



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:08 AM UTC

PDB ID : 1L8P / pdb_00001l8p
Title : Mg-phosphonoacetohydroxamate complex of S39A yeast enolase 1
Authors : Poyner, R.R.; Larsen, T.M.; Wong, S.W.; Reed, G.H.
Deposited on : 2002-03-21
Resolution : 2.10 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

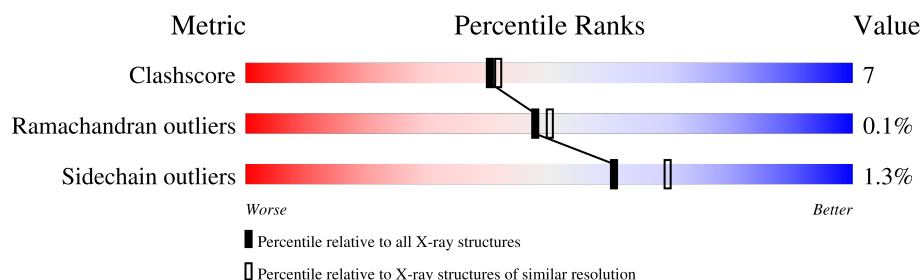
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	436	
1	B	436	
1	C	436	
1	D	436	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14636 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 enolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3290	2079	570	635	6			
1	B	436	Total	C	N	O	S	0	0	0
			3290	2079	570	635	6			
1	C	436	Total	C	N	O	S	0	0	0
			3290	2079	570	635	6			
1	D	436	Total	C	N	O	S	0	0	0
			3290	2079	570	635	6			

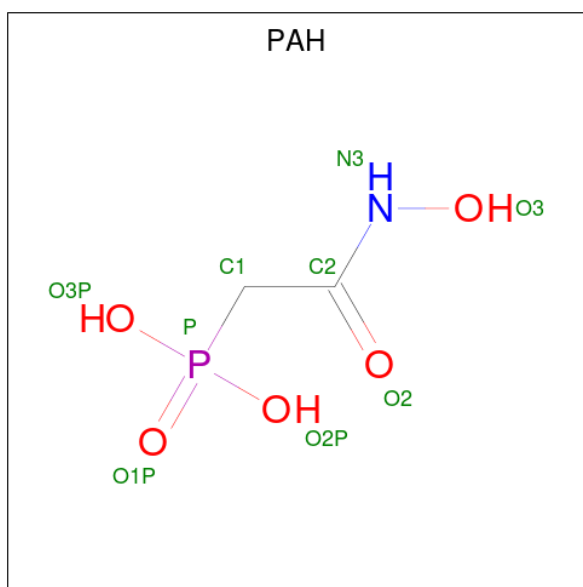
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	SER	engineered mutation	UNP P00924
B	539	ALA	SER	engineered mutation	UNP P00924
C	1039	ALA	SER	engineered mutation	UNP P00924
D	1539	ALA	SER	engineered mutation	UNP P00924

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PHOSPHONOACETOHYDROXAMIC ACID (CCD ID: PAH) (formula: C₂H₆NO₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			9	2	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			9	2	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			9	2	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			9	2	1	5	1		

- Molecule 4 is water.

