



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:36 AM GMT

PDB ID : 3DPC  
Title : Structure of E.coli Alkaline Phosphatase Mutant in Complex with a Phosphorylated Peptide  
Authors : Wang, W.H.; Jiang, T.  
Deposited on : 2008-07-07  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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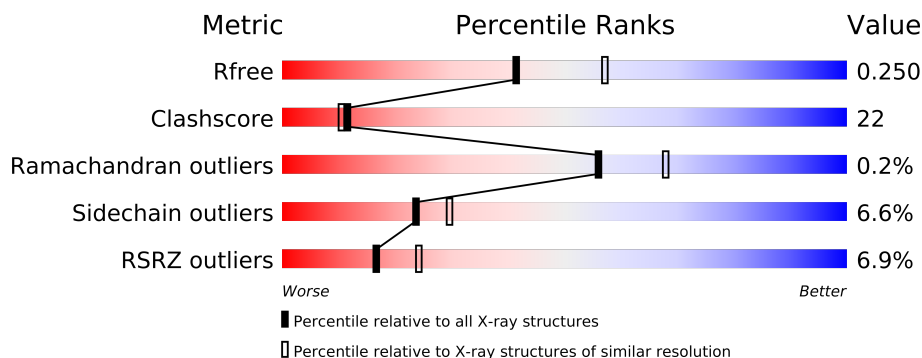
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	455	
1	B	455	
2	C	10	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	A	456	-	X
4	TRS	A	457	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6921 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3308	2047	583	666	12			
1	B	448	Total	C	N	O	S	0	0	0
			3298	2041	580	665	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	LEU	SER	ENGINEERED	UNP P00634
A	450	HIS	-	EXPRESSION TAG	UNP P00634
A	451	HIS	-	EXPRESSION TAG	UNP P00634
A	452	HIS	-	EXPRESSION TAG	UNP P00634
A	453	HIS	-	EXPRESSION TAG	UNP P00634
A	454	HIS	-	EXPRESSION TAG	UNP P00634
A	455	HIS	-	EXPRESSION TAG	UNP P00634
B	102	LEU	SER	ENGINEERED	UNP P00634
B	450	HIS	-	EXPRESSION TAG	UNP P00634
B	451	HIS	-	EXPRESSION TAG	UNP P00634
B	452	HIS	-	EXPRESSION TAG	UNP P00634
B	453	HIS	-	EXPRESSION TAG	UNP P00634
B	454	HIS	-	EXPRESSION TAG	UNP P00634
B	455	HIS	-	EXPRESSION TAG	UNP P00634

- Molecule 2 is a protein called Phosphorylated Peptide.

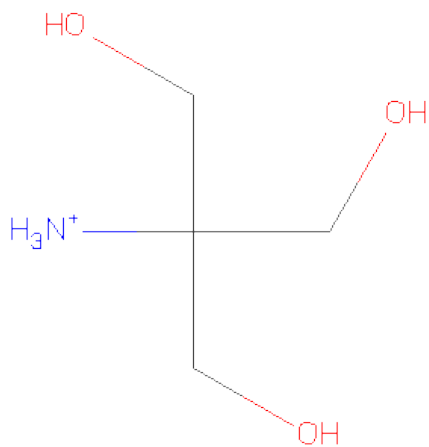
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			81	47	14	19	1			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

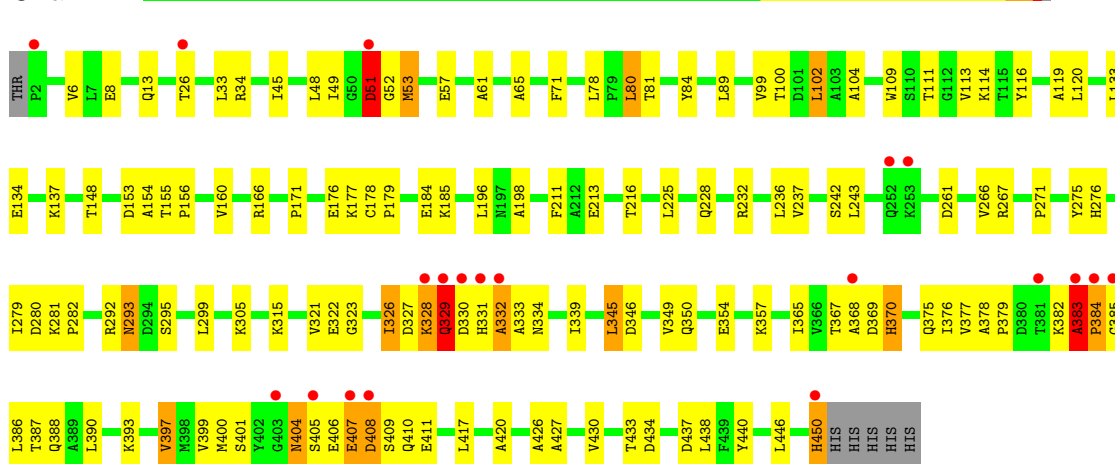
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total 97	O 97	0	0
5	B	123	Total 123	O 123	0	0
5	C	1	Total 1	O 1	0	0

