



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 02:46 AM EDT

PDB ID : 1TJ7  
Title : Structure determination and refinement at 2.44 Å resolution of Argininosuccinate lyase from E. coli  
Authors : Bhaumik, P.; Koski, M.K.; Bergman, U.; Wierenga, R.K.  
Deposited on : unknown  
Resolution : 2.44 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

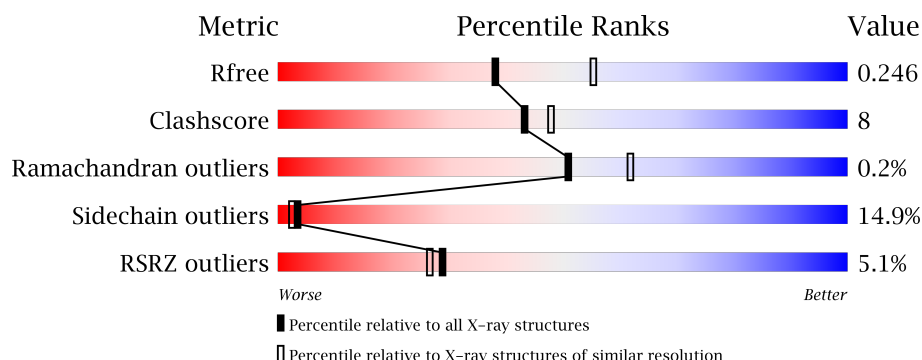
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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))
$R_{free}$	100719	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	457	<div> <div>3%</div> <div>80%</div> <div>14%</div> <div>5%</div> </div>
1	B	457	<div> <div>7%</div> <div>76%</div> <div>17%</div> <div>6%</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
2	PO4	A	601	-	-	X	X
2	PO4	B	602	-	-	-	X
3	GOL	A	602	-	-	-	X
3	GOL	A	603	-	-	X	X
3	GOL	B	603	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7289 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 Argininosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3521	2206	623	676	16			
1	B	451	Total	C	N	O	S	0	0	0
			3491	2185	618	672	16			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

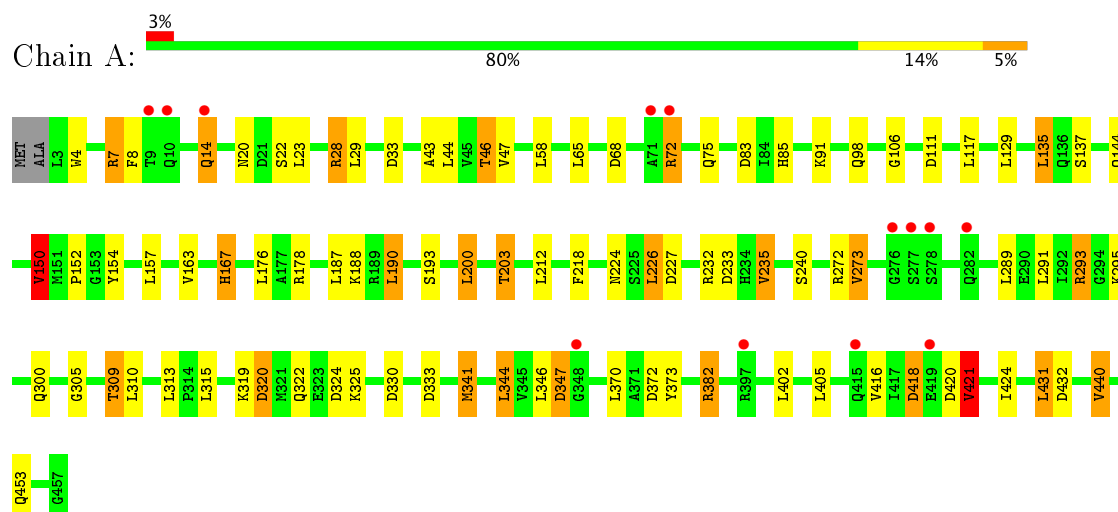
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total	O	0	0
			148	148		
4	B	101	Total	O	0	0
			101	101		

### 3 Residue-property plots [i](#)

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: Argininosuccinate lyase



#### • Molecule 1: Argininosuccinate lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.47Å 121.47Å 255.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.44 19.99 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.44) 99.8 (19.99-2.44)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.167 , 0.217 0.207 , 0.246	Depositor DCC
$R_{free}$ test set	2127 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PO4

