



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:55 AM GMT

PDB ID : 1D09  
Title : ASPARTATE TRANSCARBAMOYLASE COMPLEXED WITH N-PHOSPHONACETYL-L-ASPARTATE(PALA)  
Authors : Jin, L.; Stec, B.; Lipscomb, W.N.; Kantrowitz, E.R.  
Deposited on : 1999-09-09  
Resolution : 2.10 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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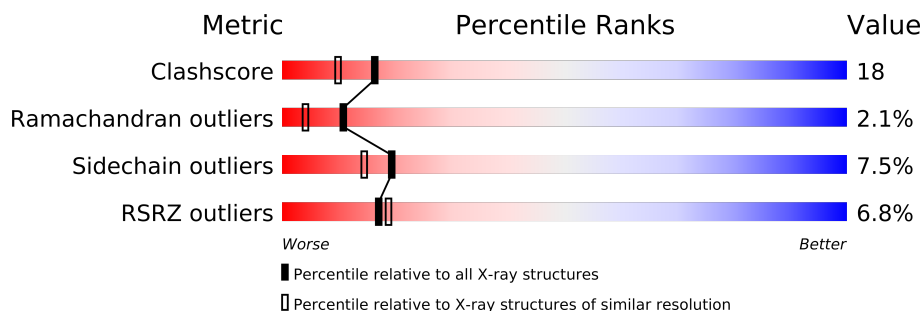
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	310	
1	C	310	
2	B	153	
2	D	153	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	PAL	C	1312	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7883 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 ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLN	GLU	CONFLICT	UNP P0A786
A	108	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLN	GLU	CONFLICT	UNP P0A786
C	108	GLN	GLU	CONFLICT	UNP P0A786

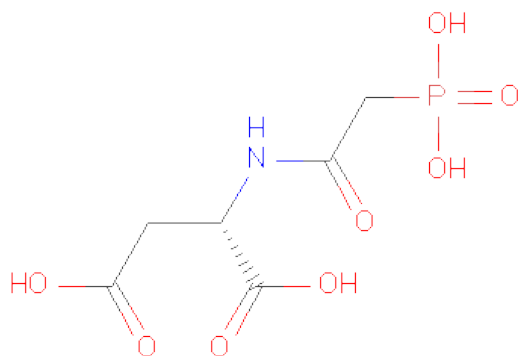
- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-(PHOSPHONACETYL)-L-ASPARTICACID (three-letter code: PAL) (formula: C<sub>6</sub>H<sub>10</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
4	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 5 is water.

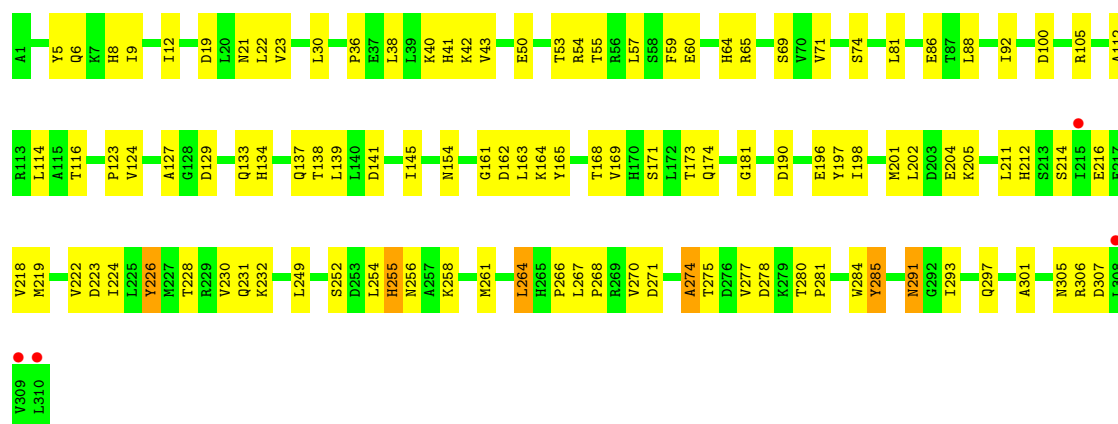
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	110	Total	O	0	0
			110	110		
5	C	305	Total	O	0	0
			305	305		
5	D	74	Total	O	0	0
			74	74		

### 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.

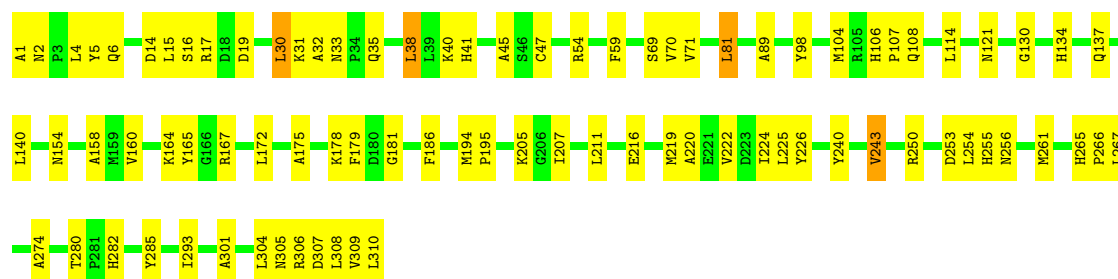
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN

Chain A: 



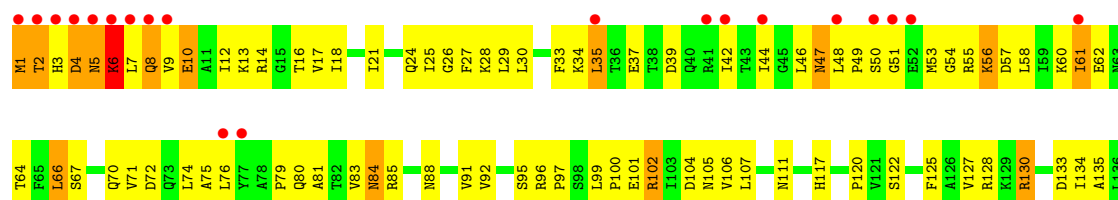
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN

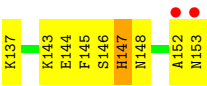
Chain C: 



#### • Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

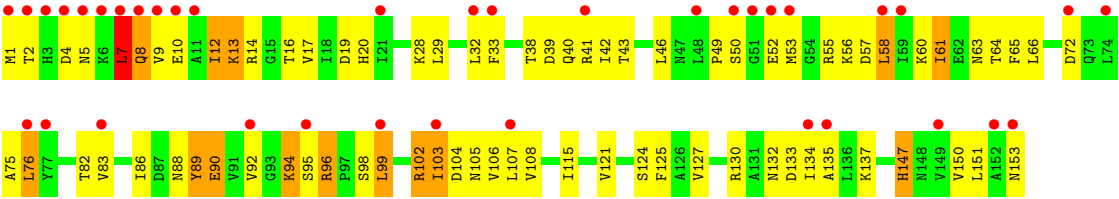
Chain B: 





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.24Å 122.24Å 156.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10 87.66 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.10) 88.9 (87.66-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.203 , 0.234 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 80.8	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 76838 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: ZN, PAL

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	1.07	4/2461 (0.2%)	1.10	4/3339 (0.1%)
1	C	1.13	3/2461 (0.1%)	1.13	4/3339 (0.1%)
2	B	0.84	0/1219	0.96	0/1647
2	D	0.81	0/1219	0.98	1/1647 (0.1%)
All	All	1.02	7/7360 (0.1%)	1.07	9/9972 (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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	TYR	CD2-CE2	7.18	1.50	1.39
1	A	226	TYR	CD2-CE2	-6.84	1.29	1.39
1	C	32	ALA	CA-CB	-5.67	1.40	1.52
1	C	89	ALA	CA-CB	-5.47	1.41	1.52
1	A	284	TRP	CB-CG	5.44	1.60	1.50
1	A	274	ALA	CA-CB	-5.14	1.41	1.52
1	A	71	VAL	CB-CG2	-5.13	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	LEU	CA-CB-CG	8.84	135.63	115.30
1	A	264	LEU	CA-CB-CG	7.81	133.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	LEU	CA-CB-CG	6.78	130.90	115.30
1	C	14	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	30	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	C	172	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	C	30	LEU	CB-CG-CD2	-5.12	102.30	111.00
2	D	7	LEU	N-CA-C	5.08	124.73	111.00
1	A	54	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	TYR	Sidechain

## 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	2415	0	2422	60	0
1	C	2415	0	2422	54	0
2	B	1201	0	1219	87	0
2	D	1201	0	1219	75	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	6	0	0
4	C	16	0	6	0	0
5	A	128	0	0	3	2
5	B	110	0	0	6	3
5	C	305	0	0	2	0
5	D	74	0	0	0	0
All	All	7883	0	7294	264	5

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 18.