### 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 errors 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.

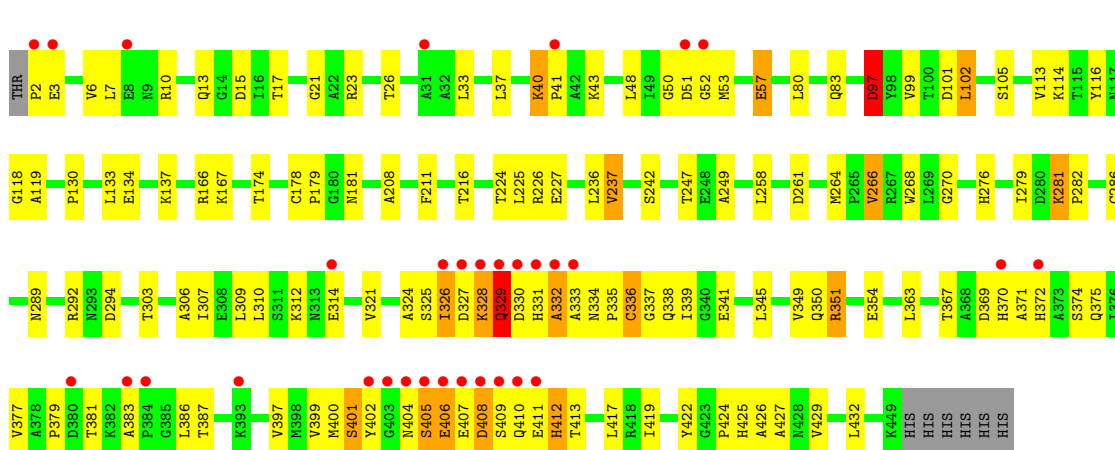
#### • Molecule 1: Alkaline phosphatase

Chain A:



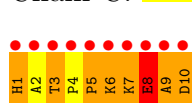
#### • Molecule 1: Alkaline phosphatase

Chain B:



#### • Molecule 2: Phosphorylated Peptide

Chain C:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.86Å 107.74Å 148.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 14.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 99.7 (14.99-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234 , 0.271 0.239 , 0.250	Depositor DCC
$R_{free}$ test set	2367 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 28.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 46934 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6921	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, PO4, TRS

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	0.35	0/3364	0.67	3/4567 (0.1%)
1	B	0.37	0/3353	0.65	2/4552 (0.0%)
2	C	0.20	0/71	0.31	0/91
All	All	0.36	0/6788	0.66	5/9210 (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	A	0	4
1	B	0	4
2	C	0	6
All	All	0	14

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	MET	N-CA-C	-5.71	95.59	111.00
1	B	332	ALA	N-CA-C	5.34	125.43	111.00
1	A	332	ALA	N-CA-C	5.33	125.40	111.00
1	B	406	GLU	N-CA-C	-5.09	97.26	111.00
1	A	51	ASP	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	327	ASP	Peptide
1	A	328	LYS	Peptide
1	A	329	GLN	Peptide
1	A	383	ALA	Peptide
1	B	327	ASP	Peptide
1	B	328	LYS	Peptide
1	B	329	GLN	Peptide
1	B	97	ASP	Peptide
2	C	1	HIS	Peptide
2	C	3	TPO	Peptide
2	C	5	PRO	Peptide
2	C	6	LYS	Peptide
2	C	8	GLU	Peptide
2	C	9	ALA	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3308	0	3254	147	0
1	B	3298	0	3249	149	0
2	C	81	0	74	32	0
3	A	5	0	0	2	0
4	A	8	0	12	1	0
5	A	97	0	0	10	0
5	B	123	0	0	8	0
5	C	1	0	0	0	0
All	All	6921	0	6589	291	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (291) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:ALA:HB2	5:A:486:HOH:O	1.41	1.20
1:B:167:LYS:CE	2:C:8:GLU:HB2	1.71	1.18

