



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:03 pm BST

PDB ID : 2YPP
Title : 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase in complex with 3 tyrosine molecules
Authors : Blackmore, N.J.; Reichau, S.; Jiao, W.; Hutton, R.D.; Baker, E.N.; Jameson, G.B.; Parker, E.J.
Deposited on : 2012-10-31
Resolution : 2.30 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 : 2.11
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) : 2.11

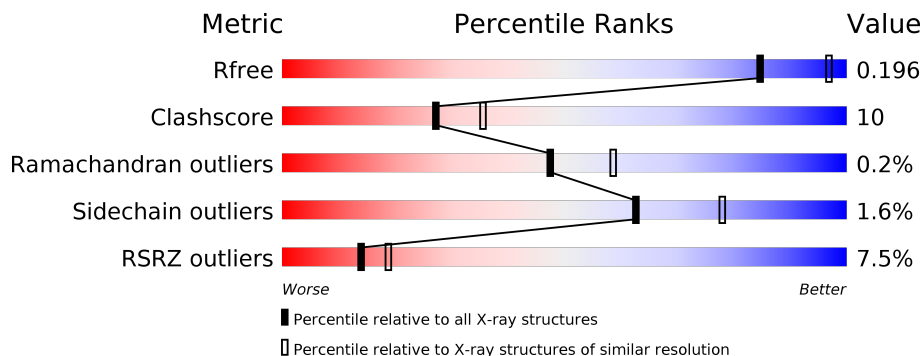
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	462	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="margin-left: 5px;">8%</div> <div style="margin-left: 5px;">80%</div> <div style="margin-left: 5px;">18%</div> <div style="margin-left: 5px;">•</div> </div>
1	B	462	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="margin-left: 5px;">7%</div> <div style="margin-left: 5px;">84%</div> <div style="margin-left: 5px;">15%</div> <div style="margin-left: 5px;">••</div> </div>

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
4	SO4	A	901	-	-	X	-

2 Entry composition [i](#)

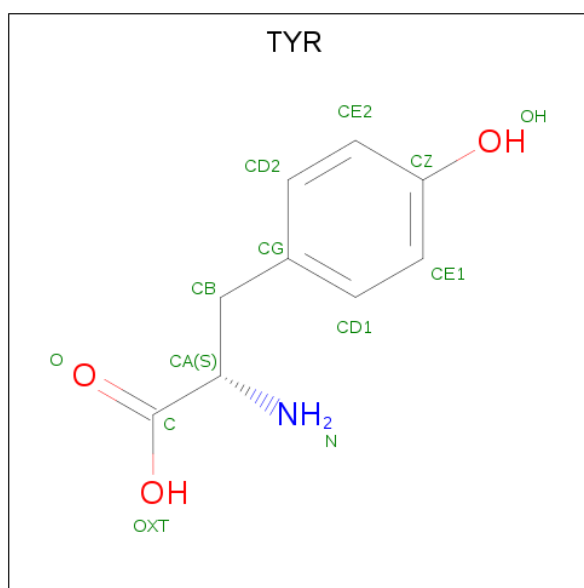
There are 7 unique types of molecules in this entry. The entry contains 7374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	Total 3566	C 2225	N 648	O 675	S 18	0	4	0
1	B	459	Total 3561	C 2223	N 649	O 671	S 18	0	4	0

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C₉H₁₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 13	C 9	N 1	O 3	0	0
2	B	1	Total 13	C 9	N 1	O 3	0	0
2	B	1	Total 13	C 9	N 1	O 3	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	2	Total Cl 2 2	0	0
6	A	1	Total Cl 1 1	0	0

