



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:55 AM UTC

PDB ID : 1G7U / pdb_00001g7u
Title : CRYSTAL STRUCTURES OF KDO8P SYNTHASE IN ITS BINARY COMPLEX WITH SUBSTRATE PHOSPHOENOL PYRUVATE
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Deposited on : 2000-11-14
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

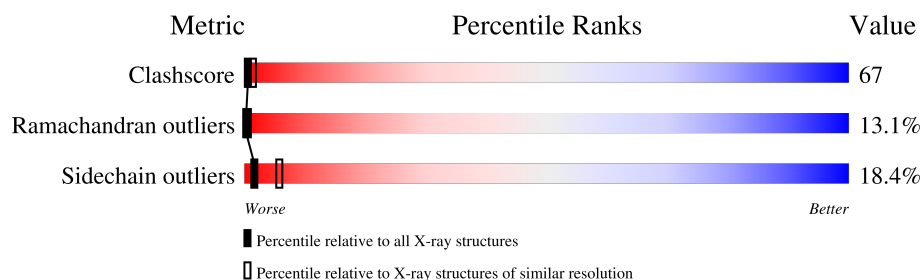
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	19% 52% 23% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2192 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.

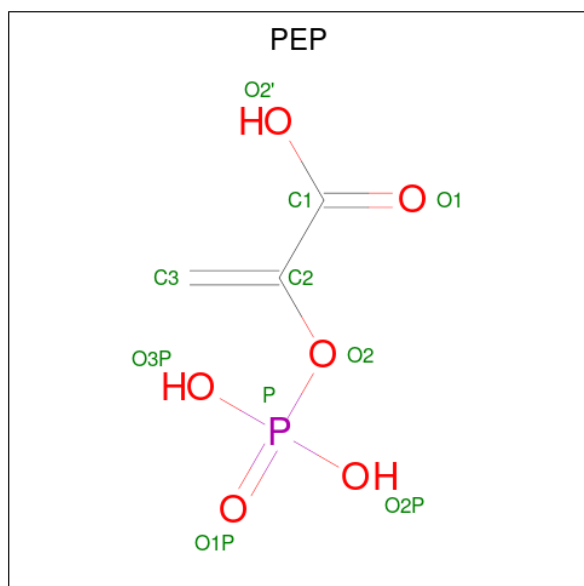
- Molecule 1 is a protein called 2-DEHYDRO-3-DEOXYPHOSPHOONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2167	1380	371	402	14	68	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	VAL	GLY	conflict	UNP P0A715

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	10	3	6	1	0	0

- Molecule 3 is water.

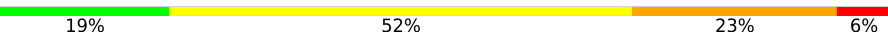
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		

