



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:51 pm BST

PDB ID : 5IZ3  
Title : P. patens sedoheptulose-1,7-bisphosphatase  
Authors : Einsle, O.; Guetle, D.  
Deposited on : 2016-03-24  
Resolution : 1.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

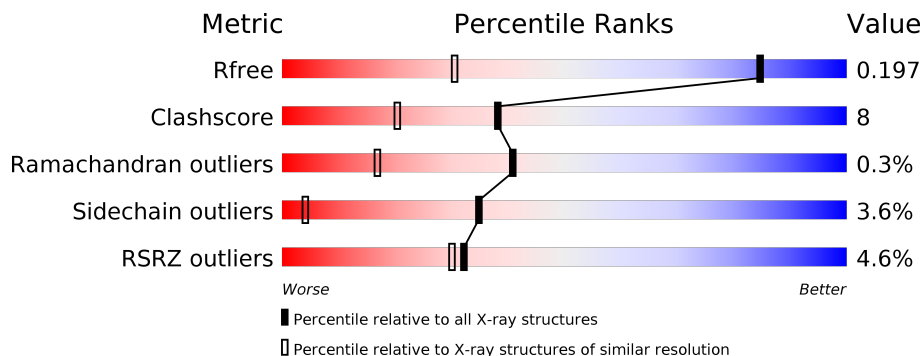
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


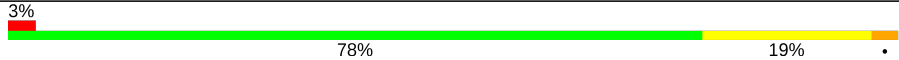
The reported resolution of this entry is 1.30 Å.

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))
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 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	316	 <p>7% 81% 16%</p>
2	B	316	 <p>3% 78% 19%</p>

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
4	PO4	B	402	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5622 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 sedoheptulose-1,7-bisphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2493	1574	415	491	13	0	7	0

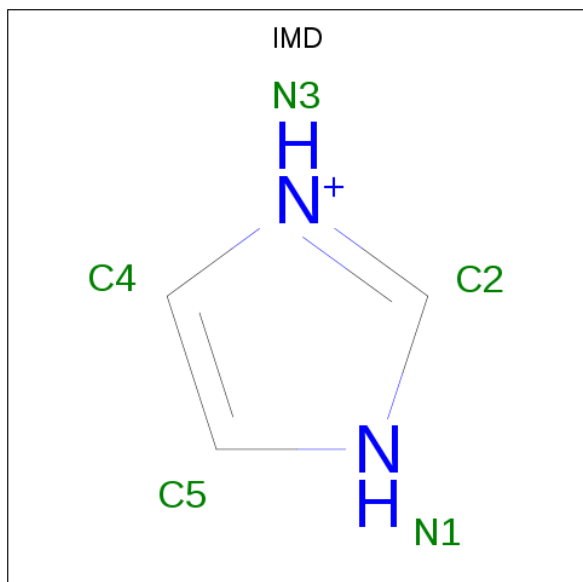
- Molecule 2 is a protein called Predicted protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	315	2499	1576	419	491	13	0	8	0

There are 3 discrepancies between the modelled and reference sequences:

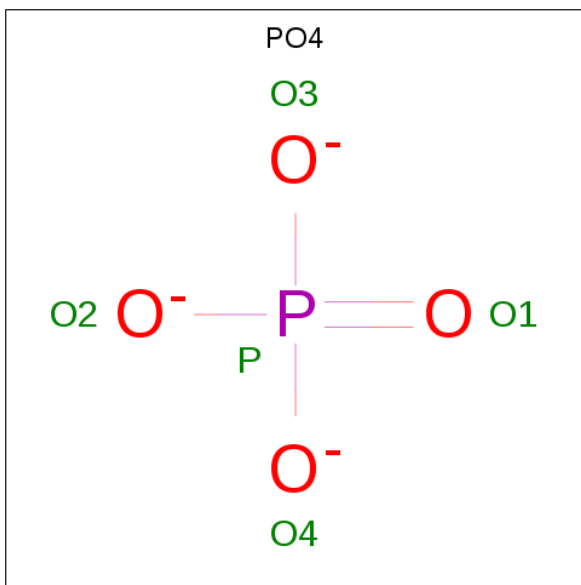
Chain	Residue	Modelled	Actual	Comment	Reference
B	126	THR	VAL	conflict	UNP A9S1S8
B	392	THR	ALA	conflict	UNP A9S1S8
B	393	VAL	THR	conflict	UNP A9S1S8