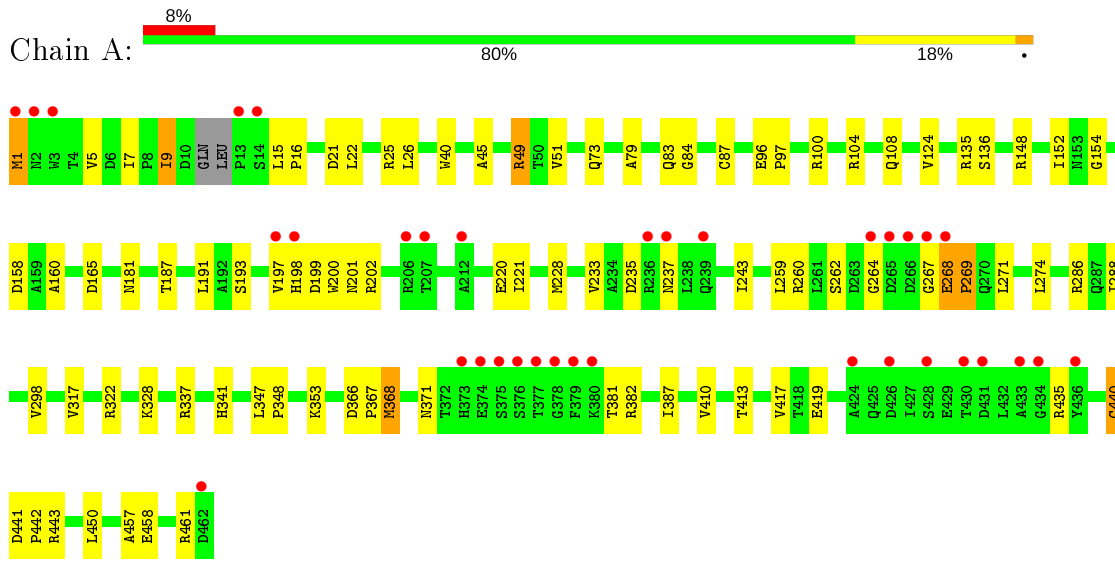
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	77	Total O 77 77	0	0
7	B	77	Total O 77 77	0	0

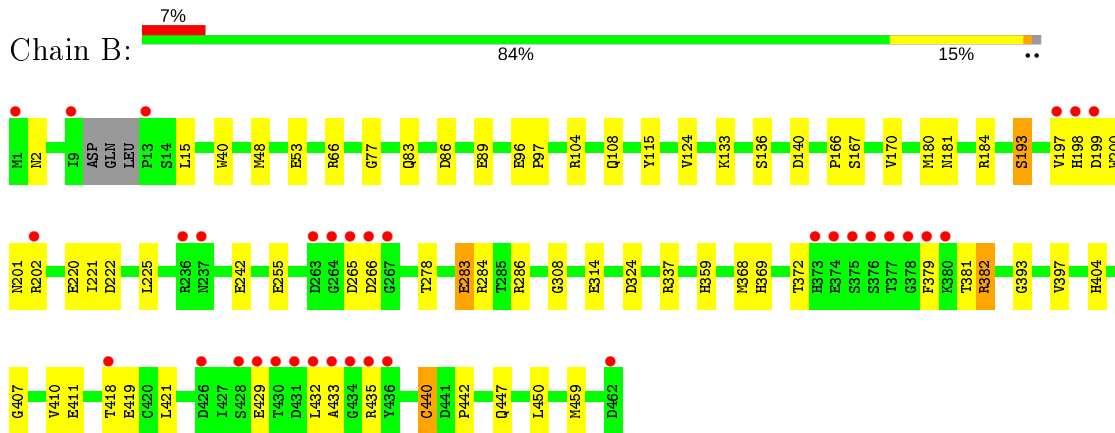
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG



- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE AROG



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.45Å 203.45Å 66.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.02 – 2.30 44.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.02-2.30) 98.7 (44.02-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.139 , 0.164 0.173 , 0.196	Depositor DCC
R_{free} test set	3451 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
Reported twinning fraction	0.791 for H, K, L 0.209 for -h,-k,l	Depositor
Outliers	0 of 69340 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7374	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, MN, SO4, CL

