



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:51 PM UTC

PDB ID : 2O53 / pdb\_00002o53  
Title : Crystal structure of apo-Aspartoacylase from human brain  
Authors : Le Coq, J.; Pavlovsky, A.; Sanishvili, R.; Viola, R.E.  
Deposited on : 2006-12-05  
Resolution : 2.70 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

<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>.

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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)  
Xtrriage (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

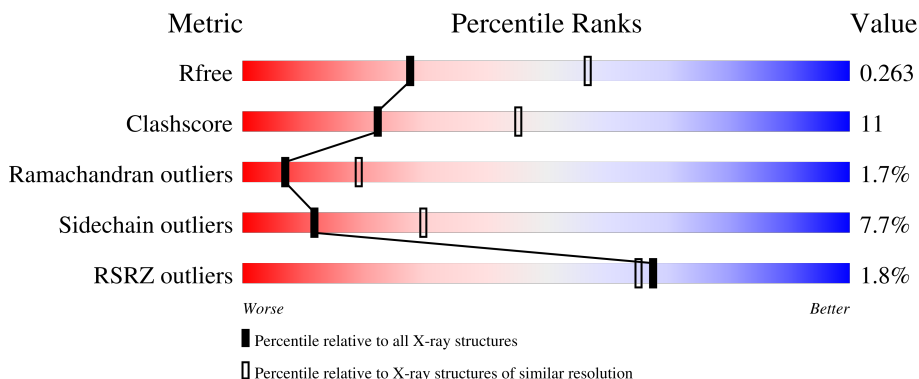
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	313	 2% 71% 21% . . .
1	B	313	 2% 70% 21% . . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4912 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 Aspartoacylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	2430	1559	411	447	13	0	0	0
1	B	302	2430	1559	411	447	13	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

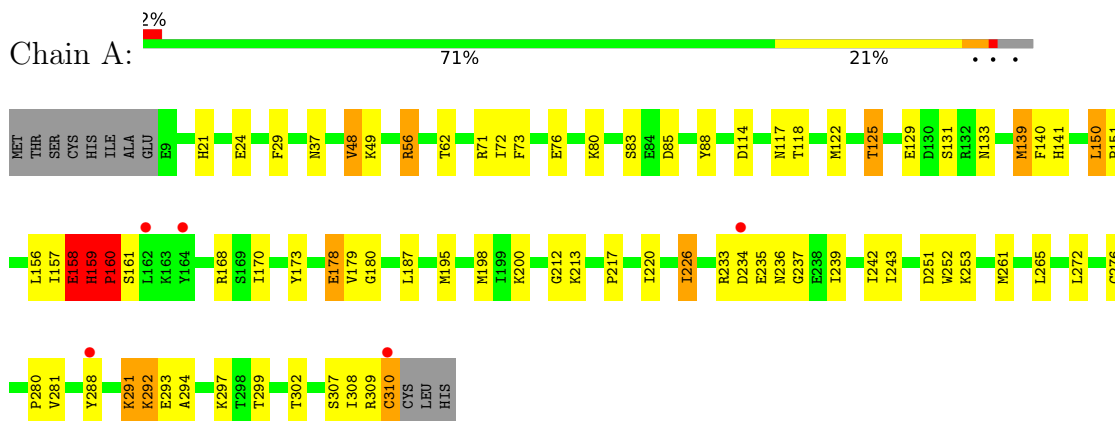
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	17	Total	O	0	0
			17	17		