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0

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



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

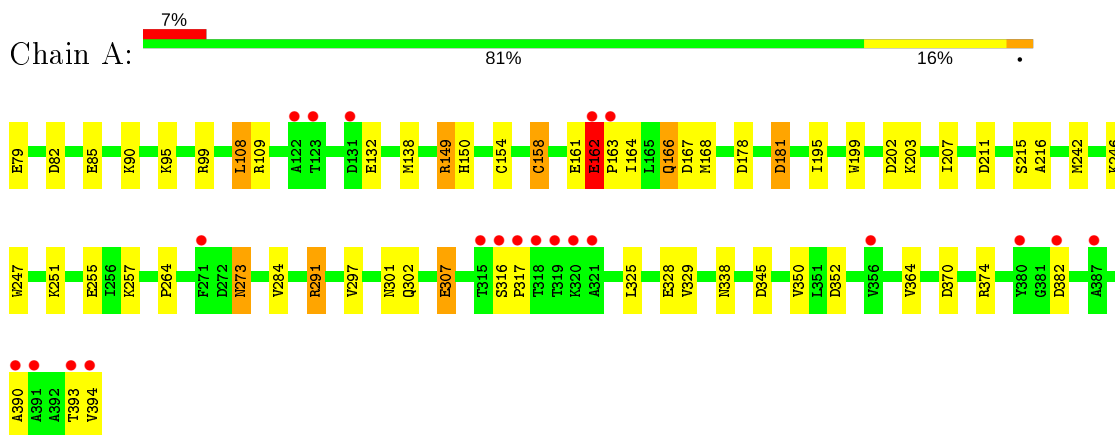
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	270	Total O 270 270	0	0
5	B	340	Total O 340 340	0	0

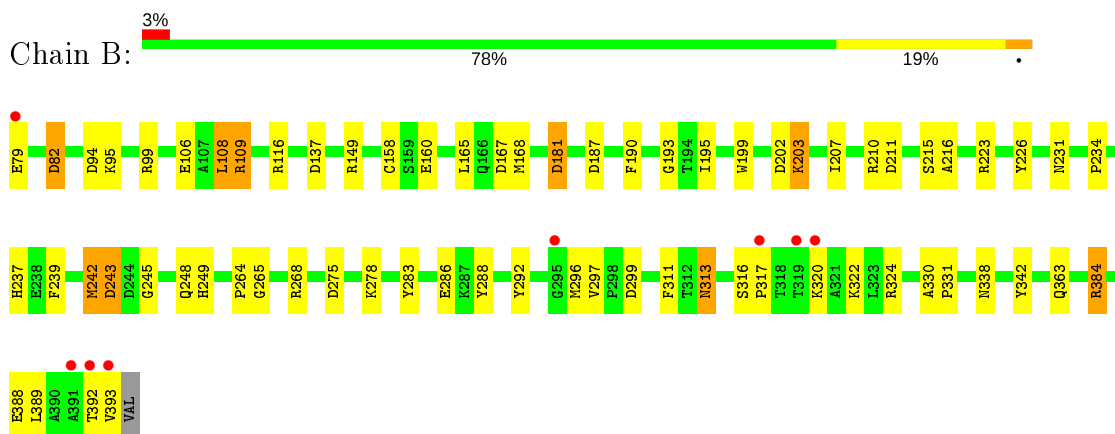
### 3 Residue-property plots [i](#)

