



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:15 AM UTC

PDB ID : 5IZ3 / pdb_00005iz3
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

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>.

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)
Xtriage (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

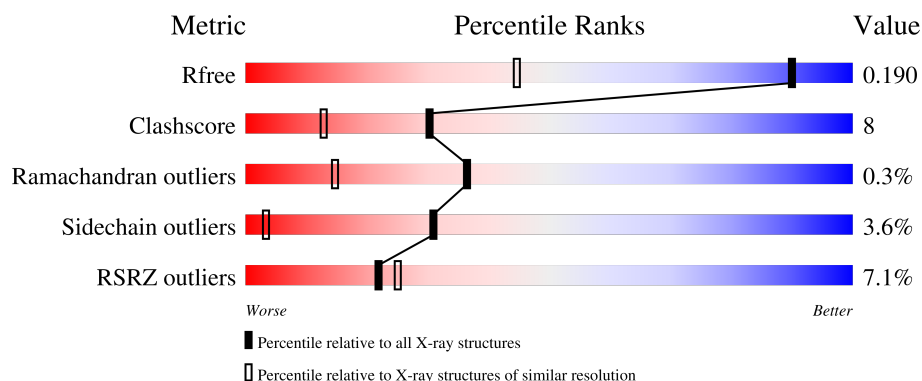
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	10% 80% 18% .
2	B	316	4% 80% 17% .

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
1	A	316	Total	C	N	O	S	0	7	0
			2493	1574	415	491	13			

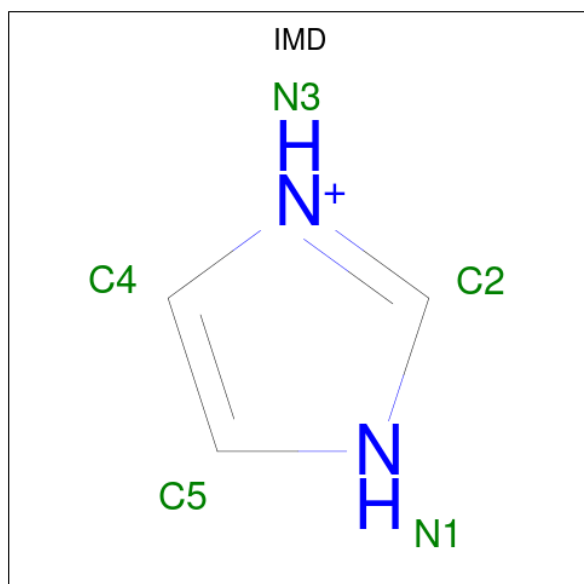
- Molecule 2 is a protein called Predicted protein.

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

There are 3 discrepancies between the modelled and reference sequences:

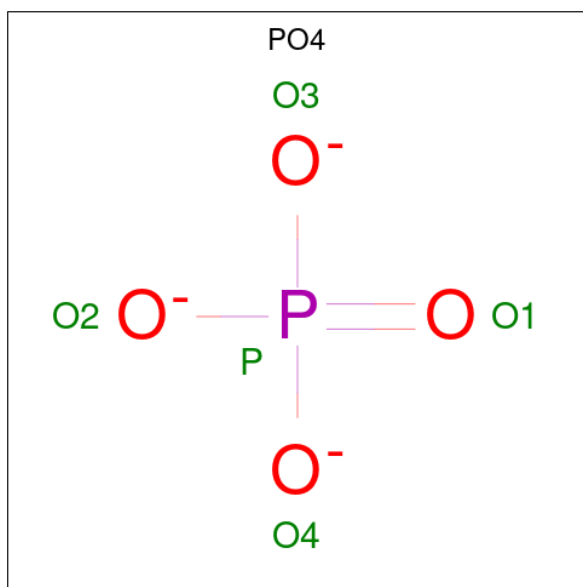
Chain	Residue	Modelled	Actual	Comment	Reference
B	126	THR	VAL	conflict	UNP A9S1S8
B	392	THR	ALA	conflict	UNP A9S1S8
B	393	VAL	THR	conflict	UNP A9S1S8