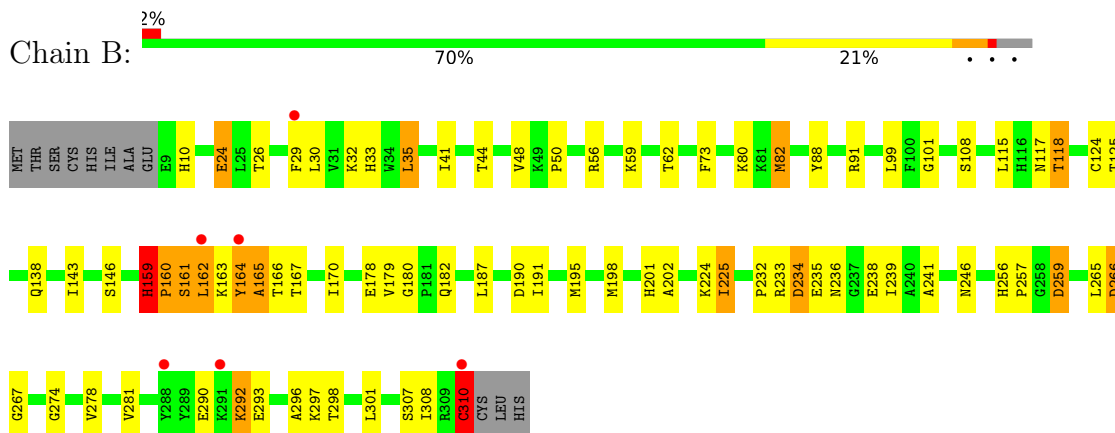
### 3 Residue-property plots [i](#)

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: Aspartoacylase



- Molecule 1: Aspartoacylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.79Å 143.79Å 104.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.3 (50.00-2.70) 81.3 (50.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.216 , 0.269 0.204 , 0.263	Depositor DCC
$R_{free}$ test set	1260 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtrriage
Anisotropy	0.542	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: PO4, ZN

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	0/2491	1.00	11/3376 (0.3%)
1	B	0.86	1/2491 (0.0%)	1.01	14/3376 (0.4%)
All	All	0.75	1/4982 (0.0%)	1.00	25/6752 (0.4%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	CYS	C-O	25.72	1.75	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	HIS	CA-C-N	13.94	137.27	119.84
1	A	159	HIS	C-N-CA	13.94	137.27	119.84
1	A	157	ILE	N-CA-C	9.52	119.61	111.90
1	B	159	HIS	CA-C-N	8.23	146.76	127.00
1	B	159	HIS	C-N-CA	8.23	146.76	127.00
1	B	159	HIS	C-N-CD	-6.85	105.53	120.60
1	B	266	ASP	N-CA-C	6.81	120.07	111.69
1	B	310	CYS	CA-C-O	-6.12	110.39	120.80
1	B	10	HIS	N-CA-C	5.83	120.93	111.37
1	B	182	GLN	CA-C-N	-5.69	114.07	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	GLN	C-N-CA	-5.69	114.07	119.76
1	B	164	TYR	CA-C-N	5.62	131.82	121.70
1	B	164	TYR	C-N-CA	5.62	131.82	121.70
1	A	160	PRO	N-CA-C	-5.45	101.24	112.47
1	A	72	ILE	N-CA-C	5.33	118.32	113.20
1	B	274	GLY	N-CA-C	-5.31	104.74	112.17
1	B	48	VAL	N-CA-C	5.25	115.63	107.28
1	A	158	GLU	N-CA-C	-5.23	102.56	110.24
1	A	150	LEU	CA-C-N	5.18	125.09	119.76
1	A	150	LEU	C-N-CA	5.18	125.09	119.76
1	A	159	HIS	N-CA-CB	-5.16	101.18	110.37
1	B	259	ASP	CA-C-N	5.13	125.13	119.90
1	B	259	ASP	C-N-CA	5.13	125.13	119.90
1	A	276	CYS	N-CA-C	5.11	116.57	108.96
1	A	48	VAL	N-CA-C	5.03	115.21	108.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLU	Peptide
1	A	159	HIS	Peptide

## 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	2430	0	2414	55	0
1	B	2430	0	2414	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	13	0	0	0	1
4	B	17	0	0	0	0
All	All	4912	0	4828	103	1

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 11.