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:383:ALA:HB3	1:A:384:PRO:HA	1.30	1.14
1:A:331:HIS:O	1:A:334:ASN:HB2	1.54	1.06
1:B:266:VAL:HG21	1:B:331:HIS:NE2	1.70	1.05
1:B:167:LYS:HE3	2:C:1:HIS:O	1.53	1.05
1:B:331:HIS:O	1:B:334:ASN:HB2	1.54	1.05
1:A:383:ALA:HB1	1:A:387:THR:HG21	1.39	1.05
1:A:102:LEU:HB2	3:A:456:PO4:O2	1.58	1.04
1:B:167:LYS:HE2	2:C:8:GLU:HB2	1.39	1.03
1:A:328:LYS:HD2	1:A:409:SER:OG	1.59	1.03
1:B:266:VAL:CG2	1:B:331:HIS:NE2	2.26	0.98
2:C:3:TPO:O	2:C:3:TPO:HG22	1.64	0.94
2:C:2:ALA:HA	2:C:5:PRO:HD3	1.51	0.92
1:A:53:MET:HE2	1:A:345:LEU:HG	1.51	0.91
1:A:382:LYS:HE2	1:B:408:ASP:OD1	1.71	0.90
1:B:331:HIS:O	1:B:334:ASN:CB	2.23	0.87
1:A:328:LYS:CD	1:A:409:SER:OG	2.23	0.87
1:A:331:HIS:O	1:A:334:ASN:CB	2.23	0.86
2:C:1:HIS:O	2:C:5:PRO:HB3	1.77	0.84
1:A:384:PRO:HD3	5:A:505:HOH:O	1.76	0.84
1:B:102:LEU:HB2	2:C:3:TPO:O3P	1.77	0.83
1:B:237:VAL:HG22	1:B:242:SER:HB3	1.59	0.83
1:A:383:ALA:CB	1:A:384:PRO:HA	2.10	0.80
2:C:8:GLU:O	2:C:8:GLU:HG2	1.81	0.79
1:B:335:PRO:HG3	1:B:402:TYR:OH	1.82	0.79
1:A:293:ASN:HD22	1:A:295:SER:H	1.28	0.79
1:B:167:LYS:CE	2:C:1:HIS:O	2.29	0.79
1:B:2:PRO:HG2	1:B:3:GLU:H	1.47	0.79
1:B:51:ASP:HB2	1:B:324:ALA:HB2	1.65	0.78
1:B:266:VAL:HG21	1:B:331:HIS:CD2	2.18	0.78
2:C:2:ALA:CA	2:C:5:PRO:HD3	2.12	0.78
1:A:382:LYS:HB3	1:B:411:GLU:OE2	1.85	0.77
1:A:368:ALA:O	1:A:417:LEU:HD13	1.83	0.77
1:B:167:LYS:CD	2:C:8:GLU:HB2	2.14	0.76
1:A:383:ALA:HB1	1:A:387:THR:CG2	2.15	0.76
1:A:382:LYS:HE3	1:B:408:ASP:OD2	1.86	0.74
2:C:2:ALA:HA	2:C:5:PRO:CD	2.17	0.73
1:A:328:LYS:HD2	1:A:409:SER:CB	2.17	0.73
1:B:167:LYS:NZ	2:C:8:GLU:HB2	2.02	0.72
1:A:329:GLN:HA	1:A:332:ALA:HB2	1.71	0.72
1:B:329:GLN:HA	1:B:332:ALA:HB2	1.71	0.72
2:C:2:ALA:CB	2:C:5:PRO:HD3	2.19	0.72
1:B:167:LYS:HE2	2:C:8:GLU:CB	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:THR:HG23	1:A:299:LEU:HD13	1.71	0.71
1:A:377:VAL:C	1:B:99:VAL:HG21	2.11	0.71
1:A:411:GLU:OE1	1:B:381:THR:HG23	1.91	0.71
2:C:3:TPO:N	2:C:4:PRO:HA	2.06	0.71
1:B:328:LYS:HD2	1:B:409:SER:HB3	1.72	0.71
1:B:276:HIS:HD2	1:B:279:ILE:HD11	1.57	0.70
1:A:427:ALA:HB1	1:B:33:LEU:HD22	1.71	0.70
1:A:237:VAL:HG13	1:A:242:SER:HB2	1.73	0.70
1:B:52:GLY:HA3	1:B:372:HIS:CE1	2.27	0.70
1:A:383:ALA:HB3	1:A:384:PRO:CA	2.18	0.69
1:B:386:LEU:HD21	1:B:406:GLU:HB2	1.73	0.69
1:B:350:GLN:O	1:B:354:GLU:HG3	1.92	0.69
1:B:379:PRO:HA	1:B:399:VAL:HG21	1.76	0.68
1:A:370:HIS:HA	1:A:417:LEU:HD11	1.75	0.68
1:A:53:MET:CE	1:A:345:LEU:HG	2.23	0.67
1:B:402:TYR:HB3	1:B:404:ASN:HD21	1.60	0.67
1:A:266:VAL:HG22	5:A:526:HOH:O	1.95	0.67
2:C:8:GLU:CG	2:C:8:GLU:O	2.43	0.66
1:B:97:ASP:C	1:B:97:ASP:OD1	2.32	0.66
1:A:382:LYS:CE	1:B:408:ASP:OD2	2.44	0.66
1:A:279:ILE:HG13	1:A:280:ASP:N	2.11	0.66
1:B:329:GLN:HG3	1:B:332:ALA:HB2	1.79	0.65
1:B:216:THR:HG21	5:B:545:HOH:O	1.95	0.65
1:B:387:THR:HG22	1:B:401:SER:HB2	1.79	0.65
1:A:48:LEU:HG	1:A:349:VAL:HG22	1.79	0.65
1:A:329:GLN:HG3	1:A:332:ALA:HB2	1.79	0.64
1:B:338:GLN:NE2	5:B:559:HOH:O	2.31	0.64
1:B:402:TYR:HB3	1:B:404:ASN:ND2	2.12	0.64
1:A:176:GLU:HG3	1:A:177:LYS:HG3	1.78	0.64
1:B:328:LYS:HD2	1:B:409:SER:CB	2.28	0.63
1:B:266:VAL:CG2	1:B:331:HIS:CE1	2.81	0.63
1:A:266:VAL:HG13	1:A:331:HIS:CE1	2.33	0.62
1:A:404:ASN:CG	1:A:410:GLN:HA	2.20	0.62
1:B:15:ASP:O	1:B:21:GLY:HA3	1.99	0.62
1:A:51:ASP:HB2	1:A:369:ASP:OD2	1.99	0.62
1:A:120:LEU:HD12	1:A:166:ARG:HA	1.81	0.62
1:A:48:LEU:HD13	1:A:321:VAL:HB	1.82	0.61
1:B:372:HIS:HB3	5:B:559:HOH:O	1.99	0.61
1:A:171:PRO:HB3	1:A:216:THR:HG23	1.81	0.61
1:B:48:LEU:HD13	1:B:321:VAL:HB	1.81	0.61
1:B:167:LYS:HD3	2:C:8:GLU:HB2	1.81	0.61
1:B:374:SER:O	1:B:375:GLN:HG3	1.99	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:335:PRO:CG	1:B:402:TYR:OH	2.49	0.61
1:B:281:LYS:HG3	1:B:282:PRO:HD2	1.80	0.61
1:B:208:ALA:HB2	1:B:258:LEU:HB3	1.83	0.61
1:A:281:LYS:HB3	1:A:282:PRO:HD2	1.82	0.61
1:B:40:LYS:HG3	1:B:41:PRO:HD2	1.84	0.60
1:A:329:GLN:HG3	1:A:332:ALA:CB	2.31	0.60
1:B:57:GLU:OE2	1:B:372:HIS:HB2	2.00	0.60
1:B:40:LYS:HE3	1:B:40:LYS:HA	1.84	0.60
2:C:9:ALA:C	2:C:10:ASP:OXT	2.38	0.60
1:B:329:GLN:HG3	1:B:332:ALA:CB	2.31	0.60
1:A:53:MET:HB3	1:A:368:ALA:HB2	1.83	0.60
1:A:382:LYS:CE	1:B:408:ASP:CG	2.70	0.59
2:C:3:TPO:N	2:C:4:PRO:CA	2.65	0.59
1:B:326:ILE:HG22	1:B:331:HIS:HB3	1.83	0.59