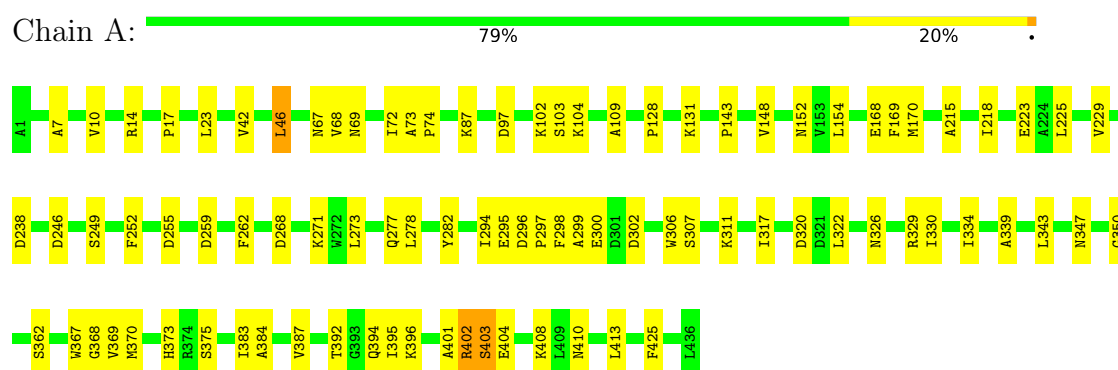
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	339	Total	O	0	0
			339	339		
4	B	388	Total	O	0	0
			388	388		
4	C	328	Total	O	0	0
			328	328		
4	D	377	Total	O	0	0
			377	377		

3 Residue-property plots

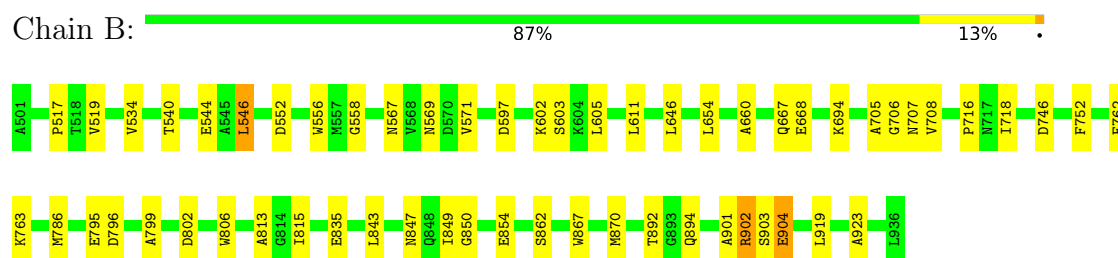
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

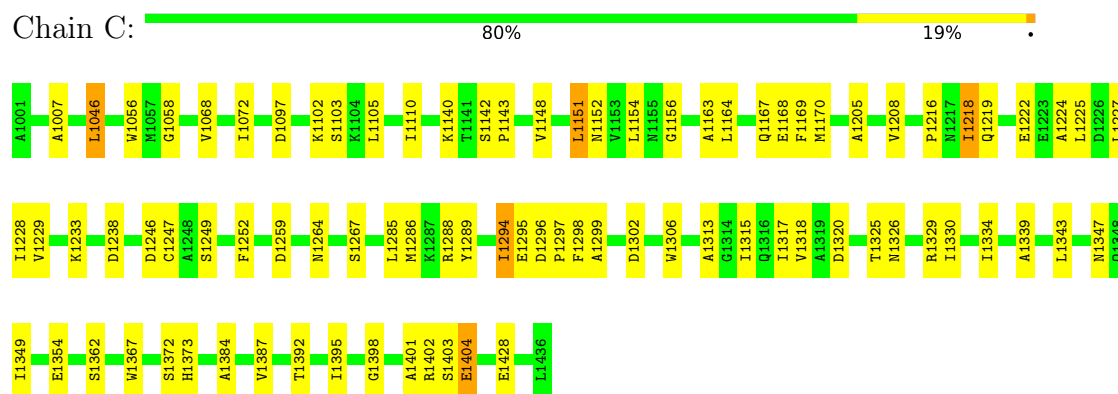
- Molecule 1: enolase 1



- Molecule 1: enolase 1

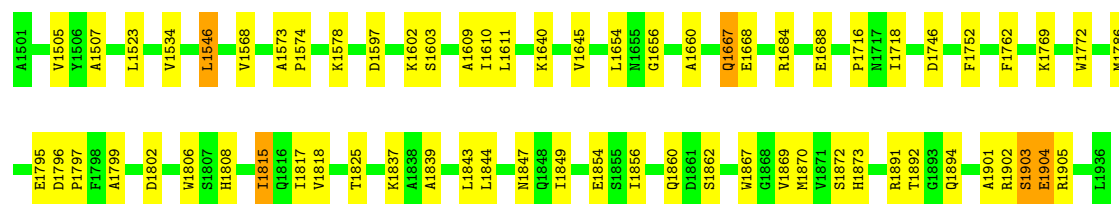


- Molecule 1: enolase 1



- Molecule 1: enolase 1

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.20Å 164.10Å 84.60Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	96.7 (20.00-2.10)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14636	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: PAH, MG