All (264) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:42:ILE:HG12	2:D:61:ILE:HG22	1.33	1.09
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.32	1.06
2:B:10:GLU:HA	2:D:8:GLN:HG3	1.49	0.94
2:D:99:LEU:HD11	2:D:134:ILE:HD13	1.50	0.91
2:B:7:LEU:HG	2:B:8:GLN:N	1.88	0.89
2:B:53:MET:HG3	2:B:56:LYS:HB3	1.55	0.88
2:D:99:LEU:HD22	2:D:127:VAL:HG11	1.56	0.87
1:C:35:GLN:NE2	1:C:310:LEU:HD22	1.90	0.87
1:C:106:HIS:ND1	1:C:107:PRO:HD2	1.93	0.82
2:D:1:MET:HB3	2:D:90:GLU:HG2	1.61	0.82
2:B:34:LYS:HB3	2:B:37:GLU:HG3	1.62	0.81
1:A:133:GLN:HE22	1:A:174:GLN:HE22	1.29	0.80
2:B:7:LEU:HG	2:B:8:GLN:H	1.50	0.77
1:C:38:LEU:HD11	1:C:308:LEU:HD11	1.65	0.77
1:A:214:SER:HB2	1:A:216:GLU:HG2	1.67	0.75
2:B:47:ASN:HD22	2:B:55:ARG:HD3	1.52	0.75
2:D:40:GLN:NE2	2:D:63:ASN:HB2	2.03	0.73
2:D:99:LEU:HD11	2:D:134:ILE:CD1	2.18	0.73
2:B:81:ALA:O	2:B:96:ARG:HG3	1.89	0.73
2:D:38:THR:HG22	2:D:40:GLN:HG2	1.72	0.72
2:B:67:SER:OG	2:B:70:GLN:HG3	1.89	0.72
2:B:134:ILE:O	2:B:147:HIS:HB3	1.90	0.72
2:D:58:LEU:HD21	2:D:60:LYS:HE3	1.69	0.72
2:B:30:LEU:HD11	2:B:44:ILE:HG12	1.72	0.71
2:D:16:THR:OG1	2:D:65:PHE:HA	1.91	0.70
2:B:137:LYS:HE2	5:B:1351:HOH:O	1.91	0.70
2:D:14:ARG:NH2	2:D:65:PHE:HE2	1.90	0.69
2:B:107:LEU:HD22	2:B:152:ALA:HB2	1.75	0.68
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.74	0.68
2:B:46:LEU:HD12	2:D:42:ILE:HB	1.74	0.67
1:A:201:MET:O	1:A:205:LYS:HG3	1.95	0.67
2:D:14:ARG:HA	2:D:86:ILE:O	1.93	0.66
2:D:17:VAL:HG21	2:D:86:ILE:HD12	1.77	0.66
1:A:218:VAL:O	1:A:222:VAL:HG13	1.95	0.66
2:B:1:MET:N	2:B:1:MET:SD	2.69	0.66
2:D:103:ILE:HD13	2:D:104:ASP:N	2.10	0.66
1:A:141:ASP:O	1:A:145:ILE:HG13	1.96	0.65
2:D:130:ARG:HE	2:D:135:ALA:HB2	1.61	0.65
2:D:58:LEU:C	2:D:58:LEU:HD23	2.17	0.65
2:B:130:ARG:HB2	2:B:135:ALA:HB2	1.79	0.65
1:C:137:GLN:O	1:C:140:LEU:HG	1.98	0.64
1:C:130:GLY:O	1:C:167:ARG:HD3	1.98	0.64
1:C:106:HIS:ND1	1:C:107:PRO:CD	2.61	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:83:VAL:HG23	2:D:95:SER:HB2	1.79	0.64
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.33	0.63
2:D:115:ILE:HG13	2:D:115:ILE:O	1.97	0.62
2:B:50:SER:OG	2:B:56:LYS:HG2	1.98	0.62
2:B:99:LEU:HD11	2:B:127:VAL:HG11	1.81	0.61
2:B:84:ASN:N	2:B:84:ASN:HD22	1.99	0.61
2:B:99:LEU:HD12	2:B:100:PRO:CD	2.19	0.61
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.00	0.61
2:B:47:ASN:ND2	2:B:55:ARG:HD3	2.15	0.61
2:B:117:HIS:HB2	5:B:1396:HOH:O	2.00	0.61
1:A:154:ASN:OD1	1:A:181:GLY:HA3	2.00	0.61
2:B:9:VAL:HG12	2:D:8:GLN:OE1	2.00	0.60
1:A:161:GLY:HA3	1:A:228:THR:HG1	1.65	0.60
2:D:82:THR:HG22	2:D:96:ARG:CZ	2.31	0.60
2:B:128:ARG:NH2	2:B:130:ARG:HG3	2.16	0.60
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.84	0.59
1:C:154:ASN:HA	1:C:181:GLY:O	2.02	0.59
2:B:17:VAL:HG13	2:B:60:LYS:HG2	1.85	0.59
2:B:143:LYS:HB2	2:B:145:PHE:CZ	2.38	0.59
2:D:32:LEU:O	2:D:33:PHE:HD1	1.85	0.58
2:B:49:PRO:HA	2:B:54:GLY:O	2.02	0.58
1:C:47:CYS:O	1:C:104:MET:HA	2.03	0.58
2:D:102:ARG:NH1	2:D:124:SER:OG	2.37	0.58
2:B:55:ARG:HH11	2:B:55:ARG:HG3	1.68	0.58
2:D:32:LEU:O	2:D:33:PHE:CD1	2.58	0.57
1:C:274:ALA:HA	5:C:1555:HOH:O	2.03	0.57
2:B:66:LEU:HD12	2:B:71:VAL:HG22	1.86	0.57
2:D:76:LEU:HG	2:D:99:LEU:HD21	1.86	0.57
1:A:196:GLU:HG3	5:A:1314:HOH:O	2.03	0.56
1:C:309:VAL:HG13	1:C:309:VAL:O	2.06	0.56
2:B:25:ILE:O	2:B:27:PHE:N	2.39	0.56
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.87	0.56
2:B:8:GLN:HB2	2:D:10:GLU:HA	1.88	0.56
2:D:106:VAL:HG23	2:D:107:LEU:HG	1.88	0.56
2:B:6:LYS:HD2	2:B:6:LYS:N	2.21	0.56
2:B:25:ILE:O	2:B:28:LYS:N	2.39	0.56
2:D:82:THR:HG22	2:D:96:ARG:NH1	2.21	0.56
1:C:17:ARG:NH2	1:C:179:PHE:HA	2.20	0.56
2:D:50:SER:OG	2:D:53:MET:HB2	2.05	0.56
2:B:39:ASP:HB3	2:D:55:ARG:NH1	2.20	0.56
1:A:293:ILE:O	1:A:297:GLN:HG3	2.06	0.56
2:B:66:LEU:O	2:B:85:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.21	0.55
2:B:42:ILE:HG12	2:B:61:ILE:HG23	1.88	0.55
1:C:114:LEU:HD11	2:D:121:VAL:HG11	1.88	0.55