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: sedoheptulose-1,7-bisphosphatase



- Molecule 2: Predicted protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.18Å 70.42Å 197.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.62 – 1.30 49.31 – 1.30	Depositor EDS
% Data completeness (in resolution range)	82.7 (98.62-1.30) 82.7 (49.31-1.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.30Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.160 , 0.191 0.169 , 0.197	Depositor DCC
$R_{free}$ test set	6340 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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, IMD

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	1.20	7/2535 (0.3%)	1.26	22/3427 (0.6%)
2	B	1.24	12/2541 (0.5%)	1.33	31/3436 (0.9%)
All	All	1.22	19/5076 (0.4%)	1.30	53/6863 (0.8%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	CYS	CB-SG	-8.76	1.67	1.82
1	A	85	GLU	CD-OE1	7.74	1.34	1.25
1	A	307	GLU	CD-OE1	-7.42	1.17	1.25
1	A	154	CYS	CB-SG	-6.64	1.71	1.82
2	B	288	TYR	CE1-CZ	-6.63	1.29	1.38
2	B	299	ASP	CG-OD1	-6.49	1.10	1.25
2	B	299	ASP	CB-CG	5.86	1.64	1.51
2	B	215	SER	CB-OG	-5.68	1.34	1.42
2	B	116	ARG	CD-NE	-5.65	1.36	1.46
2	B	160	GLU	CD-OE2	5.58	1.31	1.25
2	B	99	ARG	CZ-NH2	-5.28	1.26	1.33
2	B	363	GLN	CB-CG	-5.27	1.38	1.52
1	A	215	SER	CB-OG	-5.23	1.35	1.42
2	B	109	ARG	CD-NE	-5.23	1.37	1.46
1	A	162	GLU	C-N	-5.19	1.24	1.34
2	B	158	CYS	CB-SG	-5.16	1.73	1.81
2	B	190	PHE	CG-CD2	-5.09	1.31	1.38
1	A	328	GLU	CD-OE2	5.07	1.31	1.25
2	B	342	TYR	CE2-CZ	-5.03	1.32	1.38

All (53) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	ASP	CB-CG-OD2	-12.42	107.12	118.30
2	B	116	ARG	NE-CZ-NH1	-11.72	114.44	120.30
2	B	82	ASP	CB-CG-OD1	11.00	128.20	118.30
1	A	109	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	A	374	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	168	MET	CG-SD-CE	-10.48	83.44	100.20
2	B	168	MET	CG-SD-CE	-10.20	83.88	100.20
2	B	242	MET	CG-SD-CE	9.98	116.16	100.20
2	B	243	ASP	CB-CG-OD1	9.71	127.03	118.30
2	B	116	ARG	NE-CZ-NH2	9.13	124.86	120.30
1	A	202	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	108	LEU	CB-CG-CD1	7.59	123.90	111.00
1	A	181	ASP	CB-CG-OD2	-7.53	111.53	118.30
2	B	243	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	B	165	LEU	CB-CG-CD2	-7.19	98.78	111.00
2	B	187	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	374	ARG	NE-CZ-NH2	-6.63	116.98	120.30
2	B	109	ARG	CG-CD-NE	6.63	125.72	111.80
1	A	82	ASP	CB-CG-OD1	6.49	124.14	118.30
2	B	202	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	297	VAL	CA-CB-CG2	-6.33	101.40	110.90
1	A	291[A]	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	291[B]	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	223[A]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	B	223[B]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	B	239	PHE	CB-CG-CD2	-6.09	116.54	120.80
2	B	167	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	167	ASP	CB-CG-OD1	6.04	123.74	118.30
2	B	99	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	B	137	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	109	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	B	165	LEU	CB-CG-CD1	5.71	120.70	111.00
2	B	109	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	291[A]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	291[B]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	178	ASP	CB-CG-OD2	-5.56	113.30	118.30
2	B	384	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	B	108	LEU	CB-CG-CD1	5.53	120.40	111.00
1	A	211	ASP	CB-CG-OD1	-5.51	113.34	118.30
2	B	226	TYR	CB-CG-CD1	5.51	124.30	121.00
1	A	352	ASP	CB-CG-OD1	5.50	123.25	118.30
2	B	211	ASP	CB-CG-OD1	-5.44	113.41	118.30
2	B	324	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	283	TYR	CB-CG-CD1	5.31	124.19	121.00
2	B	94	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	352	ASP	CB-CG-OD2	-5.23	113.59	118.30
2	B	324	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	B	297	VAL	CA-CB-CG2	-5.18	103.14	110.90
1	A	345	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	370	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	B	210	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	286	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	149	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2460	45	0
2	B	2499	0	2464	31	0
3	A	5	0	5	0	0
3	B	5	0	5	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	270	0	0	16	0
5	B	340	0	0	13	1
All	All	5622	0	4934	76	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 8.