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	1.00	2/3645 (0.1%)	0.97	6/4959 (0.1%)
1	B	1.03	3/3644 (0.1%)	0.99	10/4955 (0.2%)
All	All	1.01	5/7289 (0.1%)	0.98	16/9914 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	CD-OE2	6.00	1.32	1.25
1	B	407	GLY	N-CA	-5.92	1.37	1.46
1	B	89	GLU	CD-OE2	5.22	1.31	1.25
1	A	269	PRO	N-CD	5.13	1.55	1.47
1	A	154	GLY	C-O	5.04	1.31	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	MET	CG-SD-CE	5.93	109.69	100.20
1	B	66	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	66	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	268	GLU	C-N-CD	5.68	140.34	128.40
1	B	140	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	286	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	366	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	104	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	382	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	49	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	382	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	184	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	459	MET	CG-SD-CE	-5.37	91.61	100.20
1	B	286	ARG	NE-CZ-NH2	-5.25	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	165	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	86	ASP	CB-CG-OD1	5.14	122.93	118.30

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	3566	0	3517	81	0
1	B	3561	0	3520	67	0
2	A	13	0	8	0	0
2	B	26	0	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	0	3	0
4	B	10	0	0	1	0
5	A	12	0	16	1	0
5	B	12	0	16	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	77	0	0	0	0
7	B	77	0	0	2	0
All	All	7374	0	7093	145	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 10.

