



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 AM UTC

PDB ID : 4PG8 / pdb_00004pg8
Title : Crystal structure of S. aureus Homoserine Dehydrogenase at pH8.5
Authors : Navratna, V.; Gopal, B.
Deposited on : 2014-05-01
Resolution : 2.20 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)
Xtrriage (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

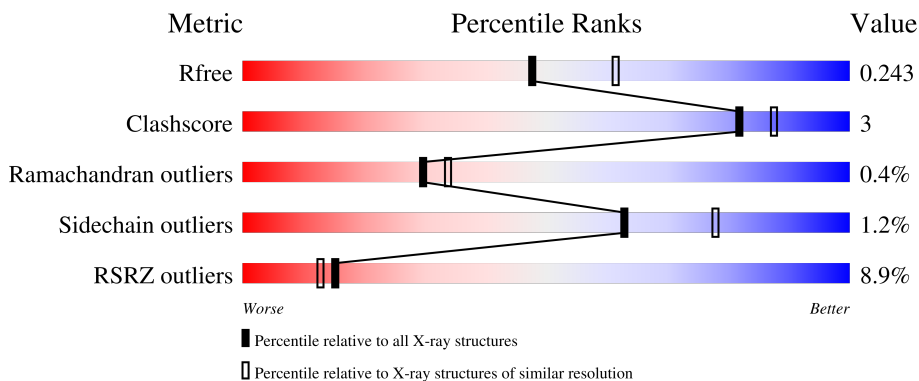
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	468	
1	B	468	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6275 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 Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	2980	1892	503	580	5	0	1	0
1	B	388	2898	1844	486	563	5	0	2	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP N6FDB4
A	-18	GLY	-	expression tag	UNP N6FDB4
A	-17	SER	-	expression tag	UNP N6FDB4
A	-16	SER	-	expression tag	UNP N6FDB4
A	-15	HIS	-	expression tag	UNP N6FDB4
A	-14	HIS	-	expression tag	UNP N6FDB4
A	-13	HIS	-	expression tag	UNP N6FDB4
A	-12	HIS	-	expression tag	UNP N6FDB4
A	-11	HIS	-	expression tag	UNP N6FDB4
A	-10	HIS	-	expression tag	UNP N6FDB4
A	-9	SER	-	expression tag	UNP N6FDB4
A	-8	SER	-	expression tag	UNP N6FDB4
A	-7	GLY	-	expression tag	UNP N6FDB4
A	-6	LEU	-	expression tag	UNP N6FDB4
A	-5	VAL	-	expression tag	UNP N6FDB4
A	-4	PRO	-	expression tag	UNP N6FDB4
A	-3	ARG	-	expression tag	UNP N6FDB4
A	-2	GLY	-	expression tag	UNP N6FDB4
A	-1	SER	-	expression tag	UNP N6FDB4
A	0	HIS	-	expression tag	UNP N6FDB4
A	427	LEU	-	expression tag	UNP N6FDB4
A	428	GLU	-	expression tag	UNP N6FDB4
A	429	ASP	-	expression tag	UNP N6FDB4
A	430	PRO	-	expression tag	UNP N6FDB4
A	431	ALA	-	expression tag	UNP N6FDB4