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	0.63	0/3578	0.92	13/4842 (0.3%)
1	B	0.65	1/3546 (0.0%)	0.94	19/4798 (0.4%)
All	All	0.64	1/7124 (0.0%)	0.93	32/9640 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	GLU	CG-CD	5.05	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	LEU	CA-CB-CG	8.55	134.96	115.30
1	B	455	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	111	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	190	LEU	CA-CB-CG	7.67	132.94	115.30
1	B	148	ASP	CB-CG-OD2	7.63	125.17	118.30
1	A	178	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	28	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	178	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	B	227	ASP	CB-CG-OD2	7.36	124.92	118.30
1	B	233	ASP	CB-CG-OD2	7.07	124.66	118.30
1	B	68	ASP	CB-CG-OD2	7.05	124.65	118.30
1	B	432	ASP	CB-CG-OD2	7.02	124.61	118.30
1	B	178	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	324	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	330	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	432	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	83	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	150	VAL	CB-CA-C	-6.11	99.79	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	179	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	287	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	185	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	94	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	421	VAL	CB-CA-C	-5.42	101.11	111.40
1	A	233	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	347	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	455	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	293	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	420	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	324	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	293	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	372	ASP	CB-CG-OD2	5.04	122.83	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	3521	0	3502	57	0
1	B	3491	0	3475	58	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
3	A	12	0	16	4	0
3	B	6	0	8	4	0
4	A	148	0	0	15	0
4	B	101	0	0	3	0
All	All	7289	0	7001	108	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 8.