All (145) 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:418:THR:O	1:B:432:LEU:HD23	1.39	1.20
1:A:197:VAL:HA	1:A:200:TRP:CE3	1.88	1.08
1:B:197:VAL:HA	1:B:200:TRP:CZ3	1.89	1.08
1:A:22:LEU:HD21	1:A:271:LEU:HD13	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[A]:SER:OG	4:A:901:SO4:S	2.21	0.98
1:B:265:ASP:O	1:B:266:ASP:HB2	1.61	0.97
1:A:417:VAL:HG22	1:A:435:ARG:O	1.66	0.95
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.04	0.91
1:A:457:ALA:O	1:A:461:ARG:HG3	1.72	0.90
1:A:197:VAL:HA	1:A:200:TRP:CZ3	2.08	0.88
1:A:96[A]:GLU:OE1	1:A:100[A]:ARG:NH2	2.08	0.87
1:B:418:THR:O	1:B:432:LEU:CD2	2.22	0.86
1:B:48:MET:HE3	1:B:170:VAL:CG2	2.07	0.85
1:B:48:MET:HE3	1:B:170:VAL:HG21	1.61	0.83
1:A:136[A]:SER:OG	4:A:901:SO4:O4	1.99	0.79
1:B:372:THR:HG22	1:B:382:ARG:HE	1.48	0.79
1:B:48:MET:HE1	1:B:167:SER:HA	1.65	0.77
1:B:368:MET:HE3	1:B:410:VAL:HG12	1.67	0.75
1:A:417:VAL:CG2	1:A:435:ARG:O	2.34	0.75
1:A:197:VAL:HG13	1:A:200:TRP:CZ3	2.22	0.74
1:B:15:LEU:HD21	1:B:53:GLU:HB3	1.72	0.71
1:A:135:ARG:NE	4:A:901:SO4:O2	2.23	0.70
1:A:197:VAL:HG13	1:A:200:TRP:HZ3	1.57	0.68
1:A:198:HIS:O	1:A:201:ASN:HB2	1.93	0.68
1:A:268:GLU:CD	1:A:268:GLU:H	1.97	0.68
1:A:193:SER:O	1:A:197:VAL:HG23	1.95	0.66
1:B:133:LYS:CD	1:B:440:CYS:SG	2.83	0.66
1:A:26:LEU:HD11	1:A:259:LEU:CD1	2.25	0.66
1:A:317:VAL:HG21	1:A:353:LYS:HE3	1.78	0.65
1:A:367:PRO:O	1:A:371:ASN:ND2	2.31	0.63
1:A:317:VAL:CG2	1:A:353:LYS:HG3	2.29	0.63
1:B:104[B]:ARG:NH1	1:B:108:GLN:OE1	2.32	0.62
1:A:417:VAL:HG21	1:A:419:GLU:OE2	1.99	0.62
1:B:447:GLN:NE2	7:B:2045:HOH:O	2.24	0.61
1:B:96:GLU:HB3	1:B:97:PRO:HD3	1.80	0.61
1:A:191:LEU:HD12	1:A:200:TRP:HH2	1.65	0.61
1:B:48:MET:CE	1:B:170:VAL:CG2	2.78	0.61
1:A:108:GLN:NE2	1:A:450:LEU:HD21	2.15	0.61
1:B:198:HIS:CD2	1:B:225:LEU:HD12	2.35	0.61
1:A:264:GLY:HA2	1:A:267:GLY:O	2.00	0.61
1:B:197:VAL:CA	1:B:200:TRP:CZ3	2.78	0.61
1:B:379:PHE:CE2	1:B:433:ALA:HA	2.37	0.59
1:B:48:MET:CE	1:B:170:VAL:HG23	2.32	0.59
1:B:369:HIS:CE1	1:B:411:GLU:OE2	2.56	0.58
1:A:158[B]:ASP:OD1	1:A:160:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASP:HA	1:A:202:ARG:HG3	1.86	0.58
1:A:197:VAL:CA	1:A:200:TRP:CE3	2.78	0.57
1:A:413:THR:HG23	1:A:443:ARG:HD2	1.86	0.57