2:D:40:GLN:O	2:D:42:ILE:HG13	2.06	0.54
2:D:13:LYS:HA	2:D:89:TYR:CD2	2.41	0.54
2:B:8:GLN:HB2	2:D:9:VAL:O	2.08	0.54
1:C:5:TYR:CD1	1:C:306:ARG:HA	2.43	0.54
2:B:47:ASN:ND2	2:D:39:ASP:HB2	2.22	0.54
2:B:111:ASN:O	2:B:117:HIS:HE1	1.90	0.54
2:D:12:ILE:N	2:D:12:ILE:HD13	2.23	0.54
2:B:24:GLN:HG3	2:B:28:LYS:HE3	1.90	0.53
2:D:94:LYS:NZ	2:D:96:ARG:HH21	2.07	0.53
2:D:102:ARG:HB2	2:D:125:PHE:O	2.07	0.53
1:C:1:ALA:HA	1:C:306:ARG:O	2.09	0.53
1:C:38:LEU:HD11	1:C:308:LEU:CD1	2.37	0.53
2:D:94:LYS:HZ1	2:D:96:ARG:HH21	1.56	0.53
1:A:197:TYR:CE1	1:A:198:ILE:HD11	2.44	0.53
2:B:83:VAL:C	2:B:84:ASN:HD22	2.12	0.53
1:C:160:VAL:HG21	1:C:225:LEU:HD11	1.90	0.53
2:D:130:ARG:NE	2:D:135:ALA:HB2	2.22	0.53
2:D:103:ILE:C	2:D:103:ILE:HD13	2.30	0.52
2:B:21:ILE:CG2	2:B:25:ILE:HB	2.39	0.52
1:A:12:ILE:HG22	1:A:12:ILE:O	2.07	0.52
2:B:91:VAL:O	2:B:91:VAL:HG13	2.10	0.52
1:A:306:ARG:HH12	1:A:307:ASP:CG	2.13	0.52
2:B:81:ALA:O	2:B:97:PRO:HD2	2.09	0.52
2:B:3:HIS:CD2	5:B:1387:HOH:O	2.63	0.52
2:B:14:ARG:HG2	2:B:88:ASN:H	1.75	0.52
1:A:211:LEU:O	1:A:212:HIS:CD2	2.63	0.51
1:A:270:VAL:HA	5:A:1416:HOH:O	2.10	0.51
2:B:18:ILE:O	2:B:58:LEU:HD12	2.09	0.51
1:A:226:TYR:CZ	1:A:266:PRO:HD3	2.45	0.51
2:B:33:PHE:CE2	2:B:74:LEU:HD23	2.46	0.51
2:D:4:ASP:HB3	2:D:9:VAL:HG21	1.93	0.51
2:B:4:ASP:O	2:B:5:ASN:HB2	2.11	0.50
1:C:114:LEU:CD1	2:D:121:VAL:HG11	2.41	0.50
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.94	0.50
2:B:106:VAL:HG12	2:B:107:LEU:HD23	1.93	0.50
1:A:50:GLU:HB3	1:A:105:ARG:HG2	1.93	0.50
1:A:138:THR:OG1	1:A:171:SER:HB3	2.12	0.50
1:A:40:LYS:O	1:A:41:HIS:HB2	2.11	0.50
2:D:52:GLU:HG3	2:D:53:MET:SD	2.52	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:220:ALA:HB2	1:C:256:ASN:HD22	1.76	0.50
2:D:40:GLN:O	2:D:42:ILE:N	2.44	0.50
2:B:9:VAL:HB	2:D:7:LEU:O	2.12	0.49
2:D:103:ILE:CD1	2:D:106:VAL:HG22	2.42	0.49
2:D:29:LEU:HD22	2:D:33:PHE:CE2	2.47	0.49
2:B:29:LEU:O	2:B:35:LEU:HD12	2.12	0.49
5:A:1422:HOH:O	2:B:120:PRO:HG3	2.11	0.49
1:A:230:VAL:O	1:A:232:LYS:N	2.44	0.49
1:A:12:ILE:CG2	1:A:12:ILE:O	2.60	0.49
1:C:219:MET:HE3	1:C:254:LEU:HA	1.94	0.49
2:B:21:ILE:HG22	2:B:25:ILE:HB	1.95	0.49
2:B:61:ILE:HB	2:B:64:THR:HB	1.95	0.49
1:C:164:LYS:HE2	1:C:165:TYR:CZ	2.47	0.49
1:C:266:PRO:O	1:C:267:LEU:HB2	2.13	0.48
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.49	0.48
1:C:70:VAL:HG12	1:C:71:VAL:N	2.27	0.48
2:B:107:LEU:N	2:B:107:LEU:HD23	2.28	0.48
2:D:125:PHE:HA	2:D:137:LYS:O	2.13	0.48
2:D:50:SER:O	2:D:53:MET:N	2.46	0.48
1:A:223:ASP:O	1:A:224:ILE:HD13	2.14	0.48
1:C:301:ALA:O	1:C:305:ASN:HB2	2.14	0.48
1:A:164:LYS:HD3	1:A:165:TYR:CE2	2.49	0.48
1:A:219:MET:HE1	1:A:261:MET:HE1	1.96	0.48
2:B:46:LEU:HD23	2:B:57:ASP:OD1	2.14	0.47
2:B:102:ARG:HA	2:B:125:PHE:O	2.14	0.47
1:A:162:ASP:HB2	1:A:230:VAL:HA	1.96	0.47
2:B:2:THR:O	2:B:3:HIS:CG	2.68	0.47
2:B:122:SER:N	5:B:1409:HOH:O	2.44	0.47
1:A:249:LEU:HD11	1:A:254:LEU:HD21	1.96	0.47
2:B:48:LEU:HA	2:B:49:PRO:HD2	1.60	0.47
1:C:35:GLN:NE2	1:C:310:LEU:CD2	2.70	0.47
1:A:23:VAL:HG11	1:A:139:LEU:HD13	1.97	0.47
1:A:255:HIS:ND1	1:A:256:ASN:N	2.62	0.47
2:D:49:PRO:O	2:D:56:LYS:HG2	2.15	0.47
1:A:43:VAL:HG22	1:A:69:SER:HB2	1.96	0.47
2:B:107:LEU:CD2	2:B:152:ALA:HB2	2.44	0.47
2:D:40:GLN:HE21	2:D:63:ASN:HB2	1.76	0.46
2:D:13:LYS:HG3	2:D:88:ASN:HA	1.96	0.46
1:C:2:ASN:OD1	1:C:4:LEU:N	2.45	0.46
1:C:6:GLN:HA	1:C:6:GLN:NE2	2.30	0.46
1:A:197:TYR:HB3	2:B:144:GLU:HG2	1.97	0.46
2:B:16:THR:HG22	2:B:17:VAL:N	2.31	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:HIS:ND1	1:A:124:VAL:N	2.53	0.46
2:D:83:VAL:CG2	2:D:95:SER:HB2	2.44	0.46
1:C:45:ALA:HA	1:C:71:VAL:O	2.15	0.46
1:C:40:LYS:O	1:C:41:HIS:HB2	2.16	0.45
2:B:5:ASN:C	2:B:6:LYS:HD2	2.37	0.45
2:B:48:LEU:O	2:B:56:LYS:HG3	2.16	0.45
1:A:267:LEU:HB3	1:A:268:PRO:HA	1.99	0.45
2:B:85:ARG:O	2:B:92:VAL:HG22	2.16	0.45
2:B:4:ASP:O	2:B:5:ASN:CB	2.64	0.45
2:B:91:VAL:HG21	5:B:1403:HOH:O	2.17	0.45
1:C:175:ALA:O	1:C:178:LYS:HB2	2.17	0.45