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

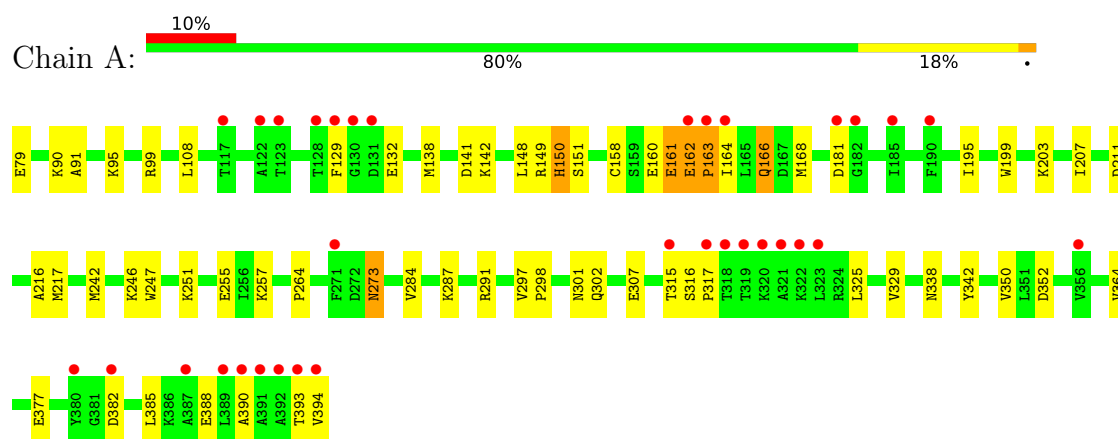
- Molecule 5 is water.