1:B:133:LYS:HD2	1:B:440:CYS:SG	2.45	0.57
1:A:7:ILE:O	1:B:2:ASN:HB2	2.05	0.56
1:A:22:LEU:HD11	1:A:271:LEU:HD22	1.88	0.56
1:B:198:HIS:CE1	1:B:221:ILE:HG22	2.40	0.56
1:A:1:MET:N	1:A:1:MET:SD	2.75	0.56
1:A:264:GLY:HA3	1:A:269:PRO:HG3	1.87	0.56
1:A:26:LEU:HD11	1:A:259:LEU:HD12	1.88	0.56
1:B:379:PHE:HE2	1:B:433:ALA:HB2	1.70	0.56
1:B:429:GLU:HA	1:B:432:LEU:HD12	1.88	0.55
1:A:413:THR:HG21	1:A:443:ARG:NH1	2.22	0.55
1:B:379:PHE:CZ	1:B:433:ALA:HA	2.42	0.55
1:A:1:MET:HE3	1:A:1:MET:HA	1.89	0.55
1:B:198:HIS:CE1	1:B:221:ILE:CG2	2.89	0.55
1:B:193:SER:O	1:B:197:VAL:HG23	2.07	0.55
1:A:1:MET:CE	1:A:1:MET:CA	2.86	0.54
1:A:260:ARG:HG3	1:A:274:LEU:HD12	1.88	0.54
1:B:197:VAL:HG22	1:B:200:TRP:CZ3	2.42	0.54
1:B:381:THR:HA	1:B:442:PRO:HG3	1.89	0.54
1:B:368:MET:CE	1:B:410:VAL:HG12	2.38	0.54
1:A:381:THR:HA	1:A:442:PRO:HG3	1.89	0.53
1:A:1:MET:CE	1:A:1:MET:HA	2.38	0.53
1:A:381:THR:HA	1:A:442:PRO:CG	2.39	0.53
1:B:108:GLN:NE2	1:B:450:LEU:HD11	2.24	0.53
1:A:96[A]:GLU:CD	1:A:100[A]:ARG:HH21	2.11	0.53
1:B:419:GLU:HB3	1:B:442:PRO:CB	2.38	0.53
1:B:199:ASP:HA	1:B:202:ARG:HD2	1.91	0.53
1:A:9:ILE:HG21	1:A:51:VAL:HG21	1.91	0.52
1:B:48:MET:CE	1:B:167:SER:HA	2.35	0.52
1:B:421:LEU:HD21	1:B:432:LEU:HD11	1.92	0.52
1:A:198:HIS:CE1	1:A:221:ILE:CG2	2.93	0.52
1:B:77:GLY:HA2	1:B:404:HIS:CD2	2.44	0.52
1:A:367:PRO:HB2	1:A:387:ILE:HG23	1.92	0.51
1:A:268:GLU:OE1	1:A:268:GLU:N	2.44	0.51
1:B:421:LEU:CD2	1:B:432:LEU:HD11	2.40	0.51
1:A:193:SER:OG	1:A:235:ASP:OD2	2.26	0.50
1:A:317:VAL:HG23	1:A:353:LYS:HG3	1.93	0.50
1:B:136:SER:HB2	4:B:903:SO4:O2	2.11	0.50
1:B:278:THR:HG23	7:B:2016:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:OE2	1:A:461:ARG:NH2	2.45	0.50
1:A:199:ASP:O	1:A:202:ARG:N	2.46	0.49
1:A:96[A]:GLU:HB3	1:A:97:PRO:HD3	1.95	0.49
1:A:187:THR:CG2	1:A:243:ILE:HD12	2.43	0.49
1:B:379:PHE:CE2	1:B:433:ALA:HB2	2.48	0.49
1:B:197:VAL:CA	1:B:200:TRP:CE3	2.89	0.48
1:B:53:GLU:OE2	2:B:801:TYR:N	2.47	0.48
1:A:237:ASN:N	1:A:237:ASN:HD22	2.11	0.48
1:A:413:THR:CG2	1:A:443:ARG:NH1	2.76	0.48
1:B:133:LYS:NZ	1:B:440:CYS:SG	2.83	0.48
1:A:83:GLN:HA	1:A:124:VAL:O	2.13	0.48
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.94	0.48