1:B:6:VAL:O	1:B:6:VAL:HG22	2.02	0.59
1:A:326:ILE:HG22	1:A:331:HIS:HB3	1.83	0.59
1:B:118:GLY:HA3	2:C:1:HIS:CG	2.37	0.59
2:C:3:TPO:O	2:C:3:TPO:CG2	2.40	0.59
1:A:328:LYS:NZ	1:A:409:SER:OG	2.31	0.59
1:B:402:TYR:CB	1:B:404:ASN:HD21	2.15	0.59
1:A:292:ARG:NH2	5:A:476:HOH:O	2.35	0.59
1:A:382:LYS:CE	1:B:408:ASP:OD1	2.47	0.58
1:B:167:LYS:NZ	2:C:8:GLU:CB	2.67	0.58
1:A:102:LEU:HD13	1:A:154:ALA:HB3	1.85	0.58
1:A:49:ILE:HD13	1:A:367:THR:HG23	1.86	0.58
1:B:426:ALA:O	1:B:429:VAL:HG22	2.04	0.58
1:B:133:LEU:C	1:B:133:LEU:HD23	2.24	0.58
1:A:228:GLN:O	1:A:232:ARG:HG3	2.04	0.58
1:A:71:PHE:N	4:A:457:TRS:N	2.52	0.57
1:A:293:ASN:ND2	1:A:295:SER:OG	2.36	0.57
1:A:376:ILE:O	1:B:413:THR:HA	2.04	0.57
1:A:404:ASN:ND2	1:A:410:GLN:HA	2.19	0.57
1:B:303:THR:O	1:B:307:ILE:HG13	2.04	0.57
1:B:405:SER:O	1:B:408:ASP:CB	2.53	0.57
1:A:228:GLN:HB2	5:A:474:HOH:O	2.04	0.57
1:B:167:LYS:CE	2:C:8:GLU:CB	2.65	0.56
1:B:52:GLY:HA3	1:B:372:HIS:ND1	2.19	0.56
1:B:15:ASP:OD1	1:B:17:THR:HB	2.04	0.56
1:A:184:GLU:HG2	1:A:185:LYS:HD3	1.87	0.56
1:B:226:ARG:NH1	1:B:236:LEU:HD21	2.19	0.56
1:B:381:THR:HG22	1:B:383:ALA:H	1.70	0.56
1:B:52:GLY:HA2	1:B:370:HIS:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:GLY:HA3	1:A:345:LEU:CD2	2.37	0.55
1:A:243:LEU:HD12	1:A:243:LEU:O	2.06	0.55
1:A:390:LEU:O	1:A:397:VAL:HA	2.06	0.55
1:A:84:TYR:HA	1:A:433:THR:O	2.07	0.55
1:A:65:ALA:O	1:A:393:LYS:HD2	2.06	0.55
1:A:383:ALA:CB	1:A:384:PRO:CA	2.82	0.55
1:A:53:MET:C	1:A:368:ALA:HB2	2.26	0.55
1:A:34:ARG:NH1	1:B:37:LEU:O	2.41	0.54
1:A:267:ARG:HA	1:A:292:ARG:HD2	1.89	0.54
1:B:6:VAL:O	1:B:6:VAL:CG2	2.55	0.54
1:A:450:HIS:N	1:A:450:HIS:ND1	2.38	0.54
1:A:279:ILE:CG1	1:A:280:ASP:N	2.70	0.53
1:A:267:ARG:HA	1:A:292:ARG:CD	2.38	0.53
1:B:266:VAL:HG22	1:B:331:HIS:CE1	2.42	0.53
1:B:286:CYS:CB	1:B:336:CYS:SG	2.97	0.53
1:B:13:GLN:HG2	1:B:26:THR:HG22	1.91	0.53
1:B:51:ASP:HB2	1:B:324:ALA:CB	2.36	0.53
1:B:48:LEU:HG	1:B:349:VAL:HG22	1.90	0.53
1:A:346:ASP:O	1:A:350:GLN:HG3	2.08	0.53
1:B:130:PRO:HA	1:B:134:GLU:OE1	2.09	0.53
1:A:365:ILE:HD13	1:A:438:LEU:HD11	1.91	0.53
1:A:116:TYR:CZ	1:A:119:ALA:HB2	2.43	0.52
1:A:370:HIS:CA	1:A:417:LEU:HD11	2.40	0.52
1:A:329:GLN:CA	1:A:332:ALA:HB2	2.39	0.52
1:B:167:LYS:HE2	2:C:5:PRO:HG3	1.92	0.51
1:A:45:ILE:CD1	1:A:446:LEU:HG	2.41	0.51
1:A:387:THR:HG22	1:A:401:SER:HB3	1.93	0.51
1:B:6:VAL:O	1:B:7:LEU:C	2.48	0.51
1:A:382:LYS:HE3	1:B:408:ASP:CG	2.28	0.50
1:B:351:ARG:NH2	5:B:550:HOH:O	2.44	0.50
1:B:118:GLY:HA3	2:C:1:HIS:ND1	2.26	0.50
1:A:116:TYR:CE1	1:A:119:ALA:HB2	2.46	0.50
1:B:113:VAL:HG22	1:B:114:LYS:O	2.11	0.50
1:B:370:HIS:CG	1:B:412:HIS:CE1	3.00	0.50
1:A:51:ASP:OD1	1:A:51:ASP:C	2.47	0.50
1:B:97:ASP:OD1	1:B:97:ASP:O	2.30	0.50
2:C:2:ALA:HB1	2:C:5:PRO:HD3	1.94	0.50
1:B:7:LEU:HD13	1:B:10:ARG:NE	2.27	0.50
1:A:379:PRO:HA	1:A:399:VAL:HG21	1.94	0.49
1:A:292:ARG:HG2	5:A:470:HOH:O	2.13	0.49
1:B:329:GLN:CA	1:B:332:ALA:HB2	2.39	0.49
2:C:5:PRO:CG	2:C:8:GLU:HB3	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:GLY:HA3	1:A:345:LEU:HD22	1.94	0.49
1:A:49:ILE:O	1:A:322:GLU:HA	2.13	0.49
1:A:387:THR:HG22	1:A:401:SER:CB	2.43	0.49
1:A:102:LEU:CB	3:A:456:PO4:O2	2.47	0.49
1:A:78:LEU:H	1:A:78:LEU:HD12	1.77	0.48
1:B:97:ASP:O	1:B:99:VAL:N	2.46	0.48
1:A:275:TYR:O	1:A:276:HIS:HB2	2.12	0.48
1:A:382:LYS:CB	1:B:411:GLU:OE2	2.60	0.48
1:B:174:THR:HG23	1:B:178:CYS:HB2	1.96	0.48
1:B:374:SER:HB3	1:B:402:TYR:CD2	2.49	0.48
1:B:224:THR:OG1	1:B:227:GLU:HG3	2.13	0.48
1:B:312:LYS:HD2	5:B:556:HOH:O	2.13	0.48
5:A:483:HOH:O	1:B:413:THR:HB	2.14	0.47
1:B:226:ARG:HH11	1:B:236:LEU:HD21	1.78	0.47
1:A:383:ALA:CB	1:A:387:THR:HG21	2.27	0.47
1:A:89:LEU:HG	1:A:114:LYS:HB3	1.96	0.47
1:B:333:ALA:O	1:B:335:PRO:HD3	2.14	0.47
1:A:6:VAL:HG21	1:A:357:LYS:HE2	1.97	0.47
1:B:372:HIS:CD2	1:B:410:GLN:HG3	2.50	0.47
1:B:6:VAL:HG12	1:B:422:TYR:CE1	2.49	0.47
1:B:178:CYS:N	1:B:179:PRO:HD3	2.29	0.47
1:B:247:THR:O	5:B:556:HOH:O	2.20	0.47
1:A:53:MET:HE2	1:A:345:LEU:CG	2.36	0.46
1:B:402:TYR:CB	1:B:404:ASN:ND2	2.75	0.46
1:A:33:LEU:HB3	1:B:37:LEU:CD1	2.45	0.46
1:A:178:CYS:N	1:A:179:PRO:HD3	2.30	0.46
1:A:387:THR:HA	1:A:400:MET:O	2.16	0.46
1:A:78:LEU:N	1:A:78:LEU:HD12	2.29	0.46
1:B:405:SER:O	1:B:408:ASP:HB2	2.16	0.46