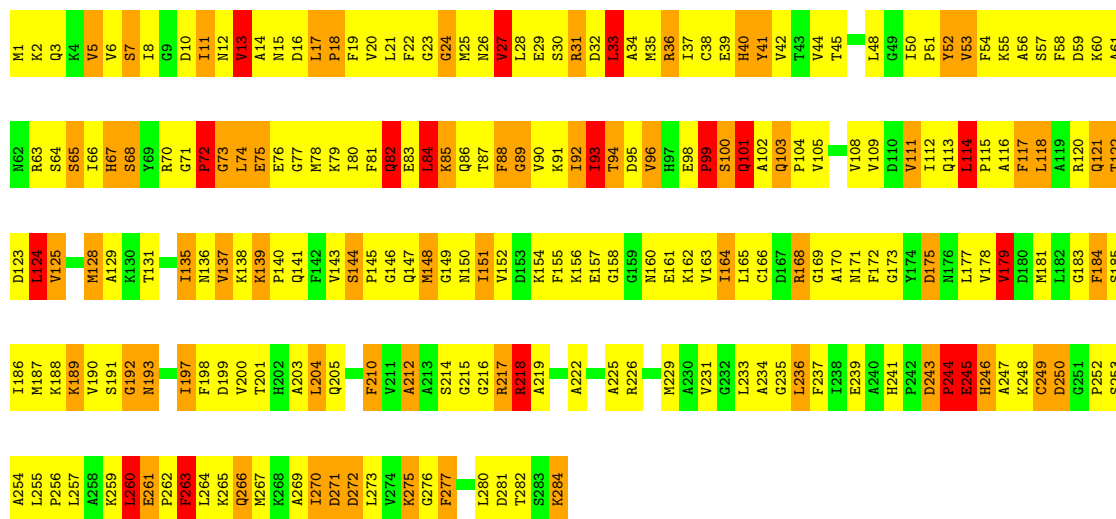
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: 2-DEHYDRO-3-DEOXYPHOSPHOCTONATE ALDOLASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	117.90 Å 117.90 Å 117.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.228 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2192	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.95	2/2207 (0.1%)	1.66	50/2977 (1.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	MET	SD-CE	-7.12	1.61	1.79
1	A	27	VAL	CA-CB	5.63	1.62	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	N-CA-C	-13.91	100.44	112.12
1	A	17	LEU	CA-C-N	11.40	134.09	119.84
1	A	17	LEU	C-N-CA	11.40	134.09	119.84
1	A	212	ALA	N-CA-C	-10.60	88.22	110.80
1	A	71	GLY	CA-C-N	10.58	133.06	119.84
1	A	71	GLY	C-N-CA	10.58	133.06	119.84
1	A	246	HIS	N-CA-C	-10.22	100.22	111.36
1	A	125	VAL	N-CA-C	-9.72	101.39	110.53
1	A	210	PHE	N-CA-C	-9.27	91.06	110.80
1	A	243	ASP	CA-C-N	9.23	131.37	119.84
1	A	243	ASP	C-N-CA	9.23	131.37	119.84
1	A	217	ARG	N-CA-C	9.13	122.19	108.31
1	A	98	GLU	CA-C-N	8.98	131.07	119.84
1	A	98	GLU	C-N-CA	8.98	131.07	119.84
1	A	263	PHE	N-CA-C	-8.21	101.92	111.03
1	A	65	SER	N-CA-C	8.11	128.07	110.80
1	A	93	ILE	N-CA-C	7.60	117.79	108.06
1	A	59	ASP	N-CA-C	7.59	119.21	108.74
1	A	128	MET	N-CA-C	-7.48	103.27	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	LYS	N-CA-C	-7.38	103.53	112.54
1	A	231	VAL	N-CA-C	-7.17	106.10	112.12
1	A	33	LEU	N-CA-C	-6.80	103.80	111.07
1	A	219	ALA	N-CA-C	6.70	120.44	109.72
1	A	197	ILE	N-CA-C	6.69	118.44	108.46
1	A	144	SER	N-CA-C	-6.52	101.56	109.83
1	A	94	THR	N-CA-C	6.40	120.00	108.48
1	A	22	PHE	N-CA-C	-6.18	97.80	108.56
1	A	36	ARG	N-CA-C	-6.10	103.79	111.11
1	A	5	VAL	N-CA-C	6.08	121.98	109.34
1	A	271	ASP	N-CA-C	-6.02	104.72	111.28
1	A	139	LYS	N-CA-C	6.00	118.32	109.50
1	A	266	GLN	N-CA-C	-5.98	103.52	111.24
1	A	149	GLY	N-CA-C	-5.95	105.95	115.66
1	A	179	VAL	CB-CA-C	-5.93	100.20	110.65
1	A	260	LEU	N-CA-C	5.93	118.26	111.02
1	A	117	PHE	N-CA-C	5.91	119.75	112.54
1	A	24	GLY	N-CA-C	5.89	117.97	110.20
1	A	52	TYR	N-CA-C	5.86	119.06	108.69
1	A	7	SER	N-CA-C	5.68	118.00	108.73
1	A	114	LEU	CA-C-N	5.43	125.74	119.93
1	A	114	LEU	C-N-CA	5.43	125.74	119.93
1	A	72	PRO	N-CA-C	5.40	123.60	112.47
1	A	13	VAL	N-CA-C	-5.40	102.10	109.55
1	A	249	CYS	N-CA-C	-5.29	106.69	112.72
1	A	173	GLY	N-CA-C	-5.28	102.56	112.22
1	A	111	VAL	CB-CA-C	-5.12	105.66	111.59
1	A	40	HIS	N-CA-C	5.06	117.53	111.71
1	A	64	SER	N-CA-C	5.06	121.58	110.80
1	A	169	GLY	N-CA-C	-5.03	107.17	111.95
1	A	124	LEU	N-CA-C	-5.01	107.30	113.41

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	2167	0	2203	283	0
2	A	10	0	2	2	0
3	A	15	0	0	5	0
All	All	2192	0	2205	283	0

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 67.