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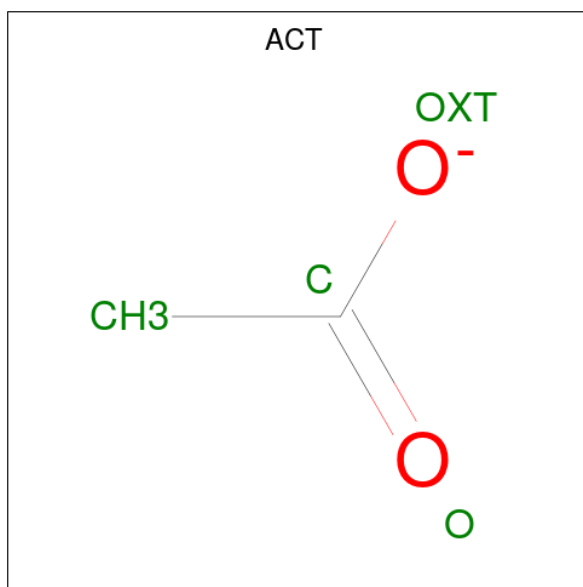
Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	-	expression tag	UNP N6FDB4
A	433	ASN	-	expression tag	UNP N6FDB4
A	434	LYS	-	expression tag	UNP N6FDB4
A	435	ALA	-	expression tag	UNP N6FDB4
A	436	ARG	-	expression tag	UNP N6FDB4
A	437	LYS	-	expression tag	UNP N6FDB4
A	438	GLU	-	expression tag	UNP N6FDB4
A	439	ALA	-	expression tag	UNP N6FDB4
A	440	GLU	-	expression tag	UNP N6FDB4
A	441	LEU	-	expression tag	UNP N6FDB4
A	442	ALA	-	expression tag	UNP N6FDB4
A	443	ALA	-	expression tag	UNP N6FDB4
A	444	ALA	-	expression tag	UNP N6FDB4
A	445	THR	-	expression tag	UNP N6FDB4
A	446	ALA	-	expression tag	UNP N6FDB4
A	447	GLU	-	expression tag	UNP N6FDB4
A	448	GLN	-	expression tag	UNP N6FDB4
B	-19	MET	-	initiating methionine	UNP N6FDB4
B	-18	GLY	-	expression tag	UNP N6FDB4
B	-17	SER	-	expression tag	UNP N6FDB4
B	-16	SER	-	expression tag	UNP N6FDB4
B	-15	HIS	-	expression tag	UNP N6FDB4
B	-14	HIS	-	expression tag	UNP N6FDB4
B	-13	HIS	-	expression tag	UNP N6FDB4
B	-12	HIS	-	expression tag	UNP N6FDB4
B	-11	HIS	-	expression tag	UNP N6FDB4
B	-10	HIS	-	expression tag	UNP N6FDB4
B	-9	SER	-	expression tag	UNP N6FDB4
B	-8	SER	-	expression tag	UNP N6FDB4
B	-7	GLY	-	expression tag	UNP N6FDB4
B	-6	LEU	-	expression tag	UNP N6FDB4
B	-5	VAL	-	expression tag	UNP N6FDB4
B	-4	PRO	-	expression tag	UNP N6FDB4
B	-3	ARG	-	expression tag	UNP N6FDB4
B	-2	GLY	-	expression tag	UNP N6FDB4
B	-1	SER	-	expression tag	UNP N6FDB4
B	0	HIS	-	expression tag	UNP N6FDB4
B	427	LEU	-	expression tag	UNP N6FDB4
B	428	GLU	-	expression tag	UNP N6FDB4
B	429	ASP	-	expression tag	UNP N6FDB4
B	430	PRO	-	expression tag	UNP N6FDB4
B	431	ALA	-	expression tag	UNP N6FDB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	432	ALA	-	expression tag	UNP N6FDB4
B	433	ASN	-	expression tag	UNP N6FDB4
B	434	LYS	-	expression tag	UNP N6FDB4
B	435	ALA	-	expression tag	UNP N6FDB4
B	436	ARG	-	expression tag	UNP N6FDB4
B	437	LYS	-	expression tag	UNP N6FDB4
B	438	GLU	-	expression tag	UNP N6FDB4
B	439	ALA	-	expression tag	UNP N6FDB4
B	440	GLU	-	expression tag	UNP N6FDB4
B	441	LEU	-	expression tag	UNP N6FDB4
B	442	ALA	-	expression tag	UNP N6FDB4
B	443	ALA	-	expression tag	UNP N6FDB4
B	444	ALA	-	expression tag	UNP N6FDB4
B	445	THR	-	expression tag	UNP N6FDB4
B	446	ALA	-	expression tag	UNP N6FDB4
B	447	GLU	-	expression tag	UNP N6FDB4
B	448	GLN	-	expression tag	UNP N6FDB4

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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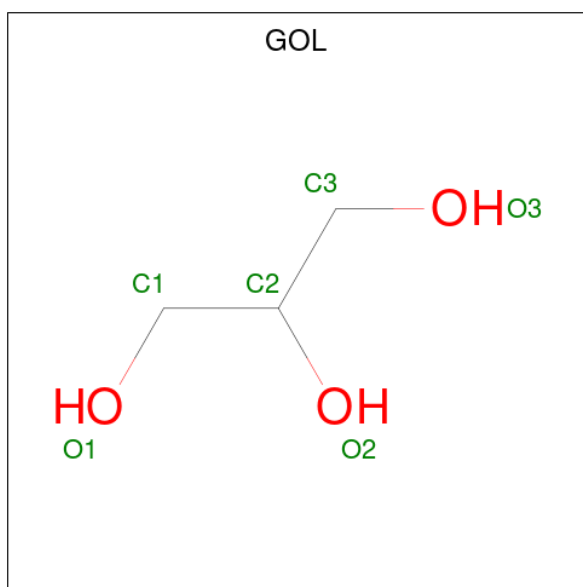
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