All (76) 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)
2:B:149:ARG:NH1	5:B:501:HOH:O	1.61	1.25
1:A:242:MET:HG3	5:A:657:HOH:O	1.04	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:MET:HG3	5:B:530:HOH:O	1.01	1.19
1:A:162:GLU:O	5:A:501:HOH:O	1.66	1.12
2:B:243:ASP:OD1	5:B:502:HOH:O	1.81	0.97
1:A:149:ARG:NH1	5:A:503:HOH:O	1.98	0.96
1:A:181:ASP:OD2	5:A:502:HOH:O	1.85	0.94
2:B:389:LEU:O	2:B:393:VAL:HG12	1.86	0.76
2:B:275:ASP:OD1	5:B:503:HOH:O	2.04	0.76
1:A:390:ALA:C	1:A:393:THR:HG22	2.07	0.75
1:A:251:LYS:NZ	1:A:307:GLU:OE2	2.16	0.74
1:A:162:GLU:CG	5:A:505:HOH:O	2.35	0.73
1:A:393:THR:HG23	1:A:394:VAL:HG13	1.71	0.72
1:A:390:ALA:O	1:A:393:THR:HG22	1.90	0.71
1:A:255:GLU:HG3	1:A:257:LYS:CE	2.21	0.70
1:A:161:GLU:OE1	5:A:504:HOH:O	2.10	0.69
1:A:242:MET:CE	5:A:657:HOH:O	2.39	0.69
2:B:106:GLU:OE1	5:B:504:HOH:O	2.11	0.68
1:A:255:GLU:HG3	1:A:257:LYS:HE3	1.76	0.67
1:A:166:GLN:NE2	5:A:505:HOH:O	2.26	0.66
2:B:268:ARG:NH1	5:B:505:HOH:O	2.27	0.66
1:A:255:GLU:HG3	1:A:257:LYS:NZ	2.10	0.66
1:A:390:ALA:O	1:A:393:THR:CG2	2.45	0.65
2:B:181[A]:ASP:N	2:B:181[A]:ASP:OD1	2.27	0.64
2:B:278:LYS:NZ	5:B:503:HOH:O	2.31	0.64
2:B:109:ARG:NH2	2:B:245:GLY:HA3	2.13	0.64
2:B:181[A]:ASP:OD2	2:B:195[A]:ILE:CD1	2.46	0.63
1:A:138[B]:MET:SD	5:A:563:HOH:O	2.56	0.62
2:B:242:MET:HE2	2:B:248:GLN:HB3	1.84	0.60
1:A:273:ASN:C	1:A:273:ASN:HD22	2.05	0.60
2:B:199:TRP:CE2	2:B:207:ILE:HD12	2.37	0.60
2:B:237:HIS:HD2	2:B:249:HIS:NE2	2.00	0.60
2:B:203[A]:LYS:HD3	5:B:543:HOH:O	2.03	0.59
1:A:162:GLU:HG3	5:A:505:HOH:O	1.98	0.58
1:A:79:GLU:OE1	1:A:90:LYS:NZ	2.37	0.58
1:A:242:MET:SD	5:A:657:HOH:O	2.53	0.56
1:A:162:GLU:HG2	1:A:162:GLU:O	2.06	0.55
1:A:301:ASN:HB3	5:B:585:HOH:O	2.07	0.54
1:A:316:SER:HB2	1:A:317:PRO:HD2	1.91	0.52