All (283) 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:A:125:VAL:HG21	1:A:154:LYS:HE2	1.31	1.12
1:A:125:VAL:HG11	1:A:154:LYS:HG3	1.33	1.07
1:A:99:PRO:HD3	1:A:124:LEU:HD22	1.48	0.95
1:A:241:HIS:ND1	1:A:245:GLU:HG2	1.87	0.90
1:A:245:GLU:HB2	1:A:248:LYS:HB2	1.52	0.88
1:A:248:LYS:HB3	1:A:254:ALA:HB2	1.54	0.88
1:A:172:PHE:HB2	1:A:178:VAL:HG23	1.59	0.85
1:A:41:TYR:CD1	1:A:260:LEU:HD11	2.12	0.84
1:A:96:VAL:HG21	1:A:124:LEU:HD11	1.60	0.84
1:A:217:ARG:HG3	1:A:218:ARG:H	1.45	0.82
1:A:115:PRO:HB2	1:A:118:LEU:HD22	1.61	0.81
1:A:2:LYS:HD3	1:A:3:GLN:N	1.96	0.80
1:A:140:PRO:HB2	1:A:143:VAL:HG23	1.63	0.80
1:A:14:ALA:HB3	1:A:17:LEU:HB2	1.61	0.80
1:A:244:PRO:O	1:A:245:GLU:HB2	1.82	0.79
1:A:78:MET:SD	1:A:108:VAL:CG2	2.71	0.78
1:A:141:GLN:NE2	1:A:168:ARG:HE	1.82	0.77
1:A:222:ALA:O	1:A:226:ARG:HG3	1.84	0.77
1:A:81:PHE:CD1	1:A:92:ILE:HD12	2.20	0.77
1:A:41:TYR:HD1	1:A:260:LEU:HD11	1.50	0.76
1:A:48:LEU:HD21	1:A:265:LYS:HZ2	1.50	0.76
1:A:92:ILE:HG12	1:A:109:VAL:HA	1.68	0.75
1:A:141:GLN:HE21	1:A:168:ARG:HE	1.35	0.74
1:A:45:THR:HG21	1:A:52:TYR:HB2	1.70	0.73
1:A:95:ASP:HA	1:A:113:GLN:O	1.88	0.73
1:A:78:MET:SD	1:A:108:VAL:HG22	2.29	0.72
1:A:48:LEU:HD21	1:A:265:LYS:NZ	2.04	0.72
1:A:217:ARG:HG3	1:A:218:ARG:N	2.04	0.71
1:A:154:LYS:HA	1:A:157:GLU:HB3	1.73	0.70
1:A:92:ILE:HG13	1:A:109:VAL:HG12	1.72	0.70
1:A:78:MET:SD	1:A:108:VAL:HG21	2.30	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:HIS:CG	1:A:245:GLU:HA	2.28	0.69
1:A:14:ALA:CB	1:A:17:LEU:HD22	2.23	0.69
1:A:20:VAL:HG22	1:A:51:PRO:HG3	1.76	0.67
1:A:263:PHE:O	1:A:266:GLN:HB2	1.93	0.67
1:A:36:ARG:HD3	3:A:307:HOH:O	1.94	0.67
1:A:140:PRO:HB2	1:A:143:VAL:CG2	2.25	0.67
1:A:74:LEU:HD12	1:A:78:MET:HG2	1.76	0.67
1:A:96:VAL:CG2	1:A:124:LEU:HD11	2.24	0.66
1:A:256:PRO:HB2	1:A:259:LYS:HB2	1.77	0.66
1:A:112:ILE:HD12	1:A:128:MET:HE2	1.77	0.66
1:A:241:HIS:CG	1:A:245:GLU:HG2	2.30	0.66
1:A:124:LEU:HD12	1:A:128:MET:HG3	1.76	0.66
1:A:168:ARG:NH1	1:A:168:ARG:HG2	2.10	0.66
1:A:14:ALA:HB3	1:A:17:LEU:HD22	1.78	0.65
1:A:241:HIS:HB2	1:A:245:GLU:HG2	1.77	0.65
1:A:266:GLN:O	1:A:270:ILE:HG13	1.97	0.65
1:A:241:HIS:CE1	1:A:245:GLU:HA	2.31	0.64
1:A:25:MET:HB3	1:A:37:ILE:HG21	1.78	0.64
1:A:81:PHE:HD1	1:A:92:ILE:HD12	1.62	0.64
1:A:112:ILE:CD1	1:A:128:MET:HE2	2.26	0.64
1:A:15:ASN:OD1	1:A:234:ALA:HB2	1.96	0.64
1:A:23:GLY:O	1:A:55:LYS:HB3	1.97	0.64
1:A:129:ALA:C	1:A:131:THR:H	2.04	0.64
1:A:16:ASP:HA	1:A:275:LYS:HD2	1.80	0.64