1:A:112:ALA:O	1:A:116:THR:HG23	2.16	0.45
1:C:106:HIS:CG	1:C:107:PRO:CD	3.00	0.45
1:C:255:HIS:CE1	5:C:1329:HOH:O	2.69	0.45
1:A:306:ARG:HG2	1:A:306:ARG:HH11	1.81	0.45
1:C:280:THR:C	1:C:282:HIS:H	2.18	0.45
2:D:147:HIS:O	2:D:151:LEU:HG	2.17	0.44
1:C:158:ALA:HB2	1:C:222:VAL:HG11	1.99	0.44
2:B:79:PRO:O	2:B:97:PRO:HG2	2.17	0.44
1:C:17:ARG:CZ	1:C:179:PHE:HA	2.48	0.44
2:D:46:LEU:HA	2:D:57:ASP:OD1	2.18	0.44
1:A:291:ASN:HD22	1:A:291:ASN:HA	1.57	0.44
2:D:1:MET:HA	2:D:90:GLU:OE1	2.17	0.44
2:B:104:ASP:O	2:B:106:VAL:HG23	2.17	0.44
1:C:15:LEU:O	1:C:178:LYS:HE2	2.18	0.44
1:C:186:PHE:HB2	1:C:211:LEU:HD23	1.99	0.44
1:C:30:LEU:HA	1:C:30:LEU:HD23	1.56	0.44
1:C:33:ASN:ND2	1:C:35:GLN:HE22	2.15	0.43
2:D:150:VAL:O	2:D:153:ASN:ND2	2.51	0.43
2:D:4:ASP:CG	2:D:5:ASN:N	2.72	0.43
2:B:12:ILE:HD13	2:B:14:ARG:O	2.18	0.43
1:A:129:ASP:OD1	1:A:129:ASP:N	2.51	0.43
2:B:46:LEU:O	2:B:48:LEU:N	2.51	0.43
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.19	0.43
2:D:16:THR:CG2	2:D:17:VAL:N	2.82	0.43
2:D:32:LEU:HG	2:D:32:LEU:O	2.19	0.43
2:D:19:ASP:O	2:D:20:HIS:HB2	2.18	0.43
2:B:133:ASP:HB3	5:B:1369:HOH:O	2.19	0.43
1:A:275:THR:O	1:A:278:ASP:HB2	2.18	0.43
1:A:145:ILE:HG12	1:A:264:LEU:HD11	2.01	0.43
1:C:4:LEU:HA	1:C:4:LEU:HD23	1.78	0.42
2:B:62:GLU:C	2:B:64:THR:H	2.22	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:51:GLY:O	2:B:54:GLY:N	2.52	0.42
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.72	0.42
1:C:205:LYS:HA	1:C:205:LYS:HD3	1.78	0.42
1:A:280:THR:HB	1:A:281:PRO:HD2	2.01	0.42
1:C:33:ASN:ND2	1:C:35:GLN:NE2	2.67	0.42
2:D:13:LYS:HD3	2:D:89:TYR:OH	2.19	0.42
2:B:137:LYS:HA	2:B:144:GLU:HA	2.02	0.42
1:C:205:LYS:HB2	1:C:207:ILE:HG12	2.00	0.42
1:A:274:ALA:O	1:A:277:VAL:HG23	2.19	0.42
1:C:16:SER:O	1:C:19:ASP:HB2	2.18	0.42
1:A:198:ILE:O	1:A:202:LEU:HG	2.20	0.42
2:B:66:LEU:HB3	2:B:71:VAL:HG23	2.01	0.42
2:B:101:GLU:HG3	2:B:102:ARG:HG2	2.01	0.42
2:B:75:ALA:HA	2:B:79:PRO:HA	2.02	0.42
1:C:31:LYS:O	1:C:31:LYS:HG2	2.20	0.42
1:A:163:LEU:HA	1:A:169:VAL:HG21	2.02	0.42
1:A:60:GLU:O	1:A:64:HIS:CD2	2.73	0.41
1:C:224:ILE:HA	1:C:224:ILE:HD13	1.90	0.41
1:C:114:LEU:HD11	2:D:121:VAL:CG1	2.49	0.41
1:A:5:TYR:CE2	1:A:6:GLN:HG2	2.56	0.41
2:B:21:ILE:HB	2:B:57:ASP:HB3	2.02	0.41
2:D:88:ASN:ND2	2:D:89:TYR:CE1	2.88	0.41
2:B:111:ASN:O	2:B:117:HIS:CE1	2.71	0.41
1:A:55:THR:HG21	1:A:127:ALA:HB1	2.02	0.41
1:A:88:LEU:O	1:A:92:ILE:HG12	2.21	0.41
1:A:19:ASP:O	1:A:22:LEU:HB3	2.20	0.41
1:A:173:THR:HG21	1:A:198:ILE:CG2	2.51	0.41
1:C:81:LEU:HD23	1:C:81:LEU:C	2.41	0.41
1:A:258:LYS:HE3	1:A:258:LYS:HB2	1.90	0.41
1:A:9:ILE:HD12	1:A:9:ILE:HG23	1.81	0.41
1:A:138:THR:OG1	1:A:171:SER:CB	2.69	0.41
2:D:61:ILE:HD13	2:D:61:ILE:N	2.35	0.41
1:A:270:VAL:HG12	1:A:271:ASP:N	2.36	0.41
2:B:102:ARG:NH1	2:B:102:ARG:HB2	2.36	0.41
2:D:66:LEU:HA	2:D:66:LEU:HD23	1.78	0.41
2:D:72:ASP:O	2:D:75:ALA:HB3	2.21	0.41
2:D:16:THR:HG22	2:D:17:VAL:N	2.36	0.41
2:D:108:VAL:H	2:D:153:ASN:CG	2.23	0.41
1:A:301:ALA:O	1:A:305:ASN:HB2	2.21	0.41
2:D:90:GLU:HA	2:D:90:GLU:OE1	2.20	0.41
2:D:13:LYS:O	2:D:86:ILE:HG22	2.21	0.41
1:C:265:HIS:HA	1:C:266:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:LYS:HA	1:A:100:ASP:OD2	2.21	0.41
2:D:104:ASP:O	2:D:105:ASN:HB2	2.21	0.40
2:B:48:LEU:HG	2:B:56:LYS:HE2	2.03	0.40
1:C:240:TYR:O	1:C:243:VAL:HG22	2.20	0.40
1:A:53:THR:O	1:A:57:LEU:HB2	2.20	0.40
1:C:293:ILE:HA	1:C:293:ILE:HD13	1.75	0.40
2:B:146:SER:C	2:B:148:ASN:N	2.75	0.40
2:D:103:ILE:CG2	2:D:107:LEU:HD12	2.51	0.40
2:D:127:VAL:HG13	2:D:134:ILE:HG21	2.03	0.40
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.97	0.40
1:C:15:LEU:O	1:C:178:LYS:CE	2.70	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:1367:HOH:O	5:A:1367:HOH:O[2_655]	0.32	1.88
5:B:1367:HOH:O	5:B:1367:HOH:O[3_565]	0.38	1.82
5:A:1353:HOH:O	5:A:1353:HOH:O[4_555]	0.41	1.79
5:B:1365:HOH:O	5:B:1365:HOH:O[3_565]	0.47	1.73
5:B:1392:HOH:O	5:B:1392:HOH:O[3_565]	1.60	0.60