1:B:372:HIS:CB	5:B:559:HOH:O	2.60	0.46
1:B:53:MET:HG2	1:B:53:MET:O	2.15	0.46
1:A:13:GLN:HE21	1:A:26:THR:CG2	2.28	0.46
1:A:440:TYR:CE2	1:B:23:ARG:HD2	2.52	0.46
1:B:116:TYR:CZ	1:B:119:ALA:HB2	2.50	0.46
1:A:236:LEU:HD23	5:A:498:HOH:O	2.16	0.45
1:A:332:ALA:C	1:A:334:ASN:H	2.19	0.45
1:B:326:ILE:HD11	1:B:341:GLU:HG2	1.97	0.45
1:B:166:ARG:CZ	2:C:2:ALA:O	2.64	0.45
1:B:332:ALA:C	1:B:334:ASN:H	2.20	0.45
1:B:402:TYR:CD1	1:B:402:TYR:N	2.85	0.45
1:A:378:ALA:N	1:B:99:VAL:HG21	2.31	0.45
1:A:61:ALA:HA	1:A:339:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:370:HIS:HA	1:B:417:LEU:CD2	2.46	0.45
1:B:2:PRO:CG	1:B:3:GLU:N	2.80	0.45
1:A:33:LEU:HD22	1:B:427:ALA:HB1	1.99	0.44
1:B:83:GLN:O	1:B:432:LEU:HA	2.17	0.44
1:B:40:LYS:HA	1:B:40:LYS:CE	2.47	0.44
1:B:424:PRO:O	1:B:425:HIS:HB2	2.18	0.44
2:C:7:LYS:HB3	2:C:8:GLU:H	1.52	0.44
1:B:268:TRP:CZ3	1:B:339:ILE:HG22	2.53	0.44
1:A:51:ASP:OD1	1:A:52:GLY:N	2.51	0.44
1:A:52:GLY:HA2	1:A:57:GLU:HG2	2.00	0.44
1:B:334:ASN:OD1	1:B:337:GLY:N	2.40	0.44
1:B:166:ARG:HD3	2:C:2:ALA:H	1.83	0.44
1:B:48:LEU:HD22	1:B:48:LEU:N	2.33	0.43
1:A:331:HIS:HE1	5:A:540:HOH:O	2.01	0.43
1:B:363:LEU:HD13	1:B:424:PRO:O	2.18	0.43
1:A:405:SER:O	1:A:408:ASP:O	2.36	0.43
1:A:370:HIS:N	1:A:370:HIS:ND1	2.62	0.43
1:B:405:SER:O	1:B:406:GLU:C	2.55	0.43
1:A:111:THR:OG1	1:A:113:VAL:HG12	2.19	0.43
1:B:137:LYS:HB3	1:B:137:LYS:HE2	1.86	0.43
1:A:331:HIS:O	1:A:334:ASN:HB3	2.13	0.43
1:A:155:THR:HB	5:A:487:HOH:O	2.19	0.43
1:B:289:ASN:O	1:B:292:ARG:HB2	2.19	0.43
1:A:211:PHE:HA	1:A:225:LEU:HB2	2.01	0.43
1:A:153:ASP:OD1	1:A:154:ALA:N	2.52	0.43
1:A:370:HIS:C	1:A:417:LEU:HD11	2.39	0.43
1:B:369:ASP:OD2	1:B:370:HIS:ND1	2.40	0.43
1:A:33:LEU:HB3	1:B:37:LEU:HD13	2.01	0.43
1:A:81:THR:HG22	1:A:420:ALA:HB2	2.01	0.43
1:A:160:VAL:HB	1:A:198:ALA:CB	2.49	0.43
1:A:266:VAL:CG1	1:A:331:HIS:CE1	3.01	0.42
1:A:51:ASP:HA	1:A:369:ASP:OD2	2.18	0.42
1:A:184:GLU:HG2	1:A:185:LYS:CD	2.48	0.42
1:A:113:VAL:HG22	1:A:114:LYS:O	2.17	0.42
1:A:386:LEU:O	1:A:401:SER:HA	2.19	0.42
1:A:367:THR:OG1	1:A:368:ALA:N	2.52	0.42
1:A:49:ILE:CD1	1:A:367:THR:HG23	2.48	0.42
1:A:100:THR:O	1:A:370:HIS:CD2	2.71	0.42
1:A:134:GLU:O	1:A:137:LYS:HB3	2.19	0.42
1:B:306:ALA:O	1:B:310:LEU:HG	2.19	0.42
1:B:264:MET:O	1:B:325:SER:HB2	2.20	0.42
1:B:312:LYS:CD	5:B:556:HOH:O	2.66	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:80:LEU:HD23	1:A:426:ALA:HB3	2.01	0.42
1:B:370:HIS:CD2	1:B:371:ALA:O	2.72	0.42
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.42
1:A:237:VAL:HG11	1:A:243:LEU:HB2	2.00	0.42
1:B:367:THR:HB	1:B:419:ILE:HG13	2.02	0.42
1:A:99:VAL:HG21	1:B:377:VAL:C	2.40	0.42
1:B:2:PRO:CG	1:B:3:GLU:H	2.15	0.42
1:A:430:VAL:HG21	1:B:33:LEU:HD21	2.02	0.42
1:A:375:GLN:OE1	1:B:413:THR:HG21	2.20	0.42
1:A:133:LEU:C	1:A:133:LEU:HD23	2.40	0.42
1:B:43:LYS:HE3	1:B:314:GLU:O	2.20	0.42
1:A:350:GLN:O	1:A:354:GLU:HG3	2.19	0.41
1:B:270:GLY:HA3	1:B:336:CYS:SG	2.60	0.41
1:A:100:THR:OG1	1:A:104:ALA:HB3	2.20	0.41
1:A:100:THR:O	1:A:370:HIS:HD2	2.03	0.41
1:A:45:ILE:HD12	1:A:446:LEU:HG	2.01	0.41
1:B:178:CYS:HB3	1:B:181:ASN:OD1	2.20	0.41
1:B:40:LYS:HG3	1:B:41:PRO:CD	2.49	0.41
1:B:335:PRO:HG3	1:B:402:TYR:CZ	2.55	0.41
1:A:155:THR:HB	1:A:156:PRO:CD	2.51	0.41
1:A:271:PRO:HG2	1:A:388:GLN:NE2	2.35	0.41
1:A:384:PRO:HB2	1:A:385:GLY:H	1.70	0.41
1:A:84:TYR:CE1	1:A:417:LEU:HB2	2.55	0.41
1:A:243:LEU:HD11	1:A:305:LYS:HG2	2.03	0.41
1:A:171:PRO:HD2	1:A:213:GLU:OE1	2.20	0.41
1:A:196:LEU:HA	1:A:196:LEU:HD23	1.86	0.41
2:C:2:ALA:O	2:C:3:TPO:HB	2.21	0.40
1:A:379:PRO:HB3	1:A:399:VAL:HG23	2.03	0.40
1:B:226:ARG:HG3	1:B:236:LEU:HD21	2.02	0.40
1:A:109:TRP:CD1	1:A:109:TRP:C	2.94	0.40
1:B:211:PHE:HA	1:B:225:LEU:HB2	2.04	0.40
1:B:249:ALA:HB2	1:B:309:LEU:HD13	2.02	0.40
1:B:329:GLN:CG	1:B:332:ALA:HB2	2.48	0.40
1:B:292:ARG:HA	1:B:292:ARG:HD3	1.95	0.40
1:A:434:ASP:O	1:A:437:ASP:HB2	2.21	0.40
1:B:50:GLY:HA3	1:B:345:LEU:HD22	2.03	0.40
1:A:281:LYS:HB3	1:A:282:PRO:CD	2.49	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	447/455 (98%)	416 (93%)	29 (6%)	2 (0%)	43	52
1	B	446/455 (98%)	420 (94%)	26 (6%)	0	100	100
2	C	7/10 (70%)	4 (57%)	3 (43%)	0	100	100
All	All	900/920 (98%)	840 (93%)	58 (6%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	PRO
1	A	383	ALA