1:A:41:TYR:O	1:A:45:THR:HG23	1.98	0.63
1:A:261:GLU:HB3	1:A:262:PRO:HD3	1.80	0.63
1:A:24:GLY:N	1:A:41:TYR:CE2	2.65	0.62
1:A:191:SER:O	1:A:193:ASN:N	2.32	0.62
1:A:181:MET:HA	1:A:184:PHE:CE2	2.35	0.62
1:A:8:ILE:CG2	1:A:91:LYS:HG2	2.29	0.61
1:A:245:GLU:HG3	1:A:248:LYS:NZ	2.15	0.61
1:A:1:MET:SD	1:A:193:ASN:OD1	2.59	0.61
1:A:245:GLU:OE1	1:A:247:ALA:HB3	2.00	0.61
1:A:118:LEU:O	1:A:121:GLN:HB2	2.01	0.61
1:A:30:SER:HB2	1:A:33:LEU:HB2	1.81	0.61
1:A:113:GLN:HG3	1:A:136:ASN:HB3	1.84	0.60
1:A:139:LYS:HD2	1:A:187:MET:HE3	1.83	0.60
1:A:185:SER:HA	1:A:188:LYS:HB2	1.83	0.60
1:A:245:GLU:HG3	1:A:248:LYS:HZ3	1.65	0.60
1:A:198:PHE:HB2	1:A:233:LEU:HD13	1.84	0.60
1:A:92:ILE:CG1	1:A:109:VAL:HA	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HB3	1:A:284:LYS:NZ	2.16	0.60
1:A:172:PHE:HB2	1:A:178:VAL:CG2	2.32	0.60
1:A:60:LYS:HD3	1:A:70:ARG:HA	1.83	0.59
1:A:198:PHE:HB2	1:A:233:LEU:CD1	2.33	0.59
1:A:156:LYS:HE2	1:A:161:GLU:CD	2.28	0.59
1:A:112:ILE:CG1	1:A:128:MET:HE2	2.32	0.58
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.68	0.58
1:A:241:HIS:ND1	1:A:245:GLU:HA	2.18	0.58
1:A:28:LEU:HB3	1:A:72:PRO:HG2	1.86	0.58
1:A:112:ILE:HG13	1:A:128:MET:HE2	1.85	0.58
1:A:45:THR:HG21	1:A:52:TYR:CB	2.33	0.58
1:A:178:VAL:HG12	1:A:179:VAL:H	1.69	0.57
1:A:38:CYS:SG	1:A:84:LEU:HD13	2.45	0.57
1:A:156:LYS:HA	1:A:160:ASN:O	2.05	0.57
1:A:31:ARG:HA	1:A:80:ILE:CG2	2.35	0.57
1:A:58:PHE:CD1	1:A:58:PHE:C	2.82	0.57
1:A:245:GLU:HB3	1:A:248:LYS:N	2.21	0.56
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.19	0.56
1:A:23:GLY:HA3	1:A:52:TYR:HE1	1.70	0.56
1:A:103:GLN:HB3	1:A:104:PRO:HD3	1.89	0.56
1:A:30:SER:O	1:A:33:LEU:N	2.39	0.55
1:A:125:VAL:CG2	1:A:154:LYS:HE2	2.20	0.55
1:A:165:LEU:HD11	1:A:191:SER:CB	2.36	0.55
1:A:183:GLY:O	1:A:187:MET:HG3	2.06	0.55
1:A:60:LYS:HG2	3:A:305:HOH:O	2.05	0.55
1:A:93:ILE:HG13	1:A:111:VAL:O	2.06	0.55
1:A:19:PHE:HZ	1:A:264:LEU:CD2	2.20	0.55
1:A:168:ARG:NH2	3:A:311:HOH:O	2.39	0.55
1:A:245:GLU:O	1:A:249:CYS:SG	2.64	0.55
1:A:50:ILE:HG22	1:A:51:PRO:O	2.06	0.55
1:A:53:VAL:HG13	1:A:91:LYS:HB3	1.89	0.55
1:A:58:PHE:HZ	1:A:101:GLN:HE22	1.55	0.54
1:A:226:ARG:HD3	1:A:266:GLN:OE1	2.08	0.54
1:A:129:ALA:HB1	1:A:158:GLY:O	2.08	0.54
1:A:165:LEU:HD11	1:A:191:SER:OG	2.08	0.54
1:A:148:MET:O	1:A:152:VAL:HG23	2.07	0.54
1:A:2:LYS:HD3	1:A:3:GLN:H	1.69	0.53
1:A:55:LYS:HA	1:A:93:ILE:HG23	1.90	0.53
1:A:67:HIS:CD2	1:A:70:ARG:HG2	2.43	0.53