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	0.37	0/3350	0.88	9/4533 (0.2%)
1	B	0.37	0/3350	0.88	10/4533 (0.2%)
1	C	0.37	0/3350	0.87	9/4533 (0.2%)
1	D	0.38	0/3350	0.89	9/4533 (0.2%)
All	All	0.37	0/13400	0.88	37/18132 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	904	GLU	N-CA-C	-8.51	102.88	113.18
1	D	1667	GLN	N-CA-C	8.38	120.19	111.14
1	C	1148	VAL	N-CA-C	-8.24	101.54	108.63
1	A	46	LEU	N-CA-C	7.28	120.29	109.59
1	D	1904	GLU	N-CA-C	-6.86	104.78	113.01
1	A	404	GLU	N-CA-C	-6.62	105.07	113.01
1	B	667	GLN	N-CA-C	6.50	118.16	111.14
1	D	1903	SER	N-CA-C	6.44	120.60	112.87
1	B	708	VAL	N-CA-C	6.38	118.99	109.17
1	C	1046	LEU	N-CA-C	6.34	118.91	109.59
1	D	1872	SER	N-CA-C	6.33	119.05	109.23
1	C	1404	GLU	N-CA-C	-6.10	105.69	113.01
1	C	1398	GLY	N-CA-C	6.08	119.69	112.33
1	A	403	SER	N-CA-C	5.88	119.55	112.38
1	C	1318	VAL	N-CA-C	5.79	116.64	108.36
1	B	646	LEU	N-CA-C	-5.73	102.43	109.65
1	D	1818	VAL	N-CA-C	5.71	116.81	108.58
1	C	1167	GLN	N-CA-C	5.54	118.16	111.40
1	B	569	ASN	N-CA-C	5.53	117.39	111.36
1	B	546	LEU	N-CA-C	5.52	117.71	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ALA	N-CA-C	-5.51	106.61	113.55
1	A	343	LEU	N-CA-C	-5.47	100.26	108.96
1	D	1546	LEU	N-CA-C	5.40	118.00	109.96
1	D	1609	ALA	N-CA-C	-5.39	106.38	113.12
1	B	903	SER	N-CA-C	5.39	119.47	113.01
1	B	850	GLY	N-CA-C	5.33	121.09	114.37
1	C	1372	SER	N-CA-C	5.33	117.92	109.50
1	D	1843	LEU	N-CA-C	-5.30	100.53	108.96
1	B	519	VAL	N-CA-C	5.28	116.18	108.58
1	B	843	LEU	N-CA-C	-5.21	100.01	108.41
1	C	1208	VAL	N-CA-C	5.19	117.25	109.20
1	D	1645	VAL	N-CA-C	5.14	115.26	107.80
1	A	72	ILE	N-CA-C	5.11	115.34	110.53
1	C	1110	ILE	N-CA-C	5.05	115.27	110.53
1	A	368	GLY	N-CA-C	-5.04	103.90	112.51
1	A	350	GLY	N-CA-C	5.01	120.69	114.37
1	A	69	ASN	N-CA-C	5.00	116.81	111.36

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	3290	0	3301	53	0
1	B	3290	0	3298	32	0
1	C	3290	0	3298	55	0
1	D	3290	0	3298	42	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	9	0	3	0	0
3	B	9	0	3	0	0
3	C	9	0	3	0	0
3	D	9	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	339	0	0	4	0
4	B	388	0	0	2	0
4	C	328	0	0	1	0
4	D	377	0	0	3	0
All	All	14636	0	13207	174	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 7.