1:A:243:ILE:O	5:A:905:GOL:H31	2.13	0.48
1:A:73:GLN:HG2	1:A:79:ALA:HB2	1.95	0.48
1:A:382:ARG:NH1	1:A:442:PRO:O	2.47	0.47
1:B:242:GLU:OE1	5:B:902:GOL:O3	2.32	0.47
1:A:271:LEU:HD23	1:A:298:VAL:HG12	1.95	0.47
1:A:197:VAL:HG13	1:A:200:TRP:CE3	2.49	0.47
1:A:262:SER:O	1:A:269:PRO:HB3	2.15	0.47
1:A:368:MET:HB3	1:A:368:MET:HE3	1.89	0.47
1:A:198:HIS:O	1:A:201:ASN:N	2.47	0.46
1:B:48:MET:HE2	1:B:170:VAL:HG23	1.97	0.46
1:B:77:GLY:HA2	1:B:404:HIS:CG	2.51	0.46
1:A:441:ASP:HB3	1:A:442:PRO:HD2	1.98	0.46
1:B:197:VAL:HG13	1:B:200:TRP:CZ3	2.50	0.46
1:B:283:GLU:OE2	1:B:308:GLY:HA3	2.16	0.46
1:A:181:ASN:HB2	1:B:181:ASN:HB2	1.99	0.45
1:B:379:PHE:CE2	1:B:433:ALA:CB	2.99	0.45
1:B:197:VAL:HG13	1:B:200:TRP:HZ3	1.82	0.45
1:B:369:HIS:HE1	1:B:411:GLU:OE2	1.99	0.45
1:A:228:MET:CE	1:A:233:VAL:HG11	2.47	0.44
1:A:347:LEU:N	1:A:348:PRO:CD	2.80	0.44
1:B:314:GLU:CD	1:B:314:GLU:H	2.21	0.44
1:A:5:VAL:HG11	1:B:48:MET:SD	2.58	0.44
1:A:73:GLN:HG2	1:A:79:ALA:CB	2.49	0.43
1:B:393:GLY:O	1:B:397:VAL:HG23	2.18	0.43
1:A:96[B]:GLU:OE2	1:A:100[B]:ARG:NH2	2.45	0.43
1:A:15:LEU:HB3	1:A:16:PRO:HD2	2.01	0.43
1:B:104[B]:ARG:CZ	1:B:108:GLN:OE1	2.66	0.43
1:B:198:HIS:HE2	1:B:222:ASP:HB2	1.84	0.43
1:A:441:ASP:HB3	1:A:442:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:HIS:O	1:B:201:ASN:HB2	2.19	0.42
1:A:197:VAL:O	1:A:200:TRP:HB2	2.19	0.42
1:B:133:LYS:HD3	1:B:440:CYS:SG	2.58	0.42
1:B:265:ASP:O	1:B:266:ASP:CB	2.44	0.42
1:A:148:ARG:HB2	1:A:152:ILE:HB	2.01	0.42
1:A:45:ALA:O	1:A:49:ARG:HG3	2.20	0.42
1:A:84:GLY:HA2	1:A:410:VAL:O	2.20	0.41
1:A:21:ASP:O	1:A:25:ARG:HG3	2.20	0.41
1:B:324:ASP:O	1:B:359:HIS:CE1	2.72	0.41
1:B:115:TYR:OH	1:B:220:GLU:HG2	2.19	0.41
1:B:83:GLN:HA	1:B:124:VAL:O	2.21	0.41
1:A:458:GLU:HA	1:A:458:GLU:OE1	2.21	0.41
1:B:48:MET:HG3	1:B:166:PRO:O	2.21	0.41
1:A:228:MET:HE3	1:A:233:VAL:HG11	2.03	0.41
1:A:288:ILE:O	1:A:322:ARG:NH1	2.54	0.41
1:B:372:THR:CG2	1:B:382:ARG:HE	2.27	0.40
1:A:87:CYS:SG	1:A:440:CYS:HB3	2.61	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	460/462 (100%)	447 (97%)	12 (3%)	1 (0%)	47	58
1	B	459/462 (99%)	450 (98%)	8 (2%)	1 (0%)	47	58
All	All	919/924 (100%)	897 (98%)	20 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	CYS

