



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:14 PM UTC

PDB ID : 2YPP / pdb_00002ypp
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 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

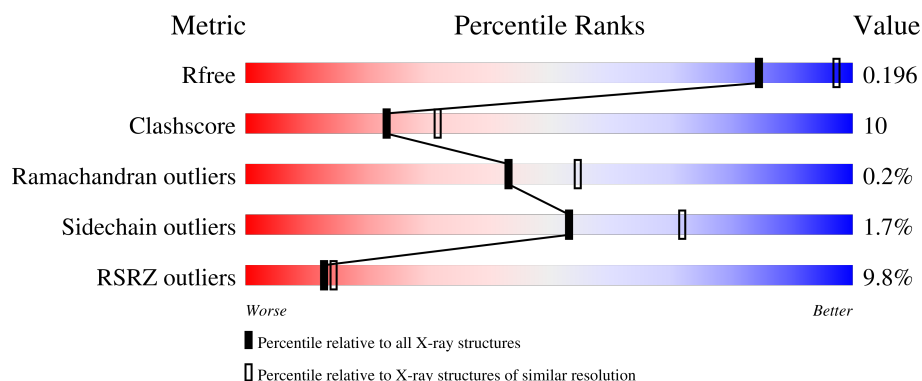
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	462	11% 76% 21% .
1	B	462	9% 78% 20% ..

2 Entry composition [i](#)

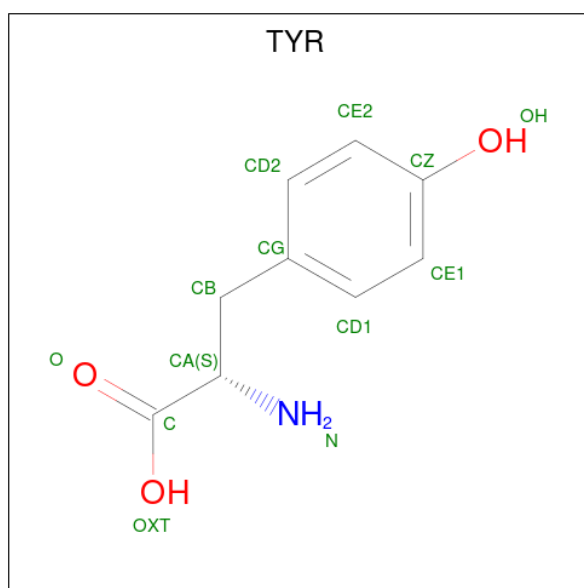
There are 7 unique types of molecules in this entry. The entry contains 7374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	460	Total	C	N	O	S	0	4	0
			3566	2225	648	675	18			
1	B	459	Total	C	N	O	S	0	4	0
			3561	2223	649	671	18			

- Molecule 2 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- 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	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

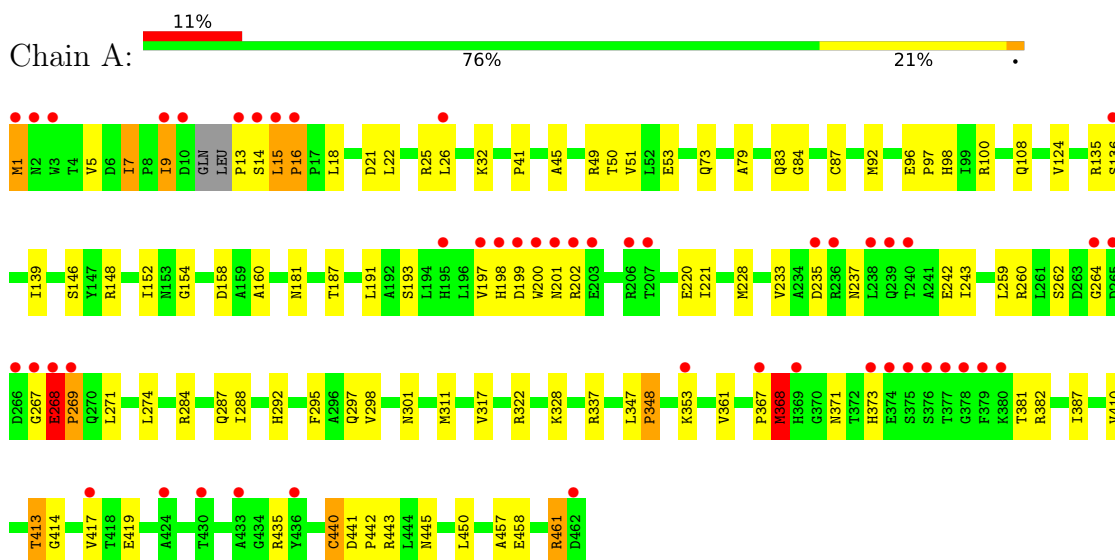
- Molecule 7 is water.