All (103) 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:310:CYS:C	1:B:310:CYS:O	1.75	1.29
1:A:261:MET:HE2	1:A:272:LEU:HA	1.35	1.07
1:A:160:PRO:HD2	1:A:161:SER:H	1.16	1.06
1:A:159:HIS:CD2	1:A:160:PRO:HD3	1.92	1.04
1:A:160:PRO:HD2	1:A:161:SER:N	1.74	0.94
1:A:122:MET:HE1	1:A:281:VAL:HG13	1.49	0.93
1:A:160:PRO:CD	1:A:161:SER:H	1.74	0.91
1:A:160:PRO:CD	1:A:161:SER:N	2.33	0.90
1:B:159:HIS:HB3	1:B:160:PRO:C	1.99	0.87
1:A:159:HIS:CG	1:A:160:PRO:HD3	2.08	0.87
1:A:179:VAL:CG2	1:A:198:MET:HE1	2.15	0.77
1:B:73:PHE:CE1	1:B:167:THR:HG22	2.23	0.73
1:B:24:GLU:HG2	1:B:117:ASN:HB2	1.71	0.70
1:B:124:CYS:SG	1:B:198:MET:HE2	2.32	0.68
1:B:115:LEU:HD13	1:B:195:MET:HE3	1.77	0.67
1:B:82:MET:HE1	1:B:91:ARG:HB2	1.76	0.66
1:B:29:PHE:CD1	1:B:187:LEU:HD21	2.34	0.63
1:A:71:ARG:HE	1:A:291:LYS:NZ	1.97	0.63
1:B:30:LEU:HD12	1:B:195:MET:HE2	1.81	0.63
1:B:159:HIS:HB3	1:B:161:SER:N	2.14	0.61
1:A:195:MET:HA	1:A:198:MET:CE	2.31	0.60
1:B:146:SER:HB3	1:B:201:HIS:CE1	2.36	0.60
1:A:288:TYR:HB3	1:A:293:GLU:HB2	1.83	0.60
1:A:179:VAL:HG22	1:A:198:MET:HE1	1.82	0.60
1:B:82:MET:HE3	1:B:82:MET:HA	1.85	0.59
1:A:159:HIS:CD2	1:A:159:HIS:C	2.82	0.57
1:A:261:MET:CE	1:A:272:LEU:HA	2.22	0.57
1:A:122:MET:CE	1:A:281:VAL:HG13	2.28	0.56
1:B:266:ASP:N	1:B:267:GLY:HA2	2.21	0.55
1:B:179:VAL:HG22	1:B:198:MET:HE1	1.89	0.55
1:A:308:ILE:C	1:A:309:ARG:HD3	2.31	0.55
1:A:21:HIS:CE1	3:A:315:PO4:O3	2.60	0.54
1:A:122:MET:HE2	1:A:252:TRP:CZ2	2.42	0.54
1:B:232:PRO:HG2	1:B:241:ALA:HB3	1.89	0.54
1:A:133:ASN:HD21	1:A:173:TYR:HD1	1.57	0.53
1:B:146:SER:HB3	1:B:201:HIS:ND1	2.24	0.53
1:B:164:TYR:HA	1:B:165:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:HB2	1:B:238:GLU:H	1.74	0.53
1:A:159:HIS:CG	1:A:160:PRO:CD	2.89	0.51
1:A:265:LEU:HD13	1:B:33:HIS:HB2	1.93	0.51
1:B:125:THR:HB	1:B:178:GLU:HB3	1.93	0.51
1:B:164:TYR:HA	1:B:165:ALA:CB	2.41	0.51
1:B:164:TYR:HD1	1:B:166:THR:HG23	1.76	0.51
1:B:56:ARG:HD3	1:B:88:TYR:CE1	2.45	0.51
1:B:138:GLN:HG3	1:B:308:ILE:HG12	1.92	0.50
1:A:159:HIS:CD2	1:A:160:PRO:CD	2.83	0.50
1:A:83:SER:C	1:A:85:ASP:H	2.19	0.49
1:B:164:TYR:CA	1:B:165:ALA:HB3	2.42	0.49
1:B:161:SER:O	1:B:163:LYS:N	2.45	0.49
1:B:195:MET:HA	1:B:198:MET:HE3	1.95	0.48
1:B:73:PHE:HE1	1:B:167:THR:HG22	1.72	0.48
1:A:29:PHE:CD1	1:A:187:LEU:HD11	2.49	0.47