All (108) 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:341:MET:HB2	4:A:724:HOH:O	1.22	1.29
1:A:293:ARG:CD	4:A:740:HOH:O	2.00	1.08
1:A:293:ARG:HD2	1:B:320:ASP:OD2	1.59	1.02
1:B:135:LEU:HD13	1:B:176:LEU:HD11	1.49	0.93
1:B:40:TRP:CH2	1:B:207:ILE:HD13	2.08	0.88
1:A:315:LEU:HB2	3:A:603:GOL:H2	1.57	0.86
1:B:274:THR:HG21	1:B:284:LYS:HE3	1.59	0.85
1:A:293:ARG:HD3	4:A:740:HOH:O	1.69	0.82
1:A:293:ARG:HB2	4:A:740:HOH:O	1.78	0.82
1:A:293:ARG:NE	4:A:740:HOH:O	2.05	0.82
1:A:341:MET:SD	4:A:724:HOH:O	2.39	0.81
1:A:224:ASN:HD22	1:A:227:ASP:H	1.30	0.79
1:A:150:VAL:HG13	1:A:431:LEU:HD21	1.65	0.78
1:B:20:ASN:ND2	1:B:319:LYS:HE2	1.99	0.77
1:B:179:ASP:OD2	1:B:248:HIS:HD2	1.68	0.76
1:B:224:ASN:HD22	1:B:227:ASP:H	1.32	0.76
2:A:601:PO4:O3	2:B:602:PO4:O4	2.04	0.75
1:B:106:GLY:O	1:B:203:THR:HG23	1.86	0.74
1:A:7:ARG:NH1	4:A:606:HOH:O	2.21	0.73
1:A:8:PHE:HE2	1:B:274:THR:HG22	1.53	0.72
1:A:293:ARG:CB	4:A:740:HOH:O	2.33	0.72
3:B:603:GOL:O2	4:B:688:HOH:O	2.09	0.70
1:A:320:ASP:OD2	1:B:293:ARG:HD2	1.92	0.70
1:B:26:ASP:O	1:B:84:ILE:HG12	1.91	0.70
1:B:163:VAL:HA	1:B:440:VAL:HG21	1.73	0.69
1:B:40:TRP:CH2	1:B:207:ILE:CD1	2.75	0.69
1:A:341:MET:CB	4:A:724:HOH:O	2.01	0.68
1:B:282:GLN:H	1:B:282:GLN:HE21	1.40	0.67
1:B:135:LEU:HD13	1:B:176:LEU:CD1	2.24	0.67
1:A:28:ARG:NH2	1:A:333:ASP:OD2	2.27	0.66
1:A:315:LEU:CB	3:A:603:GOL:H2	2.24	0.66
1:B:133:ARG:HH11	1:B:133:ARG:HB2	1.61	0.65
1:A:135:LEU:HD13	1:A:176:LEU:HD11	1.80	0.63
1:A:106:GLY:O	1:A:203:THR:HG23	1.99	0.63
1:A:295:LYS:HE3	1:B:323:GLU:OE2	1.99	0.62
1:B:224:ASN:HD21	1:B:226:LEU:HB2	1.64	0.62
1:B:224:ASN:ND2	1:B:227:ASP:H	1.99	0.61
1:A:8:PHE:CE2	1:B:274:THR:HG22	2.37	0.59
1:A:319:LYS:HG3	1:B:291:LEU:HD13	1.83	0.59
1:A:106:GLY:O	1:A:203:THR:CG2	2.52	0.58
1:A:273:VAL:HG23	1:A:344:LEU:HD13	1.86	0.57
1:A:43:ALA:O	1:A:46:THR:HB	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:TYR:HB2	3:B:603:GOL:H11	1.87	0.56
1:A:418:ASP:O	1:A:421:VAL:HG22	2.07	0.55
1:A:305:GLY:O	1:A:309:THR:HG23	2.07	0.55
1:B:40:TRP:HH2	1:B:207:ILE:HD13	1.66	0.55
1:B:415:GLN:HE21	1:B:415:GLN:H	1.53	0.55
1:B:232:ARG:HB3	1:B:235:VAL:HG13	1.89	0.54
1:B:20:ASN:HD21	1:B:319:LYS:HE2	1.71	0.54
1:A:117:LEU:HD23	4:A:641:HOH:O	2.07	0.54
1:A:315:LEU:C	3:A:603:GOL:H31	2.28	0.54
1:A:163:VAL:HA	1:A:440:VAL:HG21	1.88	0.54
1:B:282:GLN:H	1:B:282:GLN:NE2	2.05	0.54
1:A:144:GLN:HE21	1:A:453:GLN:HE22	1.55	0.54
1:B:274:THR:CG2	1:B:284:LYS:HG3	2.38	0.53
1:A:305:GLY:O	1:A:309:THR:CG2	2.56	0.53
1:A:224:ASN:HD21	1:A:226:LEU:HB2	1.74	0.53
1:A:341:MET:CG	4:A:724:HOH:O	2.42	0.53
1:A:293:ARG:CD	1:B:320:ASP:OD2	2.46	0.53
1:B:154:TYR:CD1	3:B:603:GOL:H12	2.44	0.52
1:A:315:LEU:O	3:A:603:GOL:H31	2.10	0.52
1:A:20:ASN:HD21	1:A:319:LYS:NZ	2.07	0.51
1:A:224:ASN:ND2	1:A:227:ASP:H	2.03	0.51
1:A:33:ASP:OD1	1:A:85:HIS:HD2	1.93	0.51
1:B:319:LYS:HE3	1:B:322:GLN:NE2	2.25	0.51
1:B:434:ARG:HG3	1:B:440:VAL:HG12	1.92	0.51
1:B:133:ARG:NH1	1:B:133:ARG:HB2	2.23	0.50
1:B:432:ASP:HA	1:B:441:SER:HB2	1.92	0.50
1:B:106:GLY:O	1:B:203:THR:CG2	2.56	0.50
1:B:154:TYR:HD1	3:B:603:GOL:H12	1.75	0.50
1:B:246:MET:HG3	1:B:299:VAL:HG21	1.93	0.50
1:B:167:HIS:HD2	4:B:609:HOH:O	1.95	0.50
1:A:373:TYR:CE2	1:A:421:VAL:HG13	2.47	0.50
1:A:167:HIS:HD2	4:A:616:HOH:O	1.95	0.50
1:A:193:SER:HB2	1:A:218:PHE:CD2	2.48	0.48
1:B:54:GLU:HB3	1:B:99:LEU:HD11	1.95	0.48
1:A:272:ARG:HD3	4:B:691:HOH:O	2.14	0.47
1:B:20:ASN:HD21	1:B:319:LYS:CE	2.27	0.47
1:B:274:THR:HG21	1:B:284:LYS:CE	2.38	0.46
1:A:167:HIS:CD2	4:A:616:HOH:O	2.69	0.46
1:B:203:THR:HB	1:B:205:TYR:H	1.80	0.46
1:B:274:THR:HG21	1:B:284:LYS:HG3	1.98	0.46
1:B:452:ALA:O	1:B:456:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:H	1:A:14:GLN:NE2	2.14	0.45
1:B:230:SER:HB3	1:B:316:ALA:O	2.16	0.45
1:B:319:LYS:HE3	1:B:322:GLN:HE22	1.82	0.45
1:B:26:ASP:OD1	1:B:84:ILE:HG13	2.15	0.45
1:A:293:ARG:CG	4:A:740:HOH:O	2.44	0.44
1:A:72:ARG:HG2	1:A:72:ARG:O	2.18	0.44
1:B:40:TRP:CZ3	1:B:207:ILE:HD13	2.53	0.43
1:A:152:PRO:HB2	1:A:154:TYR:CZ	2.54	0.43
1:B:74:GLN:H	1:B:74:GLN:HE21	1.64	0.43
1:B:136:GLN:HB3	1:B:456:LEU:HD21	1.99	0.43
1:B:180:GLU:O	1:B:184:GLN:HG3	2.20	0.42
2:A:601:PO4:O4	1:B:278:SER:OG	2.25	0.42
1:A:382:ARG:NH1	1:A:382:ARG:HG2	2.35	0.42
1:A:7:ARG:O	1:A:7:ARG:HG3	2.18	0.42
1:A:300:GLN:HG2	1:B:308:MET:SD	2.60	0.42
1:A:293:ARG:NH2	4:A:750:HOH:O	2.48	0.41
1:A:22:SER:OG	1:A:83:ASP:HB3	2.20	0.41
1:B:96:VAL:HG11	1:B:99:LEU:HD23	2.03	0.41
1:A:319:LYS:HE3	1:A:322:GLN:NE2	2.35	0.41
1:A:4:TRP:CZ2	1:B:275:SER:HB2	2.56	0.41
1:B:434:ARG:O	1:B:441:SER:HB3	2.21	0.41
1:A:65:LEU:HD21	1:A:91:LYS:HB3	2.04	0.40
1:B:232:ARG:HD2	1:B:324:ASP:OD2	2.22	0.40
1:A:232:ARG:HB3	1:A:235:VAL:HG13	2.04	0.40
1:B:270:SER:O	1:B:274:THR:HB	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	453/457 (99%)	446 (98%)	6 (1%)	1 (0%)	51 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	449/457 (98%)	440 (98%)	8 (2%)	1 (0%)	51	62
All	All	902/914 (99%)	886 (98%)	14 (2%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	B	200	LEU