2:B:181[A]:ASP:OD1	2:B:193:GLY:O	2.27	0.52
1:A:162:GLU:HG2	5:A:505:HOH:O	2.05	0.50
2:B:322:LYS:CE	5:B:505:HOH:O	2.59	0.50
1:A:393:THR:HG23	1:A:394:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:GLU:O	2:B:392:THR:HG23	2.12	0.49
2:B:242:MET:HE3	2:B:248:GLN:CD	2.32	0.48
2:B:296[A]:MET:HG2	5:B:507:HOH:O	2.13	0.48
1:A:164:ILE:HG13	1:A:164:ILE:O	2.13	0.48
1:A:199:TRP:CE2	1:A:207:ILE:HD12	2.49	0.47
2:B:181[A]:ASP:OD2	2:B:195[A]:ILE:HG13	2.14	0.47
1:A:203:LYS:HE2	1:A:203:LYS:HA	1.95	0.47
1:A:242:MET:CG	5:A:657:HOH:O	1.88	0.47
2:B:234:PRO:O	2:B:237:HIS:HE1	1.97	0.47
1:A:150:HIS:HB3	5:A:737:HOH:O	2.15	0.46
1:A:158:CYS:SG	1:A:163:PRO:HA	2.56	0.46
2:B:296[A]:MET:SD	2:B:311:PHE:CZ	3.09	0.45
1:A:255:GLU:CG	1:A:257:LYS:NZ	2.79	0.45
1:A:325:LEU:HA	1:A:329:VAL:HB	1.98	0.45
1:A:195[B]:ILE:HD12	1:A:216:ALA:O	2.17	0.45
1:A:99:ARG:HH21	1:A:99:ARG:HG3	1.82	0.44
2:B:313:ASN:ND2	5:B:514:HOH:O	2.50	0.44
2:B:237:HIS:CD2	2:B:249:HIS:NE2	2.84	0.44
2:B:296[A]:MET:CG	5:B:507:HOH:O	2.67	0.43
1:A:291[B]:ARG:HB3	1:A:302:GLN:HE22	1.84	0.43
1:A:149:ARG:HD2	5:A:703:HOH:O	2.18	0.43
1:A:291[A]:ARG:HB2	1:A:302:GLN:HE22	1.84	0.42
1:A:162:GLU:HA	1:A:163:PRO:HD2	1.66	0.42
1:A:393:THR:CG2	1:A:394:VAL:HG13	2.46	0.42
2:B:265:GLY:HA2	2:B:292:TYR:CZ	2.55	0.42
2:B:195[B]:ILE:HD12	2:B:216:ALA:O	2.19	0.41
1:A:246:LYS:HG2	1:A:247:TRP:N	2.36	0.41
1:A:390:ALA:O	1:A:394:VAL:HG13	2.21	0.41
1:A:350:VAL:HG11	1:A:364:VAL:HG23	2.02	0.41
1:A:284:VAL:HA	5:A:619:HOH:O	2.21	0.41
2:B:316:SER:HB2	2:B:317:PRO:HD2	2.03	0.41
2:B:181[A]:ASP:OD2	2:B:195[A]:ILE:HD12	2.18	0.40
2:B:330:ALA:HB3	2:B:331:PRO:HD3	2.03	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)
5:B:761:HOH:O	5:B:761:HOH:O[3_454]	2.12	0.08