All (174) 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:C:1168:GLU:HB2	1:C:1246:ASP:HB3	1.59	0.85
1:A:168:GLU:HB2	1:A:246:ASP:HB3	1.66	0.76
1:A:330:ILE:O	1:A:334:ILE:HG12	1.89	0.73
1:C:1362:SER:O	1:C:1367:TRP:HB2	1.91	0.70
1:C:1072:ILE:HD11	1:C:1105:LEU:HD13	1.75	0.69
1:B:668:GLU:HB2	1:B:746:ASP:HB3	1.77	0.67
1:C:1218:ILE:HD12	1:C:1224:ALA:HB2	1.78	0.65
1:B:799:ALA:HB3	1:B:802:ASP:HB2	1.80	0.63
1:A:7:ALA:HB2	1:A:68:VAL:HG11	1.81	0.62
1:C:1163:ALA:HB3	1:C:1219:GLN:HA	1.82	0.62
1:C:1246:ASP:HA	1:C:1295:GLU:HB3	1.81	0.61
1:C:1205:ALA:HB1	1:C:1216:PRO:HB3	1.82	0.61
1:D:1799:ALA:HB3	1:D:1802:ASP:HB2	1.83	0.60
1:C:1330:ILE:O	1:C:1334:ILE:HG12	2.02	0.60
1:D:1815:ILE:H	1:D:1815:ILE:HD13	1.66	0.60
1:C:1299:ALA:HB3	1:C:1302:ASP:HB2	1.84	0.59
1:D:1668:GLU:HB2	1:D:1746:ASP:HB3	1.84	0.59
1:D:1746:ASP:HA	1:D:1795:GLU:HB3	1.84	0.59
1:A:296:ASP:OD2	1:A:320:ASP:HB3	2.05	0.57
1:A:298:PHE:HB2	1:A:306:TRP:CD1	2.41	0.56
1:A:154:LEU:HB3	1:A:169:PHE:HB2	1.87	0.55
1:C:1297:PRO:HD2	1:C:1306:TRP:CH2	2.40	0.55
1:A:97:ASP:O	1:A:104:LYS:HD2	2.06	0.55
1:C:1387:VAL:HG21	1:C:1395:ILE:HB	1.87	0.55
1:D:1505:VAL:HG22	1:D:1523:LEU:HD12	1.87	0.55
1:C:1152:ASN:OD1	1:C:1168:GLU:HG2	2.07	0.55
1:A:299:ALA:HB3	1:A:302:ASP:HB2	1.90	0.54
1:B:654:LEU:HD23	1:B:654:LEU:C	2.33	0.54
1:C:1140:LYS:HG2	1:C:1142:SER:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1384:ALA:O	1:C:1387:VAL:HG12	2.08	0.54
1:A:104:LYS:HE3	4:A:2589:HOH:O	2.07	0.54
1:D:1849:ILE:HG12	1:D:1854:GLU:HB3	1.89	0.54
1:B:716:PRO:HG2	1:B:718:ILE:HG13	1.89	0.53
1:C:1401:ALA:O	1:C:1402:ARG:HB2	2.06	0.53
1:B:746:ASP:HA	1:B:795:GLU:HB3	1.88	0.53
1:A:170:MET:SD	1:A:396:LYS:HD2	2.49	0.53
1:C:1286:MET:HE3	1:C:1315:ILE:HG12	1.91	0.53
1:B:567:ASN:O	1:B:571:VAL:HB	2.09	0.52
1:D:1507:ALA:HB2	1:D:1568:VAL:HG11	1.91	0.52
1:D:1825:THR:O	1:D:1825:THR:HG22	2.09	0.52
1:A:362:SER:O	1:A:367:TRP:HB2	2.09	0.52
1:C:1317:ILE:O	1:C:1339:ALA:HB1	2.10	0.52
1:C:1349:ILE:HG12	1:C:1354:GLU:HB3	1.91	0.52
1:C:1225:LEU:O	1:C:1229:VAL:HG23	2.09	0.52
1:D:1769:LYS:HG2	1:D:1772:TRP:CZ2	2.45	0.51
1:C:1154:LEU:HD21	1:C:1218:ILE:HD11	1.93	0.51
1:C:1233:LYS:HA	1:C:1238:ASP:OD2	2.11	0.51
1:C:1404:GLU:HB3	1:D:1903:SER:HB2	1.92	0.51
1:D:1869:VAL:O	1:D:1892:THR:HB	2.11	0.51
1:C:1288:ARG:HG3	1:C:1289:TYR:CD2	2.46	0.51
1:A:370:MET:HA	1:A:394:GLN:HG3	1.93	0.51
1:C:1164:LEU:HD22	1:C:1218:ILE:CD1	2.40	0.51
1:A:317:ILE:O	1:A:339:ALA:HB1	2.10	0.51
1:D:1684:ARG:O	1:D:1688:GLU:HG3	2.11	0.51
1:B:540:THR:HB	1:B:544:GLU:CD	2.36	0.50
1:D:1534:VAL:HG13	1:D:1611:LEU:HD23	1.93	0.50
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.92	0.50
1:A:334:ILE:HD13	1:A:367:TRP:CE2	2.46	0.50
1:C:1164:LEU:HD21	1:C:1169:PHE:CE2	2.47	0.50