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

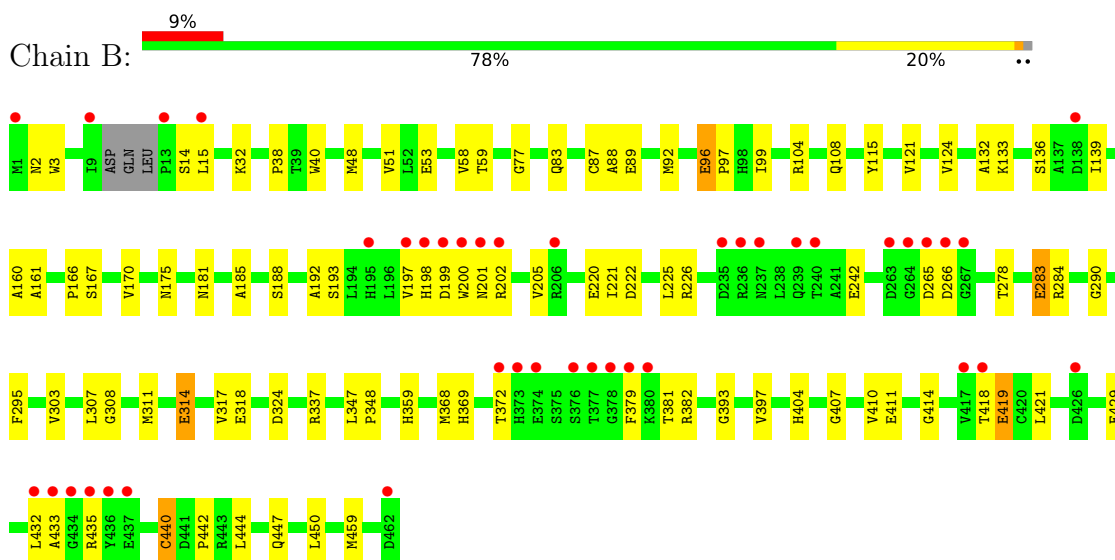
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

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	4219 reflections (6.02%)	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 , 40.0	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: SO4, MN, CL, GOL