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

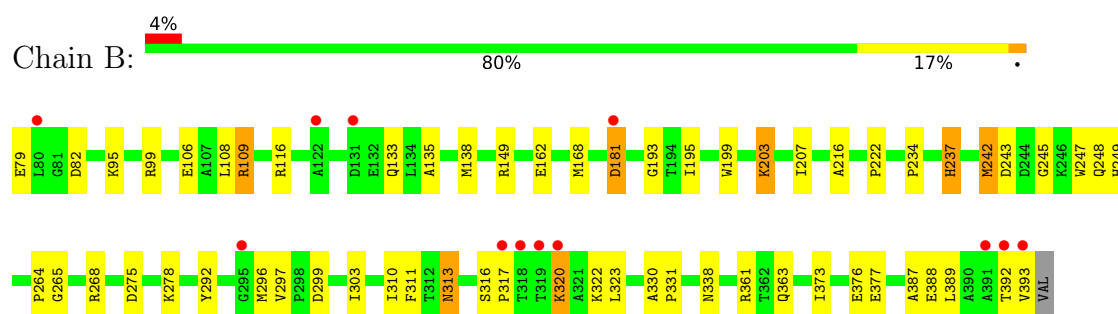
3 Residue-property plots

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: 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, α , β , γ	45.18Å 70.42Å 197.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.62 – 1.30 98.62 – 1.30	Depositor EDS
% Data completeness (in resolution range)	82.7 (98.62-1.30) 82.7 (98.62-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.160 , 0.191 0.159 , 0.190	Depositor DCC
R_{free} test set	6340 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.52	16/2535 (0.6%)	1.34	9/3427 (0.3%)
2	B	1.51	16/2541 (0.6%)	1.33	9/3436 (0.3%)
All	All	1.52	32/5076 (0.6%)	1.33	18/6863 (0.3%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	C-N	-11.21	1.24	1.33
1	A	297	VAL	CA-C	-7.93	1.44	1.52
2	B	299	ASP	CG-OD1	-7.86	1.10	1.25
1	A	163	PRO	N-CA	-7.09	1.39	1.47
2	B	373	ILE	CA-CB	-7.07	1.46	1.54
2	B	162	GLU	C-O	-6.96	1.16	1.24
2	B	247	TRP	C-O	6.83	1.32	1.24
2	B	116	ARG	CD-NE	-6.72	1.36	1.46
2	B	133	GLN	CA-C	-6.50	1.44	1.52
2	B	168	MET	SD-CE	-6.42	1.63	1.79
2	B	303	ILE	CA-C	-6.28	1.44	1.52
2	B	109	ARG	CD-NE	-6.20	1.37	1.46
2	B	297	VAL	CA-C	-6.15	1.46	1.52
1	A	211	ASP	C-O	-6.14	1.16	1.24
1	A	377	GLU	N-CA	5.98	1.53	1.46
1	A	91	ALA	N-CA	-5.80	1.38	1.46
2	B	377	GLU	N-CA	5.64	1.53	1.46
2	B	361	ARG	C-O	5.61	1.31	1.23
2	B	99	ARG	CZ-NH2	-5.58	1.26	1.33
1	A	141	ASP	C-O	5.44	1.30	1.24
1	A	298	PRO	N-CA	-5.40	1.40	1.47
1	A	160	GLU	N-CA	-5.24	1.39	1.46
2	B	387	ALA	N-CA	5.23	1.52	1.46
1	A	150	HIS	CA-CB	5.14	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TYR	CA-C	-5.12	1.46	1.52
1	A	385	LEU	N-CA	-5.10	1.40	1.46
2	B	363	GLN	CD-OE1	5.06	1.33	1.23
2	B	320	LYS	C-O	5.05	1.30	1.23
1	A	352	ASP	CG-OD1	5.05	1.34	1.25
1	A	217	MET	CB-CG	-5.03	1.37	1.52
1	A	315	THR	N-CA	5.03	1.51	1.45
1	A	148	LEU	N-CA	5.02	1.52	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	MET	CG-SD-CE	-7.94	83.44	100.90
2	B	168	MET	CG-SD-CE	-7.74	83.88	100.90
2	B	116	ARG	NE-CZ-NH1	-7.06	114.44	121.50
2	B	242	MET	CG-SD-CE	6.94	116.16	100.90
2	B	247	TRP	CA-C-O	-6.86	112.78	120.54
2	B	116	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	B	109	ARG	CG-CD-NE	6.24	125.72	112.00
1	A	142	LYS	N-CA-C	6.10	117.93	111.28
1	A	162	GLU	CA-C-O	6.07	126.94	121.06
2	B	237	HIS	CB-CG-CD2	-6.00	123.41	131.20
1	A	162	GLU	CA-C-N	5.81	126.75	120.83
1	A	162	GLU	C-N-CA	5.81	126.75	120.83
2	B	376	GLU	O-C-N	5.39	127.62	122.07
1	A	297	VAL	CA-CB-CG2	-5.29	101.40	110.40
2	B	222	PRO	N-CA-CB	-5.17	98.54	103.45
1	A	151	SER	O-C-N	5.15	128.61	122.27
1	A	161	GLU	CB-CA-C	-5.12	102.14	110.85
1	A	129	PHE	N-CA-C	-5.06	99.01	108.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2460	48	0
2	B	2499	0	2464	36	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	18	0
5	B	340	0	0	14	1
All	All	5622	0	4934	84	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 (84) 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
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
1:A:390:ALA:C	1:A:393:THR:HG22	2.07	0.80
2:B:242:MET:HE2	2:B:248:GLN:HB3	1.66	0.76
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:251:LYS:NZ	1:A:307:GLU:OE2	2.16	0.74
1:A:242:MET:HE2	5:A:657:HOH:O	1.88	0.73
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
2:B:106:GLU:OE1	5:B:504:HOH:O	2.11	0.68
1:A:242:MET:CE	5:A:657:HOH:O	2.39	0.67
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:273:ASN:C	1:A:273:ASN:HD22	2.05	0.65
1:A:390:ALA:O	1:A:393:THR:CG2	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181[A]:ASP:OD1	2:B:181[A]:ASP:N	2.27	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: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:278:LYS:NZ	5:B:503:HOH:O	2.31	0.59
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:O	1:A:162:GLU:HG2	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
2:B:388:GLU:O	2:B:392:THR:HG23	2.12	0.49
2:B:296[A]:MET:HG2	5:B:507:HOH:O	2.13	0.48
1:A:164:ILE:O	1:A:164:ILE:HG13	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:HA	1:A:203:LYS:HE2	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
2:B:296[A]:MET:HE3	2:B:296[A]:MET:HB3	1.80	0.46
2:B:296[B]:MET:HE3	2:B:323:LEU:HD13	1.97	0.46
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:138[A]:MET:HE3	5:B:716:HOH:O	2.16	0.45
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
2:B:296[A]:MET:HE1	2:B:311:PHE:CE1	2.52	0.45
2:B:135:ALA:HB3	2:B:138[B]:MET:HE3	1.98	0.45
1:A:99:ARG:HG3	1:A:99:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:NZ	5:A:513:HOH:O	2.46	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
2:B:242:MET:HE3	2:B:248:GLN:CD	2.45	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
1:A:255:GLU:HG3	1:A:257:LYS:HZ2	1.85	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%)	36	15
2	B	321/316 (102%)	314 (98%)	6 (2%)	1 (0%)	36	15
All	All	642/632 (102%)	627 (98%)	13 (2%)	2 (0%)	36	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	264	PRO
1	A	264	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	268/261 (103%)	258 (96%)	10 (4%)	30	3
2	B	269/262 (103%)	257 (96%)	12 (4%)	24	2
All	All	537/523 (103%)	515 (96%)	22 (4%)	31	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
1	A	166	GLN
1	A	273	ASN
1	A	287	LYS
1	A	338	ASN
1	A	382	ASP
1	A	388	GLU
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	310	ILE
2	B	313	ASN
2	B	320	LYS