### 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	340/346 (98%)	323 (95%)	17 (5%)	34	45
1	B	339/346 (98%)	315 (93%)	24 (7%)	21	26
2	C	7/7 (100%)	3 (43%)	4 (57%)	0	0
All	All	686/699 (98%)	641 (93%)	45 (7%)	24	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	51	ASP
1	A	80	LEU
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	261	ASP
1	A	293	ASN
1	A	315	LYS
1	A	326	ILE
1	A	329	GLN
1	A	330	ASP
1	A	345	LEU
1	A	370	HIS
1	A	397	VAL
1	A	404	ASN
1	A	407	GLU
1	A	408	ASP
1	A	450	HIS
1	B	40	LYS
1	B	57	GLU
1	B	80	LEU
1	B	97	ASP
1	B	101	ASP
1	B	102	LEU
1	B	105	SER
1	B	237	VAL
1	B	261	ASP
1	B	266	VAL
1	B	281	LYS
1	B	294	ASP
1	B	326	ILE
1	B	329	GLN
1	B	330	ASP
1	B	336	CYS
1	B	351	ARG
1	B	397	VAL
1	B	400	MET
1	B	401	SER
1	B	405	SER
1	B	407	GLU
1	B	408	ASP
1	B	412	HIS
2	C	6	LYS
2	C	7	LYS
2	C	8	GLU
2	C	10	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	230	GLN
1	A	291	GLN
1	A	293	ASN
1	A	338	GLN
1	A	404	ASN
1	B	13	GLN
1	B	230	GLN
1	B	235	GLN
1	B	276	HIS
1	B	391	ASN
1	B	404	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	C	3	2	10,10,11	6.00	5 (50%)	12,14,16	1.79	2 (16%)