1:A:260:LEU:O	1:A:263:PHE:HB3	2.08	0.53
1:A:248:LYS:CB	1:A:254:ALA:HB2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:HIS:CB	1:A:245:GLU:HG2	2.38	0.52
1:A:35:MET:O	1:A:39:GLU:HB3	2.09	0.52
1:A:21:LEU:HD13	1:A:264:LEU:HD21	1.90	0.52
1:A:165:LEU:HD11	1:A:191:SER:HB2	1.91	0.52
1:A:241:HIS:CD2	1:A:245:GLU:HA	2.44	0.52
1:A:60:LYS:HG2	1:A:61:ALA:N	2.25	0.52
1:A:105:VAL:O	1:A:109:VAL:HG22	2.09	0.52
1:A:178:VAL:HG12	1:A:179:VAL:N	2.25	0.52
1:A:11:ILE:CG2	1:A:51:PRO:HB2	2.39	0.52
1:A:145:PRO:HB2	1:A:186:ILE:HG22	1.92	0.52
1:A:31:ARG:HA	1:A:80:ILE:HG12	1.92	0.52
1:A:129:ALA:C	1:A:131:THR:N	2.67	0.52
1:A:245:GLU:HB3	1:A:248:LYS:H	1.75	0.52
1:A:85:LYS:O	1:A:89:GLY:N	2.43	0.52
1:A:125:VAL:HG13	1:A:155:PHE:CD2	2.45	0.52
1:A:73:GLY:O	1:A:74:LEU:C	2.53	0.51
1:A:75:GLU:O	1:A:79:LYS:HE3	2.09	0.51
1:A:115:PRO:HB2	1:A:118:LEU:CD2	2.35	0.51
1:A:145:PRO:HB3	1:A:187:MET:HG3	1.90	0.51
1:A:28:LEU:HB2	1:A:57:SER:O	2.09	0.51
1:A:26:ASN:OD1	1:A:27:VAL:N	2.43	0.51
1:A:38:CYS:SG	1:A:84:LEU:CD1	2.99	0.51
1:A:30:SER:C	1:A:32:ASP:N	2.68	0.51
1:A:67:HIS:CD2	1:A:67:HIS:O	2.64	0.51
1:A:67:HIS:HD2	1:A:70:ARG:HG2	1.76	0.51
1:A:145:PRO:HB2	1:A:186:ILE:CG2	2.41	0.51
1:A:189:LYS:HD3	1:A:190:VAL:HG13	1.93	0.51
1:A:245:GLU:CB	1:A:248:LYS:HB2	2.34	0.51
1:A:38:CYS:O	1:A:42:VAL:HG23	2.10	0.51
1:A:74:LEU:HD12	1:A:78:MET:CG	2.41	0.50
1:A:222:ALA:O	1:A:267:MET:HE1	2.11	0.50
1:A:241:HIS:CG	1:A:245:GLU:CA	2.94	0.50
1:A:5:VAL:HG13	1:A:13:VAL:O	2.11	0.50
1:A:40:HIS:ND1	1:A:40:HIS:O	2.45	0.50
1:A:239:GLU:HB2	1:A:248:LYS:HE3	1.92	0.50
1:A:136:ASN:HD21	1:A:166:CYS:HB2	1.76	0.50
1:A:117:PHE:C	1:A:118:LEU:HD13	2.37	0.50
1:A:24:GLY:H	1:A:41:TYR:HE2	1.52	0.50
1:A:128:MET:O	1:A:131:THR:HB	2.11	0.50
1:A:197:ILE:HG22	1:A:235:GLY:N	2.27	0.50
1:A:25:MET:SD	1:A:37:ILE:HG13	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HD11	1:A:135:ILE:HD12	1.94	0.49
1:A:191:SER:O	1:A:192:GLY:C	2.55	0.49
1:A:241:HIS:ND1	1:A:245:GLU:CG	2.68	0.49
1:A:76:GLU:O	1:A:80:ILE:HD12	2.13	0.49
1:A:199:ASP:HA	1:A:237:PHE:HB3	1.93	0.49
1:A:129:ALA:HA	1:A:160:ASN:HD22	1.77	0.48
1:A:168:ARG:NH2	2:A:300:PEP:O2P	2.47	0.48
1:A:225:ALA:HB3	1:A:267:MET:HE3	1.95	0.48
1:A:31:ARG:HA	1:A:80:ILE:HG23	1.96	0.48
1:A:34:ALA:O	1:A:37:ILE:N	2.47	0.48
1:A:67:HIS:O	1:A:68:SER:C	2.56	0.48
1:A:185:SER:O	1:A:188:LYS:N	2.46	0.48
1:A:217:ARG:CG	1:A:218:ARG:H	2.12	0.48
1:A:19:PHE:CG	1:A:19:PHE:O	2.66	0.48