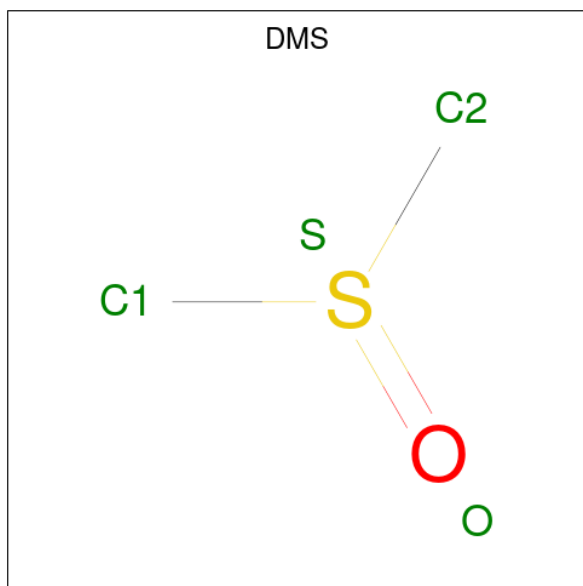
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	154	154	154	0	0
6	B	148	148	148	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.87Å 117.51Å 119.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.20 – 2.20 39.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.20-2.20) 100.0 (39.20-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.237 0.206 , 0.243	Depositor DCC
R_{free} test set	2689 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6275	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: PEG, DMS, GOL, ACT

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	0.68	0/3020	0.82	1/4091 (0.0%)
1	B	0.69	0/2935	0.84	6/3971 (0.2%)
All	All	0.69	0/5955	0.83	7/8062 (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	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	51	ARG	CA-C-N	7.87	129.67	119.84
1	B	51	ARG	C-N-CA	7.87	129.67	119.84
1	B	136	ILE	CA-C-N	7.51	129.23	119.84
1	B	136	ILE	C-N-CA	7.51	129.23	119.84
1	B	264	GLU	N-CA-C	6.30	113.80	108.13
1	A	264	GLU	N-CA-C	6.16	113.68	108.13
1	B	56	SER	N-CA-C	5.15	115.09	108.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	34	ASN	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	2980	0	2917	16	0
1	B	2898	0	2845	17	0
2	A	36	0	27	2	0
2	B	28	0	21	1	0
3	A	7	0	10	0	0
3	B	14	0	20	2	0
4	B	6	0	8	2	0
5	B	4	0	6	0	0
6	A	154	0	0	1	0
6	B	148	0	0	2	0
All	All	6275	0	5854	30	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 3.

All (30) 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:ILE:C	1:B:22:ILE:CA	2.40	0.95
1:B:131:SER:CB	1:B:301:ALA:HB3	2.09	0.83
1:A:158:LEU:HD21	1:A:284:ILE:CD1	2.17	0.74
1:A:158:LEU:CD2	1:A:284:ILE:HD11	2.31	0.61
1:A:158:LEU:HD21	1:A:284:ILE:HD11	1.84	0.59
1:B:270:LYS:NZ	2:B:505:ACT:O	2.32	0.59
1:A:339:THR:O	1:A:340:ARG:CB	2.52	0.57
1:B:59:HIS:NE2	4:B:508:GOL:H32	2.21	0.56
1:B:1:MET:HE1	1:B:30:GLN:CB	2.35	0.56
1:A:273:GLN:HE21	1:B:273[B]:GLN:HE21	1.54	0.56
1:A:335:LYS:CB	1:A:337:ASP:N	2.69	0.55
1:B:45:ARG:H	3:B:509:PEG:H21	1.73	0.54
1:B:128:PHE:CZ	1:B:130:ALA:HB2	2.44	0.52
1:A:158:LEU:CD2	1:A:284:ILE:CD1	2.88	0.51
1:B:105:LYS:HE3	1:B:130:ALA:HA	1.92	0.51
1:A:72:SER:O	2:A:507:ACT:H1	2.13	0.49
1:A:383:ARG:O	2:A:504:ACT:H2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:NZ	6:A:602:HOH:O	2.47	0.47
1:B:51:ARG:HH12	3:B:509:PEG:H12	1.80	0.46
1:A:330:PRO:O	1:A:331:HIS:C	2.60	0.44
1:B:412:LYS:NZ	6:B:602:HOH:O	2.50	0.44
1:B:182:GLU:OE1	1:B:185:ARG:HD3	2.18	0.43
1:B:153:LYS:NZ	6:B:669:HOH:O	2.52	0.43
1:A:101:ILE:CD1	1:A:314:LEU:HA	2.49	0.43
1:A:116:GLU:OE1	1:A:211:TYR:OH	2.24	0.42
1:A:25:ASN:HD21	1:B:331:HIS:N	2.17	0.41
1:A:295:MET:HE1	1:B:273[B]:GLN:NE2	2.35	0.41
1:B:66:GLU:OE1	4:B:508:GOL:O3	2.37	0.41
1:B:273[B]:GLN:HG3	1:B:295:MET:HE1	2.03	0.40
1:A:289:ASP:HA	1:A:290:ALA:HA	1.78	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	391/468 (84%)	377 (96%)	12 (3%)	2 (0%)	24	27
1	B	376/468 (80%)	368 (98%)	7 (2%)	1 (0%)	36	42
All	All	767/936 (82%)	745 (97%)	19 (2%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ARG
1	A	291	VAL
1	B	54	ASN