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	TPO	C	3	2	-	1/9/11/13	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	TPO	O-C	17.65	1.23	1.11
2	C	3	TPO	OG1-CB	3.86	1.52	1.45
2	C	3	TPO	CG2-CB	-3.21	1.43	1.51
2	C	3	TPO	P-OG1	-3.05	1.50	1.59
2	C	3	TPO	CA-C	2.48	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	TPO	OG1-P-O1P	4.56	119.52	106.79
2	C	3	TPO	P-OG1-CB	2.95	133.18	120.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	TPO	OG1-CB-CA-N

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	456	-	4,4,4	1.68	2 (50%)	6,6,6	0.32	0
4	TRS	A	457	-	7,7,7	0.88	0	9,9,9	3.41	6 (66%)

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	PO4	A	456	-	-	0/0/0/0	0/0/0/0
4	TRS	A	457	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	456	PO4	P-O3	2.23	1.61	1.52
3	A	456	PO4	P-O2	2.12	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	457	TRS	C3-C-C2	-5.72	101.32	110.70
4	A	457	TRS	C2-C-C1	-5.33	101.96	110.70
4	A	457	TRS	C1-C-N	3.94	119.01	108.30
4	A	457	TRS	C2-C-N	-3.52	98.72	108.30
4	A	457	TRS	C3-C-N	3.06	116.61	108.30
4	A	457	TRS	C3-C-C1	2.23	114.36	110.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	449/455 (98%)	0.17	20 (4%) 32 42	19, 29, 57, 80	0
1	B	448/455 (98%)	0.25	32 (7%) 16 23	10, 27, 57, 80	0
2	C	10/10 (100%)	6.92	10 (100%) 0 0	34, 47, 48, 49	0
All	All	907/920 (98%)	0.28	62 (6%) 17 25	10, 28, 57, 80	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	ASP	15.3
2	C	2	ALA	13.3
1	B	331	HIS	11.3
1	A	331	HIS	11.1
1	B	403	GLY	10.8
1	A	330	ASP	10.3
1	B	2	PRO	9.6
1	B	329	GLN	8.3
2	C	9	ALA	8.2
1	B	407	GLU	8.0
1	B	408	ASP	7.9
2	C	1	HIS	7.6
2	C	4	PRO	7.6
1	B	406	GLU	7.3
2	C	10	ASP	7.2
1	B	410	GLN	6.5
2	C	5	PRO	6.3
1	B	409	SER	5.9
1	B	328	LYS	5.5
1	B	327	ASP	5.4
2	C	8	GLU	5.2
1	B	404	ASN	5.2
1	B	405	SER	5.1