1:A:86:GLN:O	1:A:87:THR:C	2.56	0.48
1:A:20:VAL:HA	1:A:51:PRO:CG	2.43	0.48
1:A:58:PHE:HZ	1:A:101:GLN:NE2	2.11	0.48
1:A:84:LEU:HA	1:A:87:THR:HB	1.96	0.48
1:A:151:ILE:O	1:A:155:PHE:CD2	2.67	0.48
1:A:239:GLU:CB	1:A:248:LYS:HE3	2.44	0.47
1:A:45:THR:CG2	1:A:52:TYR:HB2	2.41	0.47
1:A:30:SER:CB	1:A:33:LEU:HB2	2.45	0.47
1:A:54:PHE:O	1:A:92:ILE:HA	2.14	0.47
1:A:225:ALA:HB1	1:A:236:LEU:HD11	1.96	0.47
1:A:11:ILE:HG23	1:A:51:PRO:HB2	1.96	0.47
1:A:72:PRO:HB3	1:A:77:GLY:HA2	1.96	0.47
1:A:163:VAL:HG12	1:A:164:ILE:N	2.30	0.47
1:A:137:VAL:CG1	1:A:151:ILE:HG21	2.44	0.47
1:A:100:SER:C	1:A:102:ALA:H	2.23	0.47
1:A:122:THR:HG22	1:A:154:LYS:NZ	2.30	0.47
1:A:58:PHE:HD1	1:A:58:PHE:O	1.98	0.46
1:A:88:PHE:O	1:A:89:GLY:C	2.58	0.46
1:A:26:ASN:H	1:A:248:LYS:NZ	2.13	0.46
1:A:86:GLN:C	1:A:88:PHE:N	2.72	0.46
1:A:103:GLN:O	1:A:104:PRO:C	2.56	0.46
1:A:144:SER:O	1:A:145:PRO:C	2.58	0.46
1:A:181:MET:HA	1:A:184:PHE:CD2	2.51	0.46
1:A:21:LEU:O	1:A:53:VAL:HG23	2.15	0.46
1:A:45:THR:HG21	1:A:52:TYR:CG	2.51	0.46
1:A:217:ARG:O	1:A:218:ARG:HB2	2.15	0.46
1:A:256:PRO:HB2	1:A:259:LYS:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD13	1:A:105:VAL:HG22	1.98	0.46
1:A:93:ILE:HD11	1:A:113:GLN:NE2	2.31	0.46
1:A:185:SER:O	1:A:188:LYS:HB2	2.16	0.46
1:A:241:HIS:HB3	1:A:244:PRO:C	2.40	0.46
1:A:30:SER:O	1:A:32:ASP:N	2.49	0.45
1:A:148:MET:C	1:A:150:ASN:H	2.24	0.45
1:A:237:PHE:CD1	1:A:237:PHE:C	2.95	0.45
1:A:92:ILE:CG1	1:A:109:VAL:HG12	2.43	0.45
1:A:104:PRO:O	1:A:105:VAL:C	2.59	0.45
1:A:181:MET:SD	1:A:184:PHE:HE2	2.40	0.45
1:A:204:LEU:HD11	3:A:309:HOH:O	2.16	0.45
1:A:256:PRO:HB2	1:A:259:LYS:CB	2.45	0.45
1:A:3:GLN:HG3	1:A:15:ASN:HB2	1.98	0.45
1:A:120:ARG:HH11	1:A:151:ILE:CD1	2.30	0.45
1:A:65:SER:OG	1:A:66:ILE:N	2.46	0.45
1:A:122:THR:O	1:A:125:VAL:N	2.50	0.45
1:A:172:PHE:CG	1:A:178:VAL:HG21	2.52	0.45
1:A:145:PRO:O	1:A:147:GLN:N	2.50	0.45
1:A:255:LEU:HA	1:A:256:PRO:HD3	1.82	0.45
1:A:20:VAL:HA	1:A:51:PRO:HG2	1.99	0.44
1:A:124:LEU:CD1	1:A:128:MET:HG3	2.45	0.44
1:A:204:LEU:O	1:A:205:GLN:C	2.60	0.44
1:A:23:GLY:O	1:A:55:LYS:N	2.49	0.44
1:A:26:ASN:O	1:A:27:VAL:C	2.60	0.44
1:A:94:THR:HB	1:A:109:VAL:HG11	1.99	0.44
1:A:253:SER:O	1:A:254:ALA:HB2	2.17	0.44
1:A:84:LEU:O	1:A:85:LYS:O	2.36	0.44
1:A:204:LEU:HD21	3:A:309:HOH:O	2.16	0.44
1:A:273:LEU:HD13	1:A:277:PHE:CZ	2.52	0.44
1:A:66:ILE:HG22	1:A:66:ILE:O	2.18	0.44
1:A:40:HIS:HB3	1:A:257:LEU:HD21	2.00	0.44
1:A:135:ILE:HG21	1:A:155:PHE:CE1	2.52	0.44