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Mol	Chain	Res	Type
2	B	338	ASN

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

Mol	Chain	Res	Type
1	A	248	GLN
1	A	273	ASN
1	A	302	GLN
2	B	231	ASN
2	B	237	HIS
2	B	301	ASN
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 oligosaccharides 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	$\# Z > 2$
3	IMD	B	401	-	5,5,5	0.79	0	5,5,5	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IMD	A	401	-	5,5,5	0.44	0	5,5,5	0.40	0
4	PO4	B	402	-	4,4,4	1.88	2 (50%)	6,6,6	3.21	3 (50%)
4	PO4	A	402	-	4,4,4	1.81	2 (50%)	6,6,6	1.13	1 (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
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	A	402	PO4	P-O2	-2.70	1.46	1.54
4	B	402	PO4	P-O2	-2.62	1.47	1.54
4	B	402	PO4	P-O1	-2.59	1.44	1.50
4	A	402	PO4	P-O4	-2.19	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	PO4	O4-P-O3	5.29	124.36	107.91
4	B	402	PO4	O4-P-O1	-4.24	95.96	110.95
4	B	402	PO4	O3-P-O1	-3.48	98.64	110.95
4	A	402	PO4	O3-P-O2	2.03	114.21	107.91

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	316/316 (100%)	0.52	33 (10%)	11 13	5, 16, 41, 86	12 (3%)
2	B	315/316 (99%)	0.21	12 (3%)	44 49	4, 15, 30, 95	11 (3%)
All	All	631/632 (99%)	0.37	45 (7%)	22 25	4, 15, 36, 95	23 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	7.5
2	B	393	VAL	5.8
2	B	392	THR	5.3
1	A	356	VAL	5.3
1	A	319	THR	5.1
1	A	321	ALA	4.6
1	A	122	ALA	4.5
2	B	181[A]	ASP	4.4
1	A	320	LYS	4.4
1	A	391	ALA	4.3
1	A	123	THR	4.0
2	B	320	LYS	4.0
1	A	163	PRO	3.8
1	A	393	THR	3.7
1	A	390	ALA	3.5
1	A	317	PRO	3.4
2	B	131	ASP	3.3
1	A	318	THR	3.3
1	A	129	PHE	3.2
2	B	319	THR	3.1
2	B	295	GLY	3.0
1	A	164	ILE	3.0
1	A	380	TYR	2.9
1	A	387	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	382	ASP	2.9
1	A	162	GLU	2.8
1	A	182	GLY	2.8
1	A	181	ASP	2.8
1	A	185	ILE	2.7
2	B	317	PRO	2.7
1	A	392	ALA	2.6
2	B	318	THR	2.6
1	A	131	ASP	2.5
2	B	122	ALA	2.5
1	A	128	THR	2.4
1	A	323	LEU	2.4
1	A	389	LEU	2.3
1	A	315	THR	2.3
1	A	322	LYS	2.3
1	A	117	THR	2.2
1	A	190	PHE	2.2
2	B	391	ALA	2.2
1	A	271	PHE	2.1
2	B	80	LEU	2.1
1	A	130	GLY	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	A	401	5/5	0.94	0.07	25,26,29,32	0
3	IMD	B	401	5/5	0.95	0.07	19,20,21,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	402	5/5	0.97	0.07	17,17,24,29	0
4	PO4	A	402	5/5	0.99	0.04	15,16,17,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.