1:D:1797:PRO:HD2	1:D:1806:TRP:CH2	2.47	0.50
1:C:1403:SER:HB2	1:D:1904:GLU:HB3	1.91	0.50
1:D:1597:ASP:OD2	1:D:1602:LYS:HA	2.12	0.50
1:D:1667:GLN:HG2	1:D:1668:GLU:HG3	1.92	0.50
1:A:46:LEU:HD23	1:A:103:SER:HA	1.93	0.49
1:B:786:MET:HE1	1:B:813:ALA:O	2.12	0.49
1:B:901:ALA:O	1:B:902:ARG:HB2	2.11	0.49
1:C:1169:PHE:HB3	1:C:1228:ILE:HD11	1.94	0.49
1:A:252:PHE:HB3	1:A:262:PHE:CD2	2.48	0.49
1:A:401:ALA:O	1:A:402:ARG:HB2	2.12	0.49
1:D:1901:ALA:O	1:D:1902:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:MET:HE3	1:B:815:ILE:HD13	1.94	0.48
1:A:268:ASP:OD2	1:A:271:LYS:HG3	2.14	0.48
1:B:849:ILE:HG12	1:B:854:GLU:HB3	1.95	0.48
1:C:1222:GLU:OE2	1:C:1285:LEU:HD21	2.13	0.48
1:C:1264:ASN:HD22	1:C:1267:SER:HA	1.79	0.48
1:B:597:ASP:OD2	1:B:602:LYS:HA	2.13	0.48
1:A:273:LEU:HD22	1:A:277:GLN:HB3	1.95	0.47
1:A:403:SER:OG	1:B:904:GLU:HB3	2.14	0.47
1:D:1786:MET:HE3	1:D:1815:ILE:HD12	1.95	0.47
1:D:1597:ASP:HB2	1:D:1610:ILE:HD11	1.95	0.47
1:D:1815:ILE:HD13	1:D:1815:ILE:N	2.29	0.47
1:A:307:SER:O	1:A:311:LYS:HG2	2.15	0.47
1:D:1796:ASP:HA	1:D:1806:TRP:CH2	2.50	0.47
1:D:1808:HIS:HE1	4:D:2554:HOH:O	1.98	0.47
1:D:1870:MET:HA	1:D:1894:GLN:HG3	1.96	0.47
1:A:152:ASN:OD1	1:A:168:GLU:HG2	2.15	0.47
1:B:546:LEU:HD23	1:B:603:SER:HA	1.97	0.47
1:C:1404:GLU:HB3	1:D:1903:SER:CB	2.45	0.47
1:D:1505:VAL:HG22	1:D:1523:LEU:CD1	2.45	0.47
1:A:387:VAL:HG21	1:A:395:ILE:HB	1.97	0.47
1:A:259:ASP:OD2	1:A:262:PHE:HA	2.15	0.46
1:D:1873:HIS:CD2	1:D:1873:HIS:C	2.93	0.46
1:C:1247:CYS:SG	1:C:1294:ILE:HD11	2.55	0.46
1:D:1640:LYS:HD3	1:D:1891:ARG:NH1	2.31	0.46
1:A:87:LYS:HG2	4:A:2681:HOH:O	2.15	0.46
1:B:870:MET:HA	1:B:894:GLN:HG3	1.97	0.46
1:D:1752:PHE:HB3	1:D:1762:PHE:CD2	2.51	0.46
1:C:1046:LEU:HD23	1:C:1103:SER:HA	1.97	0.46
1:A:410:ASN:HA	1:A:413:LEU:HD12	1.97	0.45
1:B:705:ALA:HB1	1:B:716:PRO:HB3	1.98	0.45
1:C:1222:GLU:H	1:C:1222:GLU:CD	2.25	0.45
1:D:1578:LYS:HE3	4:D:3299:HOH:O	2.17	0.45
1:A:225:LEU:O	1:A:229:VAL:HG23	2.17	0.45
1:A:148:VAL:HG22	1:A:425:PHE:CZ	2.52	0.45
1:A:369:VAL:O	1:A:392:THR:HB	2.16	0.45
1:D:1837:LYS:HE3	4:D:2771:HOH:O	2.17	0.44
1:C:1294:ILE:O	1:C:1294:ILE:HG23	2.18	0.44
1:A:215:ALA:HB3	1:B:707:ASN:OD1	2.17	0.44
1:C:1299:ALA:HB1	4:C:2686:HOH:O	2.18	0.44
1:D:1546:LEU:HD23	1:D:1603:SER:HA	2.00	0.44
1:D:1862:SER:O	1:D:1867:TRP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1904:GLU:HG2	1:D:1905:ARG:NE	2.33	0.44
1:A:326:ASN:O	1:A:330:ILE:HG13	2.16	0.44
1:C:1249:SER:OG	1:C:1298:PHE:C	2.61	0.44
1:C:1326:ASN:HB3	1:C:1329:ARG:CG	2.48	0.44
1:C:1373:HIS:H	1:C:1373:HIS:CD2	2.34	0.44
1:A:299:ALA:HB3	1:A:302:ASP:CB	2.48	0.43
1:C:1151:LEU:O	1:C:1170:MET:HA	2.17	0.43
1:C:1299:ALA:HB3	1:C:1302:ASP:CB	2.48	0.43
4:A:2892:HOH:O	1:B:660:ALA:HA	2.17	0.43