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	1.39	24/3645 (0.7%)	1.20	11/4959 (0.2%)
1	B	1.42	26/3644 (0.7%)	1.22	6/4955 (0.1%)
All	All	1.40	50/7289 (0.7%)	1.21	17/9914 (0.2%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	VAL	C-O	-8.04	1.15	1.24
1	A	7	ILE	N-CA	-7.79	1.40	1.45
1	B	407	GLY	N-CA	-7.40	1.37	1.45
1	A	98	HIS	N-CA	-7.26	1.37	1.46
1	A	16	PRO	CA-C	6.88	1.55	1.51
1	B	175	ASN	C-O	6.53	1.31	1.24
1	A	50	THR	C-O	-6.35	1.16	1.24
1	A	146	SER	N-CA	-6.29	1.38	1.45
1	A	414	GLY	C-O	-6.22	1.16	1.23
1	B	303	VAL	N-CA	-6.15	1.39	1.46
1	B	88	ALA	C-O	-6.11	1.17	1.24
1	A	92	MET	C-O	-6.03	1.16	1.24
1	B	188	SER	C-O	-5.97	1.16	1.24
1	A	18	LEU	CA-C	5.82	1.59	1.53
1	A	7	ILE	CA-C	-5.81	1.48	1.52
1	A	53	GLU	C-O	-5.80	1.16	1.24
1	A	268	GLU	C-N	5.79	1.41	1.33
1	B	414	GLY	C-O	-5.74	1.17	1.23
1	A	154	GLY	C-O	5.70	1.31	1.23
1	A	295	PHE	C-O	-5.66	1.17	1.24
1	B	192	ALA	C-O	-5.56	1.16	1.24
1	B	295	PHE	N-CA	5.54	1.52	1.46
1	B	132	ALA	CA-C	-5.53	1.45	1.52
1	B	242	GLU	CA-C	-5.52	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ILE	C-O	-5.49	1.18	1.24
1	B	58	VAL	C-O	5.49	1.30	1.24
1	B	96	GLU	N-CA	-5.46	1.41	1.46
1	B	51	VAL	N-CA	5.46	1.52	1.46
1	B	161	ALA	N-CA	-5.46	1.39	1.46
1	B	160	ALA	C-O	-5.40	1.17	1.24
1	B	317	VAL	CA-CB	5.31	1.60	1.54
1	A	154	GLY	N-CA	5.28	1.51	1.45
1	A	242	GLU	CA-C	-5.26	1.46	1.52
1	A	292	HIS	CA-C	-5.25	1.46	1.52
1	A	269	PRO	N-CD	5.20	1.55	1.47
1	A	32	LYS	C-O	-5.19	1.17	1.23
1	B	38	PRO	C-O	-5.17	1.17	1.23
1	B	185	ALA	C-O	-5.15	1.18	1.24
1	B	318	GLU	CA-C	5.14	1.59	1.52
1	B	87	CYS	N-CA	-5.13	1.40	1.46
1	A	41	PRO	C-O	5.12	1.29	1.23
1	A	445	ASN	N-CA	-5.09	1.39	1.45
1	B	290	GLY	N-CA	5.08	1.51	1.45
1	B	3	TRP	CA-C	-5.08	1.46	1.52
1	A	413	THR	CB-CG2	-5.06	1.35	1.52
1	B	59	THR	CA-C	-5.06	1.46	1.52
1	A	297	GLN	C-O	-5.05	1.17	1.24
1	A	373	HIS	CA-C	5.03	1.58	1.52
1	B	459	MET	C-O	-5.02	1.17	1.24
1	B	99	ILE	C-O	5.01	1.29	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	SER	N-CA-C	7.99	119.68	110.97
1	A	268	GLU	CA-C-N	-6.62	112.95	119.76
1	A	268	GLU	C-N-CA	-6.62	112.95	119.76
1	B	419	GLU	N-CA-C	6.38	118.24	111.28
1	A	368	MET	N-CA-C	6.33	118.17	111.28
1	A	15	LEU	CA-C-N	-6.21	115.13	119.66
1	A	15	LEU	C-N-CA	-6.21	115.13	119.66
1	A	14	SER	N-CA-C	5.79	119.03	110.46
1	A	348	PRO	N-CA-C	5.53	117.45	110.70
1	B	314	GLU	N-CA-C	5.35	116.80	111.07
1	B	89	GLU	N-CA-C	-5.33	102.59	110.48
1	A	461	ARG	N-CA-C	5.31	117.15	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	VAL	CB-CA-C	-5.22	104.28	111.49
1	A	301	ASN	CA-C-N	-5.20	114.40	119.76
1	A	301	ASN	C-N-CA	-5.20	114.40	119.76
1	B	32	LYS	CA-C-N	-5.04	114.76	119.85
1	B	32	LYS	C-N-CA	-5.04	114.76	119.85