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Mol	Chain	Res	Type	RSRZ
2	C	7	LYS	4.9
1	A	2	PRO	4.7
2	C	3	TPO	4.7
1	A	407	GLU	4.6
1	A	384	PRO	4.5
1	B	332	ALA	4.3
1	A	368	ALA	4.2
2	C	6	LYS	4.1
1	A	403	GLY	4.0
1	B	384	PRO	3.8
1	A	328	LYS	3.5
1	A	332	ALA	3.5
1	B	370	HIS	3.1
1	B	314	GLU	3.0
1	B	402	TYR	2.9
1	A	383	ALA	2.9
1	B	31	ALA	2.9
1	A	450	HIS	2.7
1	A	385	GLY	2.7
1	A	408	ASP	2.7
1	B	52	GLY	2.6
1	B	411	GLU	2.4
1	B	333	ALA	2.4
1	B	326	ILE	2.3
1	A	381	THR	2.3
1	A	405	SER	2.3
1	B	41	PRO	2.3
1	B	372	HIS	2.2
1	A	329	GLN	2.2
1	B	380	ASP	2.2
1	A	252	GLN	2.2
1	B	3	GLU	2.2
1	A	26	THR	2.2
1	B	383	ALA	2.2
1	B	8	GLU	2.1
1	A	51	ASP	2.0
1	B	393	LYS	2.0
1	B	51	ASP	2.0
1	A	253	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPO	C	3	11/12	0.45	0.42	20,20,52,55	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TRS	A	457	8/8	0.34	6.78	41,44,46,48	0
3	PO4	A	456	5/5	0.51	2.97	51,54,57,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.