1:A:154:LYS:O	1:A:157:GLU:HB3	2.18	0.44
1:A:276:GLY:O	1:A:277:PHE:C	2.60	0.44
1:A:129:ALA:HA	1:A:160:ASN:HB2	2.00	0.43
1:A:83:GLU:C	1:A:85:LYS:N	2.76	0.43
1:A:284:LYS:HB3	1:A:284:LYS:HZ2	1.83	0.43
1:A:19:PHE:HA	1:A:234:ALA:O	2.18	0.43
1:A:82:GLN:C	1:A:85:LYS:HB2	2.43	0.43
1:A:229:MET:HE2	1:A:233:LEU:HD12	2.01	0.43
1:A:139:LYS:HA	1:A:140:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:O	1:A:250:ASP:OD2	2.36	0.43
1:A:114:LEU:HD23	1:A:114:LEU:O	2.19	0.43
1:A:124:LEU:HD12	1:A:124:LEU:O	2.18	0.43
1:A:60:LYS:HB2	1:A:70:ARG:HA	2.00	0.42
1:A:200:VAL:O	1:A:200:VAL:HG22	2.18	0.42
1:A:60:LYS:CB	1:A:70:ARG:HA	2.49	0.42
1:A:6:VAL:HG21	1:A:164:ILE:HG12	2.01	0.42
1:A:82:GLN:HA	1:A:85:LYS:HG3	2.01	0.42
1:A:135:ILE:HG21	1:A:155:PHE:HE1	1.83	0.42
1:A:168:ARG:O	1:A:203:ALA:HA	2.19	0.42
1:A:229:MET:HE2	1:A:229:MET:HA	2.01	0.42
1:A:154:LYS:HA	1:A:157:GLU:CB	2.45	0.42
1:A:116:ALA:O	1:A:140:PRO:HG3	2.20	0.42
1:A:255:LEU:HD12	1:A:256:PRO:HD2	2.02	0.42
1:A:170:ALA:O	1:A:177:LEU:HA	2.19	0.42
1:A:27:VAL:O	1:A:29:GLU:HG3	2.20	0.42
1:A:218:ARG:N	1:A:218:ARG:HE	2.18	0.42
1:A:243:ASP:HA	1:A:244:PRO:HD2	1.73	0.42
1:A:229:MET:CE	1:A:233:LEU:HD12	2.50	0.41
1:A:15:ASN:ND2	1:A:188:LYS:HE2	2.35	0.41
1:A:84:LEU:O	1:A:88:PHE:CD2	2.73	0.41
1:A:143:VAL:CG1	1:A:147:GLN:HB2	2.50	0.41
1:A:168:ARG:NH2	2:A:300:PEP:P	2.93	0.41
1:A:271:ASP:O	1:A:272:ASP:C	2.62	0.41
1:A:56:ALA:HB3	1:A:81:PHE:CE1	2.55	0.41
1:A:241:HIS:HB2	1:A:245:GLU:CG	2.47	0.41
1:A:269:ALA:HA	1:A:272:ASP:HB2	2.03	0.41
1:A:7:SER:HB3	1:A:12:ASN:OD1	2.21	0.41
1:A:11:ILE:HG23	1:A:51:PRO:CB	2.50	0.41
1:A:58:PHE:CD2	1:A:94:THR:HG21	2.56	0.41
1:A:122:THR:HG22	1:A:154:LYS:HE3	2.02	0.41
1:A:6:VAL:O	1:A:13:VAL:HG23	2.20	0.41
1:A:30:SER:C	1:A:32:ASP:H	2.28	0.41
1:A:81:PHE:CD1	1:A:92:ILE:CD1	2.98	0.41
1:A:129:ALA:HB1	1:A:158:GLY:C	2.46	0.41
1:A:145:PRO:HB3	1:A:187:MET:CG	2.51	0.41
1:A:280:LEU:HG	1:A:281:ASP:H	1.85	0.41
1:A:263:PHE:CD2	1:A:263:PHE:C	2.99	0.41
1:A:99:PRO:O	1:A:100:SER:C	2.64	0.40
1:A:101:GLN:O	1:A:105:VAL:HG23	2.21	0.40
1:A:38:CYS:SG	1:A:84:LEU:HB2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:O	1:A:164:ILE:HG13	2.21	0.40
1:A:166:CYS:SG	1:A:199:ASP:HB2	2.62	0.40
1:A:226:ARG:HG3	1:A:267:MET:HE1	2.02	0.40
1:A:13:VAL:O	1:A:14:ALA:HB2	2.22	0.40
1:A:44:VAL:O	1:A:45:THR:C	2.62	0.40
1:A:28:LEU:HD22	1:A:72:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