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	3566	0	3517	83	0
1	B	3561	0	3520	69	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	1	0
4	B	10	0	0	1	0
5	A	12	0	16	1	0
5	B	12	0	16	0	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	148	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 (148) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:48:MET:HE3	1:B:170:VAL:HG23	1.39	1.04
1:A:22:LEU:HD21	1:A:271:LEU:HD13	1.45	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:A:1:MET:HE3	1:A:1:MET:HA	1.47	0.93
1:B:197:VAL:HA	1:B:200:TRP:CE3	2.04	0.91
1:B:48:MET:HE2	1:B:167:SER:HA	1.53	0.90
1:B:48:MET:HE3	1:B:170:VAL:CG2	2.00	0.90
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:372:THR:HG22	1:B:382:ARG:HE	1.48	0.79
1:A:1:MET:HE3	1:A:1:MET:CA	2.11	0.78
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:A:268:GLU:H	1:A:268:GLU:CD	1.97	0.72
1:B:15:LEU:HD21	1:B:53:GLU:HB3	1.72	0.71
1:B:368:MET:HE3	1:B:410:VAL:HG12	1.71	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: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: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:B:307:LEU:HD22	1:B:311:MET:HE3	1.83	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:48:MET:CE	1:B:170:VAL:CG2	2.78	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:PHE:CE2	1:B:433:ALA:HA	2.37	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
1:B:368:MET:HE3	1:B:410:VAL:CG1	2.34	0.58
1:A:13:PRO:HG2	1:B:92:MET:HE2	1.85	0.58
1:A:96[A]:GLU:CD	1:A:100[A]:ARG:HH21	2.11	0.58
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:SD	1:A:1:MET:N	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: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: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: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: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: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:N	1:A:268:GLU:OE1	2.44	0.51
1:B:368:MET:HE3	1:B:410:VAL:CB	2.41	0.51
1:B:421:LEU:CD2	1:B:432:LEU:HD11	2.40	0.51
1:B:48:MET:CE	1:B:167:SER:HA	2.35	0.51
1:B:368:MET:HE1	1:B:444:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:133:LYS:NZ	1:B:440:CYS:SG	2.83	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:314:GLU:H	1:B:314:GLU:CD	2.21	0.48
1:B:53:GLU:OE2	2:B:801:TYR:N	2.47	0.48
1:A:237:ASN:HD22	1:A:237:ASN:N	2.11	0.48
1:A:413:THR:CG2	1:A:443:ARG:NH1	2.76	0.48
1:A:1:MET:CA	1:A:1:MET:CE	2.86	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: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:198:HIS:O	1:A:201:ASN:N	2.47	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:287:GLN:H	1:A:287:GLN:CD	2.24	0.44
1:A:136[B]:SER:HG	1:A:284:ARG:HH21	1.64	0.44
1:A:5:VAL:HG11	1:B:48:MET:SD	2.58	0.44
1:A:347:LEU:N	1:A:348:PRO:CD	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:311:MET:HA	1:A:311:MET:HE2	2.01	0.42
1:A:368:MET:HB3	1:A:368:MET:HE3	1.66	0.42
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:A:45:ALA:O	1:A:49:ARG:HG3	2.20	0.42
1:A:148:ARG:HB2	1:A:152:ILE:HB	2.01	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:A:458:GLU:OE1	1:A:458:GLU:HA	2.21	0.41
1:B:48:MET:HG3	1:B:166:PRO:O	2.21	0.41
1:B:83:GLN:HA	1:B:124:VAL:O	2.21	0.41
1:A:288:ILE:O	1:A:322:ARG:NH1	2.54	0.41
1:A:220:GLU:CD	1:A:461:ARG:HH22	2.29	0.40
1:B:347:LEU:O	1:B:348:PRO:C	2.64	0.40
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%)	43 55
1	B	459/462 (99%)	450 (98%)	8 (2%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	919/924 (100%)	897 (98%)	20 (2%)	2 (0%)	43 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	CYS
1	B	440	CYS

