A:408[B]:ARG:NH2	2.86	0.42
1:A:12:LEU:HD11	1:A:36[A]:LEU:HG	2.01	0.42
1:A:386:ARG:HD2	1:A:391[B]:SER:OG	2.20	0.41
1:A:509:GLU:HB3	1:A:523:LEU:HG	2.02	0.41
1:A:36[B]:LEU:HD11	1:A:160:SER:CB	2.51	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	497/557 (89%)	487 (98%)	10 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	426/465 (92%)	418 (98%)	8 (2%)	57 49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	41	VAL
1	A	164	ASP
1	A	313	ILE
1	A	327	MET
1	A	423	ASP
1	A	433	ARG
1	A	516	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	303	GLN
1	A	351	HIS
1	A	439	ASN
1	A	441	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

11 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
3	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	A	607	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	A	604	-	3,3,3	0.58	0	2,2,2	0.42	0
3	EDO	A	605	-	3,3,3	0.39	0	2,2,2	0.20	0
2	GOL	A	602	-	5,5,5	0.35	0	5,5,5	0.47	0
4	SO4	A	608	-	4,4,4	0.27	0	6,6,6	0.34	0
3	EDO	A	606	-	3,3,3	0.53	0	2,2,2	0.30	0
2	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.37	0
2	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.35	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
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	A	607	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
2	GOL	A	602	-	-	4/4/4/4	-
3	EDO	A	606	-	-	0/1/1/1	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	C1-C2-C3-O3
2	A	603	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2
3	A	609	EDO	O1-C1-C2-O2
2	A	602	GOL	O2-C2-C3-O3
2	A	603	GOL	O1-C1-C2-O2
3	A	607	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	GOL	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	481/557 (86%)	0.48	62 (12%) 3 3	20, 34, 94, 124	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	PHE	8.0
1	A	333	LEU	7.7
1	A	321	VAL	7.0
1	A	329	TYR	6.8
1	A	328	ILE	6.5
1	A	191	TRP	6.0
1	A	319	ASP	5.7
1	A	313	ILE	5.6
1	A	1	MET	5.5
1	A	339	LEU	5.4
1	A	340	THR	5.3
1	A	252	GLN	5.1
1	A	325	PHE	5.0
1	A	41	VAL	4.4
1	A	326	PRO	4.4
1	A	323	GLN	4.3
1	A	315	HIS	4.2
1	A	266	GLY	4.1
1	A	335	LEU	4.0
1	A	330	ALA	3.9
1	A	341	LYS	3.8
1	A	287	LEU	3.8
1	A	40	PRO	3.7
1	A	254	ARG	3.5
1	A	324	HIS	3.5
1	A	314	SER	3.5
1	A	327	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	256	PHE	3.4
1	A	317	PRO	3.3
1	A	281	VAL	3.3
1	A	264	GLY	3.3
1	A	61	ASP	3.3
1	A	190	GLU	3.2
1	A	316	LYS	3.2
1	A	426	ARG	3.2
1	A	268	TYR	3.1
1	A	283	GLU	3.1
1	A	424	GLU	3.0
1	A	188	ASN	3.0
1	A	338	ASP	2.9
1	A	423	ASP	2.9
1	A	534	LEU	2.8
1	A	265	GLU	2.8
1	A	322	ARG	2.7
1	A	139	GLU	2.7
1	A	425	SER	2.7
1	A	332	LEU	2.7
1	A	280	ASP	2.7
1	A	253	ALA	2.6
1	A	334	ASP	2.6
1	A	189	LYS	2.6
1	A	318	ASP	2.6
1	A	140	VAL	2.5
1	A	185[A]	TRP	2.4
1	A	267	ALA	2.4
1	A	480	ASN	2.3
1	A	343	PRO	2.2
1	A	535	THR	2.2
1	A	337	MET	2.1
1	A	138	LYS	2.1
1	A	275	SER	2.0
1	A	376	VAL	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 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
4	SO4	A	608	5/5	0.75	0.30	114,115,120,122	0
2	GOL	A	602	6/6	0.86	0.42	45,60,68,73	0
5	ASP	A	610[B]	9/9	0.86	0.21	35,49,55,57	9
5	ASP	A	610[A]	9/9	0.86	0.21	29,48,53,55	9
3	EDO	A	609	4/4	0.88	0.21	56,68,68,81	0
3	EDO	A	607	4/4	0.88	0.15	39,40,59,64	0
3	EDO	A	606	4/4	0.90	0.15	36,49,50,64	0
2	GOL	A	601	6/6	0.91	0.21	39,59,71,72	0
2	GOL	A	603	6/6	0.91	0.12	45,68,81,82	0
3	EDO	A	604	4/4	0.94	0.14	29,34,36,41	0
3	EDO	A	605	4/4	0.94	0.14	31,39,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.