1:A:195:MET:HA	1:A:198:MET:HE2	1.96	0.47
1:A:217:PRO:HD3	1:A:307:SER:HB3	1.95	0.47
1:A:29:PHE:CE2	1:B:265:LEU:HD11	2.49	0.47
1:A:253:LYS:O	1:A:280:PRO:HD2	2.15	0.47
1:A:122:MET:HE2	1:A:252:TRP:CE2	2.50	0.46
1:A:159:HIS:HB2	1:A:160:PRO:CG	2.45	0.46
1:B:256:HIS:O	1:B:259:ASP:N	2.44	0.46
1:B:190:ASP:OD1	1:B:191:ILE:N	2.49	0.46
1:A:198:MET:HE3	1:A:198:MET:HB2	1.80	0.45
1:B:41:ILE:HD11	1:B:50:PRO:HG3	1.98	0.45
1:A:24:GLU:HB3	1:A:117:ASN:HB2	1.99	0.45
1:A:71:ARG:HE	1:A:291:LYS:HZ1	1.65	0.45
1:A:114:ASP:HB2	1:A:168:ARG:HB3	1.99	0.45
1:A:233:ARG:NH1	1:A:237:GLY:O	2.46	0.45
1:A:212:GLY:HA2	1:A:310:CYS:HB2	1.98	0.44
1:A:141:HIS:HB2	1:A:220:ILE:CG2	2.48	0.44
1:A:292:LYS:O	1:A:293:GLU:HG3	2.17	0.44
1:B:118:THR:HG23	1:B:180:GLY:HA3	2.00	0.44
1:B:225:ILE:HD12	1:B:296:ALA:HB1	2.00	0.44
1:A:243:ILE:HD11	1:A:294:ALA:HB1	2.01	0.43
1:B:234:ASP:N	1:B:238:GLU:O	2.52	0.43
1:B:30:LEU:HD12	1:B:195:MET:CE	2.48	0.43
1:B:143:ILE:HD11	1:B:202:ALA:HB2	2.00	0.43
1:B:256:HIS:O	1:B:259:ASP:HB2	2.19	0.43
1:A:83:SER:C	1:A:85:ASP:N	2.75	0.43
1:A:118:THR:HG23	1:A:180:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:THR:HG23	1:A:178:GLU:O	2.19	0.43
1:B:233:ARG:NH2	1:B:292:LYS:HA	2.33	0.42
1:B:73:PHE:CE2	1:B:170:ILE:HD11	2.53	0.42
1:A:73:PHE:CE2	1:A:170:ILE:HD11	2.54	0.42
1:B:278:VAL:HG11	1:B:297:LYS:HD3	2.00	0.42
1:A:76:GLU:O	1:A:80:LYS:HE3	2.20	0.42
1:B:198:MET:HE3	1:B:198:MET:HB2	1.84	0.42
1:B:164:TYR:CB	1:B:165:ALA:HB3	2.49	0.42
1:B:101:GLY:HA2	1:B:108:SER:HB2	2.02	0.41
1:B:234:ASP:HB2	1:B:238:GLU:N	2.33	0.41
1:A:131:SER:HB3	1:A:156:LEU:HD21	2.00	0.41
1:A:29:PHE:HD2	1:B:265:LEU:HD21	1.86	0.41
1:A:226:ILE:HG23	1:A:297:LYS:O	2.21	0.41
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.88	0.41
1:B:292:LYS:C	1:B:293:GLU:HG3	2.45	0.41
1:A:56:ARG:HB2	1:A:88:TYR:CZ	2.56	0.41
1:A:251:ASP:O	1:A:252:TRP:HB2	2.20	0.41
1:B:224:LYS:O	1:B:298:THR:HA	2.21	0.41
1:A:195:MET:HA	1:A:198:MET:HE3	2.02	0.41
1:A:234:ASP:C	1:A:236:ASN:H	2.29	0.41
1:B:35:LEU:HD13	1:B:50:PRO:HG2	2.03	0.40
1:A:159:HIS:CB	1:A:160:PRO:CD	2.98	0.40
1:A:139:MET:HG2	1:A:140:PHE:CD1	2.56	0.40
1:B:290:GLU:C	1:B:292:LYS:H	2.29	0.40
1:B:26:THR:HG22	1:B:195:MET:HE2	2.02	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:324:HOH:O	4:A:324:HOH:O[8_554]	1.60	0.60