### 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	370/371 (100%)	319 (86%)	51 (14%)	4	3
1	B	368/371 (99%)	309 (84%)	59 (16%)	3	2
All	All	738/742 (100%)	628 (85%)	110 (15%)	3	2

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	14	GLN
1	A	23	LEU
1	A	28	ARG
1	A	29	LEU
1	A	44	LEU
1	A	46	THR
1	A	47	VAL
1	A	58	LEU
1	A	68	ASP
1	A	72	ARG
1	A	75	GLN
1	A	98	GLN
1	A	129	LEU

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	137	SER
1	A	150	VAL
1	A	157	LEU
1	A	167	HIS
1	A	187	LEU
1	A	188	LYS
1	A	190	LEU
1	A	200	LEU
1	A	203	THR
1	A	212	LEU
1	A	226	LEU
1	A	235	VAL
1	A	240	SER
1	A	273	VAL
1	A	289	LEU
1	A	291	LEU
1	A	293	ARG
1	A	309	THR
1	A	310	LEU
1	A	313	LEU
1	A	320	ASP
1	A	325	LYS
1	A	341	MET
1	A	344	LEU
1	A	346	LEU
1	A	347	ASP
1	A	370	LEU
1	A	382	ARG
1	A	402	LEU
1	A	405	LEU
1	A	416	VAL
1	A	418	ASP
1	A	421	VAL
1	A	424	ILE
1	A	431	LEU
1	A	440	VAL
1	B	7	ARG
1	B	23	LEU
1	B	28	ARG
1	B	29	LEU
1	B	44	LEU

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Mol	Chain	Res	Type
1	B	47	VAL
1	B	58	LEU
1	B	67	GLU
1	B	68	ASP
1	B	72	ARG
1	B	74	GLN
1	B	79	SER
1	B	82	GLU
1	B	84	ILE
1	B	86	SER
1	B	91	LYS
1	B	92	LEU
1	B	101	LYS
1	B	129	LEU
1	B	133	ARG
1	B	135	LEU
1	B	157	LEU
1	B	163	VAL
1	B	187	LEU
1	B	190	LEU
1	B	203	THR
1	B	206	GLU
1	B	212	LEU
1	B	226	LEU
1	B	232	ARG
1	B	235	VAL
1	B	272	ARG
1	B	273	VAL
1	B	274	THR
1	B	279	LEU
1	B	282	GLN
1	B	289	LEU
1	B	291	LEU
1	B	293	ARG
1	B	308	MET
1	B	310	LEU
1	B	320	ASP
1	B	344	LEU
1	B	346	LEU
1	B	347	ASP
1	B	350	GLN
1	B	372	ASP