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	307/396 (78%)	304 (99%)	3 (1%)	68	81
1	B	296/396 (75%)	292 (99%)	4 (1%)	59	75
All	All	603/792 (76%)	596 (99%)	7 (1%)	63	78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	56	SER
1	A	412	LYS
1	B	105	LYS
1	B	132	VAL
1	B	284	ILE
1	B	304	LEU

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	25	ASN
1	A	65	ASN
1	A	282	ASN
1	B	65	ASN
1	B	282	ASN
1	B	316	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](#)

21 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	ACT	A	502	-	3,3,3	0.85	0	3,3,3	0.77	0
2	ACT	A	508	-	3,3,3	0.85	0	3,3,3	0.70	0
3	PEG	B	510	-	6,6,6	0.44	0	5,5,5	0.24	0
2	ACT	B	506	-	3,3,3	0.84	0	3,3,3	0.64	0
2	ACT	A	503	-	3,3,3	0.79	0	3,3,3	0.73	0
2	ACT	B	505	-	3,3,3	0.77	0	3,3,3	1.12	0
2	ACT	A	506	-	3,3,3	0.84	0	3,3,3	0.95	0
2	ACT	B	503	-	3,3,3	0.92	0	3,3,3	0.51	0
3	PEG	A	510	-	6,6,6	0.48	0	5,5,5	0.35	0
2	ACT	A	505	-	3,3,3	0.77	0	3,3,3	1.22	0
4	GOL	B	508	-	5,5,5	0.57	0	5,5,5	0.74	0
2	ACT	A	509	-	3,3,3	0.84	0	3,3,3	0.68	0
2	ACT	A	501	-	3,3,3	0.79	0	3,3,3	0.82	0
2	ACT	B	502	-	3,3,3	1.06	0	3,3,3	0.45	0
2	ACT	A	504	-	3,3,3	0.78	0	3,3,3	0.81	0
2	ACT	B	501	-	3,3,3	0.90	0	3,3,3	0.95	0
3	PEG	B	509	-	6,6,6	0.47	0	5,5,5	0.37	0
2	ACT	A	507	-	3,3,3	0.78	0	3,3,3	0.68	0
2	ACT	B	504	-	3,3,3	0.88	0	3,3,3	0.66	0
5	DMS	B	511	-	3,3,3	0.60	0	3,3,3	0.18	0
2	ACT	B	507	-	3,3,3	0.97	0	3,3,3	0.52	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	PEG	B	509	-	-	2/4/4/4	-
3	PEG	B	510	-	-	2/4/4/4	-
3	PEG	A	510	-	-	2/4/4/4	-
4	GOL	B	508	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	508	GOL	O1-C1-C2-C3
3	B	510	PEG	O2-C3-C4-O4
3	B	509	PEG	O1-C1-C2-O2
3	A	510	PEG	O1-C1-C2-O2
4	B	508	GOL	O1-C1-C2-O2
3	A	510	PEG	C4-C3-O2-C2
3	B	510	PEG	C4-C3-O2-C2
3	B	509	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	ACT	1	0
4	B	508	GOL	2	0
2	A	504	ACT	1	0
3	B	509	PEG	2	0
2	A	507	ACT	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	399/468 (85%)	0.37	33 (8%) 17 15	20, 39, 81, 110	1 (0%)
1	B	388/468 (82%)	0.34	37 (9%) 14 11	15, 36, 76, 99	2 (0%)
All	All	787/936 (84%)	0.36	70 (8%) 15 13	15, 38, 78, 110	3 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	LEU	7.9