## 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	308/310 (99%)	283 (92%)	22 (7%)	3 (1%)	22	14
1	C	308/310 (99%)	291 (94%)	17 (6%)	0	100	100
2	B	151/153 (99%)	111 (74%)	30 (20%)	10 (7%)	2	0
2	D	151/153 (99%)	114 (76%)	31 (20%)	6 (4%)	5	1
All	All	918/926 (99%)	799 (87%)	100 (11%)	19 (2%)	11	4

All (19) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	231	GLN
2	B	2	THR
2	B	5	ASN
2	B	105	ASN
2	D	7	LEU
2	D	41	ARG
2	B	13	LYS
2	B	26	GLY
2	B	130	ARG
2	D	132	ASN
2	B	6	LYS
2	D	8	GLN
2	B	10	GLU
2	B	47	ASN
2	B	35	LEU
1	A	252	SER
2	D	13	LYS
2	D	92	VAL
1	A	36	PRO

### 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	261/261 (100%)	251 (96%)	10 (4%)	44	44
1	C	261/261 (100%)	244 (94%)	17 (6%)	24	20
2	B	137/137 (100%)	122 (89%)	15 (11%)	9	5
2	D	137/137 (100%)	119 (87%)	18 (13%)	6	3
All	All	796/796 (100%)	736 (92%)	60 (8%)	19	14