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Mol	Chain	Res	Type
1	B	382	ARG
1	B	396	ILE
1	B	397	ARG
1	B	400	LYS
1	B	402	LEU
1	B	403	GLU
1	B	405	LEU
1	B	415	GLN
1	B	424	ILE
1	B	434	ARG
1	B	441	SER
1	B	456	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	20	ASN
1	A	85	HIS
1	A	144	GLN
1	A	146	ASN
1	A	156	HIS
1	A	167	HIS
1	A	224	ASN
1	A	322	GLN
1	A	361	GLN
1	A	428	GLN
1	A	443	GLN
1	A	447	GLN
1	B	20	ASN
1	B	74	GLN
1	B	146	ASN
1	B	167	HIS
1	B	224	ASN
1	B	248	HIS
1	B	282	GLN
1	B	300	GLN
1	B	322	GLN
1	B	362	GLN
1	B	398	GLN
1	B	415	GLN
1	B	444	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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	PO4	A	601	-	4,4,4	0.84	0	6,6,6	0.55	0
3	GOL	A	602	-	5,5,5	0.28	0	5,5,5	0.74	0
3	GOL	A	603	-	5,5,5	0.66	0	5,5,5	1.28	0
2	PO4	B	602	-	4,4,4	0.71	0	6,6,6	0.65	0
3	GOL	B	603	-	5,5,5	0.61	0	5,5,5	1.14	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	PO4	A	601	-	-	0/0/0/0	0/0/0/0
3	GOL	A	602	-	-	0/4/4/4	0/0/0/0
3	GOL	A	603	-	-	0/4/4/4	0/0/0/0
2	PO4	B	602	-	-	0/0/0/0	0/0/0/0
3	GOL	B	603	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PO4	2	0
3	A	603	GOL	4	0
2	B	602	PO4	1	0
3	B	603	GOL	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	455/457 (99%)	-0.14	13 (2%) 52 47	12, 18, 27, 41	0
1	B	451/457 (98%)	0.11	33 (7%) 16 13	6, 18, 27, 34	0
All	All	906/914 (99%)	-0.01	46 (5%) 29 27	6, 18, 27, 41	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	ARG	6.0
1	A	282	GLN	5.3
1	A	415	GLN	4.6
1	B	386	HIS	4.4
1	B	381	PHE	4.3
1	B	71	ALA	3.9
1	B	67	GLU	3.9
1	B	51	THR	3.8
1	B	397	ARG	3.8
1	B	375	VAL	3.7
1	A	397	ARG	3.7
1	B	396	ILE	3.5
1	B	72	ARG	3.4
1	A	9	THR	3.3
1	B	40	TRP	3.3
1	B	393	VAL	3.3
1	B	10	GLN	3.2
1	B	53	GLU	3.1
1	B	60	GLU	3.1
1	B	80	ASP	3.0
1	A	348	GLY	3.0
1	A	278	SER	3.0
1	B	380	PRO	3.0
1	B	52	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	48	GLY	2.9
1	B	96	VAL	2.8
1	B	415	GLN	2.7
1	A	10	GLN	2.7
1	B	47	VAL	2.6
1	B	98	GLN	2.6
1	B	57	GLN	2.6
1	B	74	GLN	2.6
1	A	14	GLN	2.5
1	B	379	VAL	2.5
1	B	206	GLU	2.5
1	A	72	ARG	2.4
1	B	9	THR	2.3
1	B	56	ALA	2.3
1	A	277	SER	2.3
1	B	385	HIS	2.2
1	B	97	GLY	2.1
1	B	372	ASP	2.1
1	A	419	GLU	2.1
1	A	71	ALA	2.1
1	B	399	GLY	2.1
1	A	276	GLY	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	602	6/6	0.67	0.37	6.81	72,72,72,73	0
3	GOL	A	603	6/6	0.90	0.29	5.14	40,43,45,47	0
3	GOL	B	603	6/6	0.90	0.29	4.66	41,44,46,47	0
2	PO4	B	602	5/5	0.98	0.15	4.60	37,37,38,39	0
2	PO4	A	601	5/5	0.98	0.16	3.25	46,47,48,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.