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	282/284 (99%)	182 (64%)	63 (22%)	37 (13%)	0 0

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	68	SER
1	A	85	LYS
1	A	99	PRO
1	A	137	VAL
1	A	192	GLY
1	A	212	ALA
1	A	214	SER
1	A	244	PRO
1	A	245	GLU
1	A	27	VAL
1	A	31	ARG
1	A	63	ARG
1	A	67	HIS
1	A	72	PRO

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Mol	Chain	Res	Type
1	A	75	GLU
1	A	89	GLY
1	A	100	SER
1	A	101	GLN
1	A	122	THR
1	A	146	GLY
1	A	162	LYS
1	A	252	PRO
1	A	73	GLY
1	A	123	ASP
1	A	175	ASP
1	A	277	PHE
1	A	74	LEU
1	A	184	PHE
1	A	215	GLY
1	A	84	LEU
1	A	193	ASN
1	A	82	GLN
1	A	103	GLN
1	A	216	GLY
1	A	218	ARG
1	A	96	VAL

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	234/234 (100%)	191 (82%)	43 (18%)	1 6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	11	ILE
1	A	13	VAL
1	A	18	PRO

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Mol	Chain	Res	Type
1	A	33	LEU
1	A	41	TYR
1	A	53	VAL
1	A	72	PRO
1	A	82	GLN
1	A	84	LEU
1	A	88	PHE
1	A	90	VAL
1	A	92	ILE
1	A	93	ILE
1	A	99	PRO
1	A	101	GLN
1	A	114	LEU
1	A	118	LEU
1	A	121	GLN
1	A	124	LEU
1	A	135	ILE
1	A	138	LYS
1	A	164	ILE
1	A	168	ARG
1	A	171	ASN
1	A	175	ASP
1	A	179	VAL
1	A	189	LYS
1	A	201	THR
1	A	204	LEU
1	A	210	PHE
1	A	218	ARG
1	A	236	LEU
1	A	244	PRO
1	A	245	GLU
1	A	250	ASP
1	A	260	LEU
1	A	261	GLU
1	A	263	PHE
1	A	270	ILE
1	A	272	ASP
1	A	282	THR
1	A	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	46	GLN
1	A	67	HIS
1	A	82	GLN
1	A	113	GLN
1	A	121	GLN
1	A	141	GLN
1	A	160	ASN
1	A	171	ASN
1	A	202	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEP	A	300	-	9,9,9	2.50	5 (55%)	11,13,13	2.95	5 (45%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEP	A	300	-	-	1/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	PEP	C2-C1	4.72	1.54	1.49
2	A	300	PEP	O2'-C1	-3.24	1.21	1.30
2	A	300	PEP	O1-C1	2.95	1.29	1.22
2	A	300	PEP	P-O1P	2.37	1.57	1.50
2	A	300	PEP	C3-C2	2.34	1.38	1.31

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	PEP	O2'-C1-C2	5.38	123.10	113.91
2	A	300	PEP	O1-C1-C2	-4.90	114.39	121.79
2	A	300	PEP	O2-C2-C3	-4.25	116.72	124.85
2	A	300	PEP	C3-C2-C1	3.62	129.43	122.73
2	A	300	PEP	O3P-P-O2P	2.42	116.88	107.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	PEP	C2-O2-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	PEP	2	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.