1	A	321	PHE	6.1
1	B	132	VAL	6.0
1	B	321	PHE	5.5
1	A	328	LEU	5.4
1	A	135	GLY	5.3
1	B	291	VAL	5.2
1	A	137	PRO	5.1
1	B	133	ALA	4.9
1	B	138	ILE	4.8
1	B	137	PRO	4.8
1	A	336	THR	4.7
1	A	329	PRO	4.7
1	A	334	LEU	4.6
1	A	301	ALA	4.5
1	B	330	PRO	4.5
1	B	32	THR	4.0
1	A	0	HIS	3.9
1	A	330	PRO	3.9
1	B	331	HIS	3.9
1	A	322	GLU	3.8
1	A	426	VAL	3.8
1	B	139	VAL	3.8
1	A	133	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	3.6
1	B	332	PHE	3.5
1	A	31	ASP	3.5
1	A	339	THR	3.4
1	A	290	ALA	3.4
1	B	31	ASP	3.4
1	B	334	LEU	3.2
1	B	49	LYS	3.1
1	B	52	PRO	3.1
1	B	129	GLU	3.0
1	A	331	HIS	3.0
1	A	134	GLY	2.9
1	A	332	PHE	2.9
1	A	53	LEU	2.9
1	B	130	ALA	2.9
1	B	131	SER	2.8
1	A	56	SER	2.7
1	B	188	PHE	2.7
1	B	2	LYS	2.7
1	B	353	GLU	2.7
1	B	140	ASN	2.6
1	A	341	GLU	2.6
1	B	55	ILE	2.6
1	A	55	ILE	2.5
1	A	4	LEU	2.5
1	B	51	ARG	2.5
1	B	256	ASN	2.5
1	B	48	SER	2.4
1	B	136	ILE	2.4
1	B	1	MET	2.4
1	B	33	LEU	2.4
1	B	34	ASN	2.4
1	B	300	GLY	2.4
1	A	132	VAL	2.4
1	B	54	ASN	2.3
1	A	289	ASP	2.3
1	A	335	LYS	2.3
1	B	333	GLU	2.2
1	B	221	ASN	2.2
1	A	29	ILE	2.1
1	B	50	LYS	2.1
1	B	4	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLY	2.1
1	A	149	ASN	2.0
1	A	57	GLN	2.0
1	A	340	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	B	507	4/4	0.55	0.23	52,61,62,66	0
2	ACT	A	509	4/4	0.60	0.24	67,67,72,74	0
2	ACT	A	506	4/4	0.71	0.20	48,49,51,53	0
2	ACT	B	506	4/4	0.72	0.23	65,68,69,69	0
4	GOL	B	508	6/6	0.76	0.17	46,47,50,50	0
3	PEG	B	510	7/7	0.78	0.18	67,71,76,76	0
3	PEG	A	510	7/7	0.78	0.17	51,57,62,63	0
2	ACT	A	507	4/4	0.80	0.13	55,56,57,58	0
5	DMS	B	511	4/4	0.80	0.23	66,66,68,69	0
3	PEG	B	509	7/7	0.82	0.17	64,68,70,71	0
2	ACT	B	503	4/4	0.82	0.18	50,53,56,58	0
2	ACT	B	505	4/4	0.83	0.15	51,53,54,54	0
2	ACT	B	504	4/4	0.85	0.18	52,52,54,54	0
2	ACT	A	508	4/4	0.86	0.12	48,51,51,52	0
2	ACT	A	501	4/4	0.86	0.19	50,51,51,57	0
2	ACT	A	505	4/4	0.86	0.15	42,49,49,49	0
2	ACT	A	502	4/4	0.87	0.11	38,40,43,48	0
2	ACT	B	502	4/4	0.87	0.12	40,41,41,51	0
2	ACT	A	504	4/4	0.88	0.13	61,61,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ACT	A	503	4/4	0.90	0.12	49,49,50,52	0
2	ACT	B	501	4/4	0.97	0.07	33,34,37,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.