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	59	PHE
1	A	65	ARG
1	A	74	SER

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Mol	Chain	Res	Type
1	A	134	HIS
1	A	190	ASP
1	A	204	GLU
1	A	255	HIS
1	A	285	TYR
1	A	291	ASN
2	B	1	MET
2	B	4	ASP
2	B	6	LYS
2	B	8	GLN
2	B	56	LYS
2	B	61	ILE
2	B	66	LEU
2	B	72	ASP
2	B	76	LEU
2	B	80	GLN
2	B	84	ASN
2	B	95	SER
2	B	102	ARG
2	B	147	HIS
2	B	153	ASN
1	C	54	ARG
1	C	59	PHE
1	C	69	SER
1	C	81	LEU
1	C	108	GLN
1	C	121	ASN
1	C	134	HIS
1	C	194	MET
1	C	195	PRO
1	C	216	GLU
1	C	243	VAL
1	C	250	ARG
1	C	253	ASP
1	C	261	MET
1	C	285	TYR
1	C	304	LEU
1	C	307	ASP
2	D	2	THR
2	D	12	ILE
2	D	28	LYS
2	D	43	THR

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Mol	Chain	Res	Type
2	D	58	LEU
2	D	61	ILE
2	D	64	THR
2	D	76	LEU
2	D	89	TYR
2	D	90	GLU
2	D	94	LYS
2	D	96	ARG
2	D	98	SER
2	D	99	LEU
2	D	102	ARG
2	D	103	ILE
2	D	133	ASP
2	D	147	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	33	ASN
1	A	64	HIS
1	A	147	GLN
1	A	174	GLN
1	A	242	ASN
1	A	246	GLN
1	A	256	ASN
1	A	291	ASN
2	B	47	ASN
2	B	73	GLN
2	B	84	ASN
2	B	105	ASN
2	B	117	HIS
2	B	153	ASN
1	C	6	GLN
1	C	21	ASN
1	C	33	ASN
1	C	35	GLN
1	C	147	GLN
1	C	291	ASN
2	D	40	GLN
2	D	88	ASN
2	D	105	ASN