## 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	300/313 (96%)	279 (93%)	17 (6%)	4 (1%)	9	25
1	B	300/313 (96%)	280 (93%)	14 (5%)	6 (2%)	6	16
All	All	600/626 (96%)	559 (93%)	31 (5%)	10 (2%)	7	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	PRO
1	B	159	HIS
1	B	160	PRO
1	B	162	LEU
1	A	292	LYS
1	B	161	SER
1	A	291	LYS
1	B	165	ALA
1	B	257	PRO
1	A	159	HIS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/277 (96%)	248 (93%)	19 (7%)	13	33
1	B	267/277 (96%)	245 (92%)	22 (8%)	10	27
All	All	534/554 (96%)	493 (92%)	41 (8%)	12	30

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	48	VAL
1	A	49	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	56	ARG
1	A	62	THR
1	A	125	THR
1	A	129	GLU
1	A	139	MET
1	A	158	GLU
1	A	178	GLU
1	A	200	LYS
1	A	213	LYS
1	A	226	ILE
1	A	235	GLU
1	A	239	ILE
1	A	242	ILE
1	A	299	THR
1	A	302	THR
1	A	310	CYS
1	B	24	GLU
1	B	32	LYS
1	B	35	LEU
1	B	44	THR
1	B	59	LYS
1	B	62	THR
1	B	80	LYS
1	B	82	MET
1	B	99	LEU
1	B	118	THR
1	B	162	LEU
1	B	225	ILE
1	B	234	ASP
1	B	235	GLU
1	B	236	ASN
1	B	239	ILE
1	B	246	ASN
1	B	281	VAL
1	B	292	LYS
1	B	301	LEU
1	B	307	SER
1	B	310	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	159	HIS
1	B	33	HIS
1	B	37	ASN
1	B	201	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
3	PO4	A	315	2	4,4,4	0.94	0	6,6,6	0.64	0
3	PO4	B	316	-	4,4,4	1.01	0	6,6,6	0.55	0
3	PO4	B	315	2	4,4,4	0.93	0	6,6,6	0.74	0
3	PO4	A	316	-	4,4,4	0.87	0	6,6,6	0.63	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	315	PO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	302/313 (96%)	-0.01	5 (1%) 69 67	32, 43, 62, 70	0
1	B	302/313 (96%)	-0.12	6 (1%) 65 62	29, 40, 58, 73	0
All	All	604/626 (96%)	-0.07	11 (1%) 67 65	29, 41, 61, 73	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	TYR	5.0
1	A	164	TYR	3.7
1	B	310	CYS	3.5
1	B	29	PHE	2.7
1	B	288	TYR	2.5
1	A	234	ASP	2.5
1	A	310	CYS	2.3
1	B	162	LEU	2.3
1	A	288	TYR	2.3
1	A	162	LEU	2.3
1	B	291	LYS	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	B	316	5/5	0.82	0.32	47,47,47,47	5
3	PO4	A	316	5/5	0.84	0.20	46,48,48,49	5
3	PO4	A	315	5/5	0.85	0.17	52,53,53,53	5
3	PO4	B	315	5/5	0.86	0.18	38,39,41,43	5
2	ZN	A	314	1/1	0.99	0.07	59,59,59,59	0
2	ZN	B	314	1/1	0.99	0.05	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.