1:B:534:VAL:HG13	1:B:611:LEU:HD23	2.01	0.43
1:C:1007:ALA:HB2	1:C:1068:VAL:HG11	1.99	0.43
1:B:862:SER:O	1:B:867:TRP:HB2	2.17	0.43
1:B:786:MET:HE3	1:B:815:ILE:CD1	2.48	0.43
1:A:403:SER:CB	1:B:904:GLU:HB3	2.48	0.43
1:C:1072:ILE:H	1:C:1072:ILE:HD12	1.83	0.43
1:D:1656:GLY:HA2	1:D:1660:ALA:HB2	2.01	0.43
1:C:1334:ILE:HD13	1:C:1367:TRP:CE2	2.54	0.42
1:A:383:ILE:HD11	1:A:408:LYS:HG2	2.01	0.42
1:C:1097:ASP:OD2	1:C:1102:LYS:HA	2.18	0.42
1:C:1325:THR:HG22	1:C:1325:THR:O	2.19	0.42
1:A:218:ILE:HG23	1:A:223:GLU:CD	2.45	0.42
1:A:384:ALA:O	1:A:387:VAL:HG12	2.19	0.42
1:C:1313:ALA:HB1	1:C:1317:ILE:HD11	2.00	0.42
1:A:97:ASP:OD2	1:A:102:LYS:HA	2.20	0.42
1:A:300:GLU:O	1:A:322:LEU:HD12	2.20	0.42
1:A:403:SER:HB2	1:B:904:GLU:HB3	2.01	0.42
1:D:1573:ALA:N	1:D:1574:PRO:HD2	2.35	0.42
1:D:1844:LEU:C	1:D:1844:LEU:HD23	2.45	0.42
1:A:294:ILE:CD1	1:A:297:PRO:HB3	2.50	0.42
1:B:571:VAL:HG11	1:B:605:LEU:HD21	2.02	0.42
1:A:249:SER:HA	1:A:252:PHE:CZ	2.55	0.42
1:A:278:LEU:HG	1:A:282:TYR:CE2	2.55	0.42
1:B:752:PHE:HB3	1:B:762:PHE:CD2	2.54	0.42
1:A:218:ILE:CG2	1:A:223:GLU:HB3	2.51	0.41
1:C:1295:GLU:OE2	1:C:1343:LEU:HD22	2.20	0.41
1:C:1403:SER:CB	1:D:1904:GLU:HB3	2.50	0.41
1:C:1296:ASP:OD2	1:C:1320:ASP:HB3	2.20	0.41
1:D:1716:PRO:HG2	1:D:1718:ILE:HG13	2.02	0.41
1:A:10:VAL:O	1:A:17:PRO:HA	2.21	0.41
1:B:796:ASP:HA	1:B:806:TRP:CH2	2.56	0.41
1:C:1154:LEU:C	1:C:1154:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:N	1:A:74:PRO:HD2	2.36	0.41
1:B:694:LYS:HE3	1:B:706:GLY:O	2.21	0.41
1:D:1654:LEU:HD23	1:D:1654:LEU:C	2.46	0.41
1:A:14:ARG:HH12	1:A:375:SER:CB	2.34	0.41
1:A:42:VAL:HG12	1:A:300:GLU:OE1	2.20	0.41
1:A:128:PRO:O	1:A:131:LYS:HB3	2.21	0.41
1:A:299:ALA:HB1	4:A:2900:HOH:O	2.21	0.41
1:B:552:ASP:O	1:B:558:GLY:HA2	2.21	0.41
1:C:1252:PHE:HB2	1:C:1259:ASP:O	2.21	0.41
1:C:1401:ALA:O	1:C:1402:ARG:CB	2.68	0.41
1:D:1856:ILE:O	1:D:1860:GLN:HG3	2.20	0.41
1:C:1156:GLY:HA3	1:C:1164:LEU:HD23	2.03	0.41
1:D:1817:ILE:O	1:D:1839:ALA:HB1	2.21	0.41
1:A:326:ASN:HB3	1:A:329:ARG:CG	2.52	0.40
1:B:799:ALA:HB1	4:B:3253:HOH:O	2.19	0.40
1:B:517:PRO:HG2	1:B:556:TRP:CG	2.55	0.40
1:B:763:LYS:HB2	4:B:3295:HOH:O	2.22	0.40
1:B:919:LEU:HD13	1:B:923:ALA:HB2	2.02	0.40
1:A:67:ASN:HD22	1:A:67:ASN:HA	1.63	0.40
1:A:373:HIS:CD2	1:A:373:HIS:H	2.38	0.40
1:C:1056:TRP:C	1:C:1058:GLY:N	2.79	0.40
1:C:1288:ARG:HG3	1:C:1289:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/436 (100%)	424 (98%)	9 (2%)	1 (0%)	43	44
1	B	434/436 (100%)	420 (97%)	13 (3%)	1 (0%)	43	44
1	C	434/436 (100%)	419 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	434/436 (100%)	421 (97%)	13 (3%)	0	100	100
All	All	1736/1744 (100%)	1684 (97%)	50 (3%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
1	B	902	ARG