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Mol	Chain	Res	Type
1	B	440	CYS

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	377/376 (100%)	371 (98%)	6 (2%)	62	78
1	B	377/376 (100%)	371 (98%)	6 (2%)	62	78
All	All	754/752 (100%)	742 (98%)	12 (2%)	62	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ILE
1	A	40	TRP
1	A	337	ARG
1	A	341	HIS
1	A	368	MET
1	B	40	TRP
1	B	193	SER
1	B	283	GLU
1	B	284	ARG
1	B	337	ARG
1	B	435	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	297	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 for Mogul analysis.

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
4	SO4	A	901	-	4,4,4	0.28	0	6,6,6	0.96	0
4	SO4	B	900	-	4,4,4	0.28	0	6,6,6	0.93	0
5	GOL	B	904	-	5,5,5	0.95	0	5,5,5	0.78	0
5	GOL	A	905	-	5,5,5	1.80	2 (40%)	5,5,5	2.47	3 (60%)
4	SO4	A	900	-	4,4,4	0.46	0	6,6,6	1.06	1 (16%)
4	SO4	A	904	-	4,4,4	0.16	0	6,6,6	0.53	0
5	GOL	A	902	-	5,5,5	1.04	0	5,5,5	1.04	0
5	GOL	B	902	-	5,5,5	0.92	0	5,5,5	0.85	0
4	SO4	B	903	-	4,4,4	0.31	0	6,6,6	0.93	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
5	GOL	A	905	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	904	-	-	2/4/4/4	-
5	GOL	A	902	-	-	0/4/4/4	-
5	GOL	B	902	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	GOL	O1-C1	2.54	1.53	1.42
5	A	905	GOL	O2-C2	2.17	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	GOL	O2-C2-C1	3.64	125.13	109.12
5	A	905	GOL	O2-C2-C3	-2.49	98.17	109.12
5	A	905	GOL	C3-C2-C1	-2.42	102.31	111.70
4	A	900	SO4	O4-S-O3	2.07	117.89	109.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	904	GOL	O1-C1-C2-C3
5	B	902	GOL	O1-C1-C2-C3
5	B	904	GOL	O1-C1-C2-O2
5	B	902	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	SO4	3	0
5	A	905	GOL	1	0
5	B	902	GOL	1	0
4	B	903	SO4	1	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	460/462 (99%)	0.00	35 (7%) 13 18	11, 29, 67, 103	0
1	B	459/462 (99%)	0.02	34 (7%) 14 19	10, 22, 60, 94	1 (0%)
All	All	919/924 (99%)	0.01	69 (7%) 14 19	10, 25, 62, 103	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	ASP	8.0
1	B	264	GLY	6.9
1	B	376	SER	6.7
1	B	237	ASN	6.7
1	B	197	VAL	6.6
1	B	377	THR	6.5
1	B	266	ASP	6.3
1	A	376	SER	5.9
1	B	433	ALA	5.5
1	A	13	PRO	5.5
1	B	378	GLY	5.5
1	A	377	THR	5.5
1	A	265	ASP	5.4
1	A	264	GLY	5.3
1	B	434	GLY	5.3
1	B	265	ASP	5.1
1	A	378	GLY	5.1
1	B	236	ARG	4.9
1	B	426	ASP	4.8
1	A	2	ASN	4.8
1	B	379	PHE	4.5
1	B	375	SER	4.4
1	A	462	ASP	4.2
1	A	1	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	436	TYR	3.9
1	B	13	PRO	3.8
1	A	379	PHE	3.7
1	A	433	ALA	3.7
1	A	3	TRP	3.7
1	B	1	MET	3.6
1	B	263	ASP	3.5
1	A	197	VAL	3.5
1	B	373	HIS	3.4
1	A	375	SER	3.4
1	B	430	THR	3.3
1	B	202	ARG	3.3
1	A	424	ALA	3.2
1	B	429	GLU	3.2
1	B	435	ARG	3.2
1	A	239	GLN	3.1
1	A	267	GLY	3.1
1	A	236	ARG	3.1
1	B	432	LEU	3.1
1	B	198	HIS	3.0
1	A	268	GLU	2.9
1	A	14	SER	2.9
1	A	426	ASP	2.8
1	A	430	THR	2.8
1	A	373	HIS	2.8
1	B	462	ASP	2.8
1	B	428	SER	2.7
1	B	9	ILE	2.7
1	A	198	HIS	2.6
1	B	418	THR	2.6
1	A	237	ASN	2.5
1	A	428	SER	2.5
1	B	431	ASP	2.5
1	B	199	ASP	2.3
1	A	380	LYS	2.3
1	B	374	GLU	2.3
1	A	434	GLY	2.2
1	B	267	GLY	2.2
1	A	207	THR	2.2
1	A	212	ALA	2.2
1	B	380	LYS	2.1
1	A	431	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	374	GLU	2.1
1	A	206	ARG	2.0
1	A	436	TYR	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 carbohydrates 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	901	5/5	0.86	0.19	30,36,37,37	5
5	GOL	A	905	6/6	0.86	0.19	30,36,38,40	0
4	SO4	A	904	5/5	0.89	0.21	25,27,30,34	5
5	GOL	B	904	6/6	0.92	0.16	19,30,35,37	0
5	GOL	B	902	6/6	0.93	0.12	11,11,12,13	6
2	TYR	B	800	13/13	0.94	0.12	19,20,24,27	0
4	SO4	B	903	5/5	0.96	0.18	59,64,68,73	0
6	CL	B	905	1/1	0.97	0.20	39,39,39,39	0
2	TYR	A	800	13/13	0.97	0.08	13,15,16,17	0
2	TYR	B	801	13/13	0.97	0.09	16,17,21,21	0
5	GOL	A	902	6/6	0.97	0.22	30,31,33,34	0
6	CL	A	903	1/1	0.97	0.08	39,39,39,39	0
3	MN	A	700	1/1	0.97	0.05	40,40,40,40	1
3	MN	B	700	1/1	0.99	0.04	46,46,46,46	1
6	CL	B	901	1/1	0.99	0.08	35,35,35,35	0
4	SO4	A	900	5/5	0.99	0.07	25,27,30,31	0
4	SO4	B	900	5/5	0.99	0.08	25,26,31,32	0

6.5 Other polymers

There are no such residues in this entry.