## 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	321/316 (102%)	313 (98%)	7 (2%)	1 (0%)	41	17
2	B	321/316 (102%)	314 (98%)	6 (2%)	1 (0%)	41	17
All	All	642/632 (102%)	627 (98%)	13 (2%)	2 (0%)	41	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	264	PRO
1	A	264	PRO

### 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	268/261 (103%)	259 (97%)	9 (3%)	37	5
2	B	269/262 (103%)	256 (95%)	13 (5%)	25	2
All	All	537/523 (103%)	515 (96%)	22 (4%)	35	2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95[A]	LYS
1	A	95[B]	LYS
1	A	108	LEU
1	A	132	GLU

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Mol	Chain	Res	Type
1	A	162	GLU
1	A	166	GLN
1	A	273	ASN
1	A	338	ASN
1	A	382	ASP
2	B	79	GLU
2	B	82	ASP
2	B	95	LYS
2	B	108	LEU
2	B	181[A]	ASP
2	B	181[B]	ASP
2	B	203[A]	LYS
2	B	203[B]	LYS
2	B	231	ASN
2	B	313	ASN
2	B	320	LYS
2	B	338	ASN
2	B	384	ARG

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

Mol	Chain	Res	Type
1	A	166	GLN
1	A	273	ASN
1	A	302	GLN
1	A	348	GLN
2	B	231	ASN
2	B	237	HIS
2	B	313	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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
4	PO4	A	402	-	4,4,4	1.74	2 (50%)	6,6,6	1.08	0
3	IMD	B	401	-	3,5,5	0.45	0	4,5,5	0.72	0
4	PO4	B	402	-	4,4,4	1.85	2 (50%)	6,6,6	3.10	3 (50%)
3	IMD	A	401	-	3,5,5	0.36	0	4,5,5	0.50	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
3	IMD	B	401	-	-	-	0/1/1/1
3	IMD	A	401	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	PO4	P-O1	-2.60	1.44	1.50
4	A	402	PO4	P-O2	-2.60	1.46	1.54
4	B	402	PO4	P-O2	-2.53	1.47	1.54
4	A	402	PO4	P-O4	-2.11	1.48	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	PO4	O4-P-O3	5.11	124.36	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	B	402	PO4	O4-P-O1	-4.08	95.96	110.89
4	B	402	PO4	O3-P-O1	-3.35	98.64	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	316/316 (100%)	0.21	21 (6%) 18 15	8, 17, 41, 86	5 (1%)
2	B	315/316 (99%)	-0.07	8 (2%) 57 56	7, 15, 30, 95	3 (0%)
All	All	631/632 (99%)	0.07	29 (4%) 32 30	7, 16, 36, 95	8 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	13.5
2	B	393	VAL	6.2
1	A	123	THR	6.2
2	B	392	THR	5.9
1	A	318	THR	5.6
1	A	319	THR	5.6
1	A	320	LYS	5.5
1	A	317	PRO	4.8
1	A	122	ALA	4.4
2	B	317	PRO	3.6
1	A	382	ASP	3.4
1	A	316	SER	3.4
1	A	380	TYR	2.9
1	A	163	PRO	2.9
1	A	393	THR	2.8
1	A	390	ALA	2.8
1	A	321	ALA	2.7
1	A	387	ALA	2.6
2	B	319	THR	2.5
2	B	320	LYS	2.4
1	A	162	GLU	2.4
1	A	131	ASP	2.3
1	A	356	VAL	2.3
2	B	295	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	79	GLU	2.3
1	A	271	PHE	2.3
1	A	315	THR	2.2
2	B	391	ALA	2.1
1	A	391	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. 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( $\text{\AA}^2$ )	Q<0.9
3	IMD	B	401	5/5	0.92	0.06	19,20,21,23	0
3	IMD	A	401	5/5	0.96	0.07	25,26,29,32	0
4	PO4	B	402	5/5	0.99	0.06	17,17,24,29	0
4	PO4	A	402	5/5	0.99	0.05	15,16,17,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.