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	343/343 (100%)	338 (98%)	5 (2%)	57	65
1	B	343/343 (100%)	340 (99%)	3 (1%)	70	78
1	C	343/343 (100%)	335 (98%)	8 (2%)	44	51
1	D	343/343 (100%)	341 (99%)	2 (1%)	78	86
All	All	1372/1372 (100%)	1354 (99%)	18 (1%)	61	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	143	PRO
1	A	238	ASP
1	A	255	ASP
1	A	347	ASN
1	B	835	GLU
1	B	847	ASN
1	B	892	THR
1	C	1143	PRO
1	C	1151	LEU
1	C	1218	ILE
1	C	1227	LEU

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Mol	Chain	Res	Type
1	C	1294	ILE
1	C	1347	ASN
1	C	1392	THR
1	C	1428	GLU
1	D	1815	ILE
1	D	1847	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	80	ASN
1	A	191	HIS
1	A	316	GLN
1	A	394	GLN
1	B	580	ASN
1	B	626	ASN
1	B	659	HIS
1	B	667	GLN
1	B	717	ASN
1	B	808	HIS
1	B	816	GLN
1	B	894	GLN
1	B	922	ASN
1	C	1067	ASN
1	C	1080	ASN
1	C	1155	ASN
1	C	1308	HIS
1	C	1316	GLN
1	C	1394	GLN
1	D	1580	ASN
1	D	1626	ASN
1	D	1717	ASN
1	D	1808	HIS
1	D	1816	GLN
1	D	1894	GLN
1	D	1922	ASN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 8 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	PAH	C	1440	2	8,8,8	2.26	3 (37%)	10,11,11	1.86	2 (20%)
3	PAH	D	1940	2	8,8,8	2.31	3 (37%)	10,11,11	1.72	2 (20%)
3	PAH	A	440	2	8,8,8	2.01	2 (25%)	10,11,11	1.83	3 (30%)
3	PAH	B	940	2	8,8,8	2.20	2 (25%)	10,11,11	1.86	3 (30%)