5.3.2 Protein sidechains ⓘ

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%)	372 (99%)	5 (1%)	61 77
1	B	377/376 (100%)	369 (98%)	8 (2%)	47 66
All	All	754/752 (100%)	741 (98%)	13 (2%)	53 72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ILE
1	A	268	GLU
1	A	337	ARG
1	A	368	MET
1	B	40	TRP
1	B	139	ILE
1	B	205	VAL
1	B	226	ARG
1	B	283	GLU
1	B	284	ARG
1	B	337	ARG
1	B	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	237	ASN
1	A	297	GLN
1	A	327	ASN
1	A	447	GLN
1	B	44	GLN
1	B	73	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	903	-	4,4,4	0.40	0	6,6,6	0.87	0
2	TYR	A	800	-	12,13,13	1.04	1 (8%)	13,17,17	0.89	0
2	TYR	B	800	-	12,13,13	1.89	4 (33%)	13,17,17	1.58	3 (23%)
4	SO4	A	904	-	4,4,4	0.21	0	6,6,6	0.54	0
5	GOL	A	905	-	5,5,5	1.87	2 (40%)	5,5,5	2.63	3 (60%)
4	SO4	B	900	-	4,4,4	0.37	0	6,6,6	0.85	0
5	GOL	B	902	-	5,5,5	0.95	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	900	-	4,4,4	0.54	0	6,6,6	0.96	0
2	TYR	B	801	-	12,13,13	1.50	2 (16%)	13,17,17	0.78	1 (7%)
5	GOL	A	902	-	5,5,5	1.07	0	5,5,5	1.11	0
4	SO4	A	901	-	4,4,4	0.36	0	6,6,6	0.95	0
5	GOL	B	904	-	5,5,5	0.97	0	5,5,5	0.84	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	TYR	A	800	-	-	0/8/8/8	0/1/1/1
2	TYR	B	800	-	-	0/8/8/8	0/1/1/1
5	GOL	A	905	-	-	0/4/4/4	-
5	GOL	B	902	-	-	2/4/4/4	-
2	TYR	B	801	-	-	0/8/8/8	0/1/1/1
5	GOL	A	902	-	-	0/4/4/4	-
5	GOL	B	904	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	TYR	CD2-CG	-3.43	1.32	1.38
2	B	800	TYR	CE2-CZ	-2.85	1.33	1.39
2	B	801	TYR	CE2-CZ	-2.71	1.33	1.39
2	B	801	TYR	OXT-C	-2.63	1.22	1.30
5	A	905	GOL	O1-C1	2.55	1.53	1.42
2	B	800	TYR	OXT-C	-2.28	1.23	1.30
5	A	905	GOL	O2-C2	2.23	1.49	1.43
2	B	800	TYR	CE2-CD2	-2.15	1.35	1.38
2	A	800	TYR	OXT-C	-2.01	1.24	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	GOL	O2-C2-C1	3.85	125.13	109.18
2	B	800	TYR	OH-CZ-CE2	-3.19	111.13	120.00
2	B	800	TYR	OXT-C-O	-2.69	117.98	124.08
5	A	905	GOL	O2-C2-C3	-2.66	98.17	109.18
2	B	800	TYR	OH-CZ-CE1	2.65	127.38	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	GOL	C3-C2-C1	-2.59	102.31	111.80
2	B	801	TYR	OXT-C-O	-2.35	118.76	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	SO4	1	0
5	A	905	GOL	1	0
2	B	801	TYR	1	0
4	A	901	SO4	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	460/462 (99%)	0.22	49 (10%)	11 12	9, 29, 67, 103	4 (0%)
1	B	459/462 (99%)	0.15	41 (8%)	15 17	8, 22, 60, 94	5 (1%)