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Mol	Chain	Res	Type
2	D	117	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	PAL	A	1311	-	15,15,15	1.66	2 (13%)	21,21,21	1.61	4 (19%)
4	PAL	C	1312	-	15,15,15	2.10	2 (13%)	21,21,21	2.65	5 (23%)

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
4	PAL	A	1311	-	-	0/17/17/17	0/0/0/0
4	PAL	C	1312	-	-	0/17/17/17	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1312	PAL	P-O2P	-5.45	1.43	1.54
4	C	1312	PAL	P-C1P	-4.57	1.72	1.79
4	A	1311	PAL	P-O3P	3.97	1.62	1.54
4	A	1311	PAL	P-O2P	-3.36	1.48	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1312	PAL	O2P-P-C1P	6.80	120.80	106.85
4	C	1312	PAL	O3P-P-C1P	6.16	119.49	106.85
4	C	1312	PAL	O2P-P-O1P	-4.99	99.25	112.56
4	A	1311	PAL	O2P-P-C1P	4.59	116.26	106.85
4	C	1312	PAL	O3P-P-O2P	-4.20	95.04	108.35
4	A	1311	PAL	O3P-P-O1P	-3.72	102.64	112.56
4	A	1311	PAL	C4-C2-N2	2.55	117.11	110.53
4	C	1312	PAL	O3P-P-O1P	-2.29	106.45	112.56
4	A	1311	PAL	O3P-P-C1P	-2.28	102.16	106.85

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	310/310 (100%)	-0.14	4 (1%) 74 78	4, 23, 50, 96	0
1	C	310/310 (100%)	-0.25	0 100 100	4, 18, 45, 64	0
2	B	153/153 (100%)	0.84	22 (14%) 3 3	12, 55, 85, 98	1 (0%)
2	D	153/153 (100%)	1.19	37 (24%) 1 1	15, 57, 88, 100	1 (0%)
All	All	926/926 (100%)	0.21	63 (6%) 17 19	4, 27, 77, 100	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	VAL	11.3
2	D	5	ASN	9.4
2	B	9	VAL	8.2
2	B	153	ASN	7.9
2	B	3	HIS	7.9
2	D	1	MET	7.1
1	A	310	LEU	6.6
2	D	10	GLU	5.8
2	B	4	ASP	5.7
2	D	2	THR	5.6
2	B	2	THR	5.5
2	B	1	MET	5.5
2	B	7	LEU	4.9
2	D	6	LYS	4.6
2	D	77	TYR	4.5
2	D	33	PHE	4.3
2	B	51	GLY	4.2
2	D	58	LEU	4.0
2	D	153	ASN	3.9
2	D	99	LEU	3.8
2	D	92	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	44	ILE	3.8
2	D	21	ILE	3.7
2	D	53	MET	3.6
2	D	7	LEU	3.5
2	D	4	ASP	3.4
2	B	35	LEU	3.4
2	B	152	ALA	3.4
2	D	8	GLN	3.4
2	B	8	GLN	3.3
2	B	48	LEU	3.3
2	B	76	LEU	3.3
2	D	59	ILE	3.3
2	D	83	VAL	3.1
2	D	74	LEU	3.0
2	D	41	ARG	3.0
2	B	61	ILE	3.0
1	A	215	ILE	3.0
1	A	309	VAL	2.9
2	D	152	ALA	2.9
2	D	52	GLU	2.9
2	D	76	LEU	2.8
2	D	51	GLY	2.8
2	D	103	ILE	2.7
2	D	107	LEU	2.7
2	D	32	LEU	2.6
2	B	5	ASN	2.5
2	D	3	HIS	2.5
2	B	42	ILE	2.5
2	B	52	GLU	2.5
2	D	149	VAL	2.4
1	A	308	LEU	2.4
2	B	50	SER	2.3
2	B	77	TYR	2.2
2	B	6	LYS	2.2
2	D	11	ALA	2.2
2	D	48	LEU	2.1
2	D	50	SER	2.1
2	D	134	ILE	2.1
2	D	135	ALA	2.1
2	D	72	ASP	2.1
2	D	95	SER	2.0
2	B	41	ARG	2.0

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

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

## 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	PAL	C	1312	16/16	0.13	2.13	2,16,24,30	0
4	PAL	A	1311	16/16	0.11	0.97	4,14,25,29	0
3	ZN	B	1313	1/1	0.08	-0.97	26,26,26,26	0
3	ZN	D	1314	1/1	0.05	-2.56	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.