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	PAH	C	1440	2	-	2/7/7/7	-
3	PAH	D	1940	2	-	0/7/7/7	-
3	PAH	A	440	2	-	1/7/7/7	-
3	PAH	B	940	2	-	0/7/7/7	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1940	PAH	P-C1	4.59	1.86	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1440	PAH	P-C1	4.51	1.86	1.79
3	B	940	PAH	P-C1	4.00	1.86	1.79
3	B	940	PAH	O2-C2	3.86	1.30	1.23
3	A	440	PAH	P-C1	3.82	1.85	1.79
3	C	1440	PAH	O2-C2	3.63	1.30	1.23
3	D	1940	PAH	O2-C2	3.62	1.30	1.23
3	A	440	PAH	O2-C2	3.38	1.29	1.23
3	D	1940	PAH	P-O1P	2.18	1.54	1.50
3	C	1440	PAH	P-O1P	2.11	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	940	PAH	C1-C2-N3	3.64	118.94	114.87
3	C	1440	PAH	C1-C2-N3	3.62	118.91	114.87
3	A	440	PAH	C1-C2-N3	3.45	118.73	114.87
3	D	1940	PAH	C1-C2-N3	3.22	118.47	114.87
3	C	1440	PAH	O3-N3-C2	-3.09	115.23	119.79
3	A	440	PAH	O3-N3-C2	-3.02	115.33	119.79
3	B	940	PAH	O3-N3-C2	-3.01	115.34	119.79
3	D	1940	PAH	O3-N3-C2	-2.96	115.42	119.79
3	A	440	PAH	O2-C2-N3	-2.12	120.66	123.27
3	B	940	PAH	O2-C2-N3	-2.10	120.69	123.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1440	PAH	C2-C1-P-O3P
3	A	440	PAH	C2-C1-P-O1P
3	C	1440	PAH	C2-C1-P-O1P

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.