All	All	919/924 (99%)	0.19	90 (9%)	13 14	8, 25, 62, 103	9 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	8.2
1	B	197	VAL	8.1
1	B	13	PRO	8.0
1	A	13	PRO	7.8
1	B	237	ASN	7.5
1	B	198	HIS	6.5
1	B	9	ILE	6.4
1	A	3	TRP	6.4
1	B	236	ARG	5.8
1	A	266	ASP	5.7
1	A	198	HIS	5.7
1	B	263	ASP	5.6
1	A	14	SER	5.5
1	B	434	GLY	5.1
1	B	433	ALA	5.0
1	A	376	SER	4.9
1	B	202	ARG	4.9
1	B	266	ASP	4.9
1	B	265	ASP	4.8
1	B	418	THR	4.7
1	A	197	VAL	4.5
1	B	435	ARG	4.5
1	B	1	MET	4.5
1	A	265	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	373	HIS	4.3
1	B	373	HIS	4.2
1	A	378	GLY	4.2
1	A	462	ASP	4.1
1	B	436	TYR	4.1
1	B	199	ASP	4.1
1	A	10	ASP	4.0
1	A	264	GLY	4.0
1	A	377	THR	4.0
1	B	432	LEU	4.0
1	A	1	MET	4.0
1	A	239	GLN	3.9
1	A	380	LYS	3.9
1	A	15	LEU	3.9
1	B	235	ASP	3.8
1	B	462	ASP	3.8
1	A	267	GLY	3.6
1	A	199	ASP	3.6
1	B	267	GLY	3.6
1	B	200	TRP	3.6
1	B	138	ASP	3.5
1	B	201	ASN	3.5
1	A	195	HIS	3.4
1	A	9	ILE	3.4
1	A	369	HIS	3.4
1	B	376	SER	3.3
1	B	378	GLY	3.3
1	A	430	THR	3.2
1	B	426	ASP	3.2
1	A	240	THR	3.2
1	A	268	GLU	3.1
1	A	2	ASN	3.1
1	A	238	LEU	3.1
1	A	269	PRO	3.0
1	B	379	PHE	2.9
1	B	380	LYS	2.9
1	A	375	SER	2.9
1	A	374	GLU	2.9
1	A	206	ARG	2.9
1	A	236	ARG	2.8
1	A	201	ASN	2.8
1	B	195[A]	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	136[A]	SER	2.7
1	B	377	THR	2.7
1	A	16	PRO	2.6
1	B	239	GLN	2.5
1	A	379	PHE	2.5
1	A	417	VAL	2.4
1	B	206	ARG	2.4
1	B	374	GLU	2.4
1	B	372	THR	2.4
1	A	203	GLU	2.4
1	B	15	LEU	2.3
1	A	200	TRP	2.3
1	A	235	ASP	2.3
1	A	367	PRO	2.2
1	A	436	TYR	2.2
1	B	417	VAL	2.2
1	B	437	GLU	2.2
1	A	26	LEU	2.2
1	A	202	ARG	2.2
1	B	240	THR	2.2
1	A	207	THR	2.1
1	A	433	ALA	2.1
1	A	353	LYS	2.1
1	A	424	ALA	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($\text{\AA}^2$)	Q<0.9
4	SO4	A	901	5/5	0.80	0.19	30,36,37,37	5
5	GOL	A	905	6/6	0.87	0.15	30,36,38,40	0
4	SO4	A	904	5/5	0.88	0.19	25,27,30,34	5
4	SO4	B	903	5/5	0.89	0.14	59,64,68,73	0
5	GOL	B	904	6/6	0.89	0.12	19,30,35,37	0
2	TYR	B	800	13/13	0.93	0.09	19,20,24,27	0
3	MN	A	700	1/1	0.94	0.07	40,40,40,40	1
5	GOL	B	902	6/6	0.94	0.10	11,11,12,13	6
5	GOL	A	902	6/6	0.94	0.16	30,31,33,34	0
6	CL	B	901	1/1	0.95	0.08	35,35,35,35	0
6	CL	B	905	1/1	0.95	0.10	39,39,39,39	0
6	CL	A	903	1/1	0.96	0.06	39,39,39,39	0
2	TYR	B	801	13/13	0.97	0.05	16,17,21,21	0
2	TYR	A	800	13/13	0.97	0.07	13,15,16,17	0
3	MN	B	700	1/1	0.98	0.09	46,46,46,46	1
4	SO4	A	900	5/5	0.99	0.07	25,27,30,31	0
4	SO4	B	900	5/5	0.99	0.06	25,26,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.