



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:00 am BST

PDB ID : 2O6I
Title : Structure of an Enterococcus Faecalis HD Domain Phosphohydrolase
Authors : Vorontsov, I.I.; Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Moy, S.; Col-lart, F.R.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-12-07
Resolution : 2.55 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 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

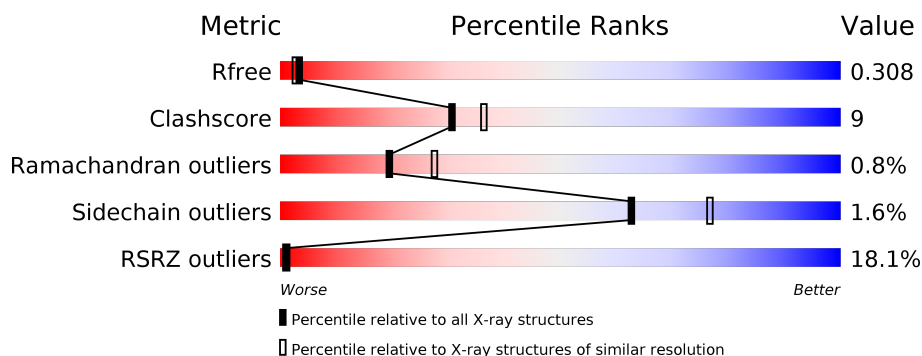
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 ≥ 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	480	<div> <div>13%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	B	480	<div> <div>20%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>• 10%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7556 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 HD domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	6	0
			3632	2325	618	676	13			
1	B	430	Total	C	N	O	S	0	12	0
			3610	2308	614	675	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	INITIATING METHIONINE	UNP Q836G9
A	-22	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-21	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-20	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-19	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-18	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-17	HIS	-	EXPRESSION TAG	UNP Q836G9
A	-16	SER	-	CLONING ARTIFACT	UNP Q836G9
A	-15	SER	-	CLONING ARTIFACT	UNP Q836G9
A	-14	GLY	-	CLONING ARTIFACT	UNP Q836G9
A	-13	VAL	-	CLONING ARTIFACT	UNP Q836G9
A	-12	ASP	-	CLONING ARTIFACT	UNP Q836G9
A	-11	LEU	-	CLONING ARTIFACT	UNP Q836G9
A	-10	GLY	-	CLONING ARTIFACT	UNP Q836G9
A	-9	THR	-	CLONING ARTIFACT	UNP Q836G9
A	-8	GLU	-	CLONING ARTIFACT	UNP Q836G9
A	-7	ASN	-	CLONING ARTIFACT	UNP Q836G9
A	-6	LEU	-	CLONING ARTIFACT	UNP Q836G9
A	-5	TYR	-	CLONING ARTIFACT	UNP Q836G9
A	-4	PHE	-	CLONING ARTIFACT	UNP Q836G9
A	-3	GLN	-	CLONING ARTIFACT	UNP Q836G9
A	-2	SER	-	CLONING ARTIFACT	UNP Q836G9
A	-1	ASN	-	CLONING ARTIFACT	UNP Q836G9
A	0	ALA	-	CLONING ARTIFACT	UNP Q836G9
B	-23	MET	-	CLONING ARTIFACT	UNP Q836G9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-21	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-20	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-19	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-18	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-17	HIS	-	EXPRESSION TAG	UNP Q836G9
B	-16	SER	-	CLONING ARTIFACT	UNP Q836G9
B	-15	SER	-	CLONING ARTIFACT	UNP Q836G9
B	-14	GLY	-	CLONING ARTIFACT	UNP Q836G9
B	-13	VAL	-	CLONING ARTIFACT	UNP Q836G9
B	-12	ASP	-	CLONING ARTIFACT	UNP Q836G9
B	-11	LEU	-	CLONING ARTIFACT	UNP Q836G9
B	-10	GLY	-	CLONING ARTIFACT	UNP Q836G9
B	-9	THR	-	CLONING ARTIFACT	UNP Q836G9
B	-8	GLU	-	CLONING ARTIFACT	UNP Q836G9
B	-7	ASN	-	CLONING ARTIFACT	UNP Q836G9
B	-6	LEU	-	CLONING ARTIFACT	UNP Q836G9
B	-5	TYR	-	CLONING ARTIFACT	UNP Q836G9
B	-4	PHE	-	CLONING ARTIFACT	UNP Q836G9
B	-3	GLN	-	CLONING ARTIFACT	UNP Q836G9
B	-2	SER	-	CLONING ARTIFACT	UNP Q836G9
B	-1	ASN	-	CLONING ARTIFACT	UNP Q836G9
B	0	ALA	-	CLONING ARTIFACT	UNP Q836G9

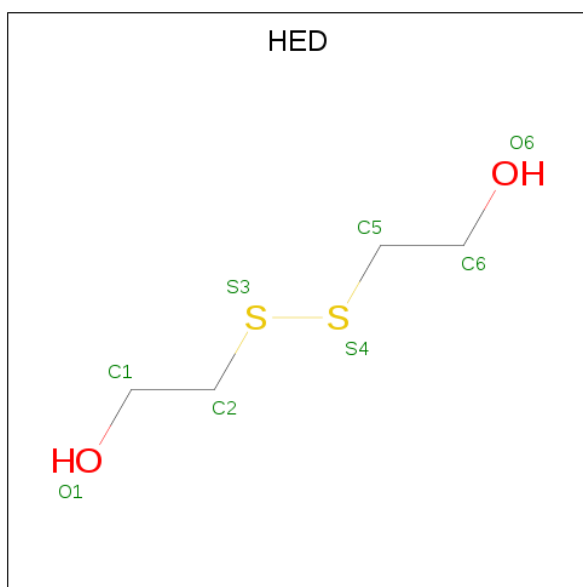
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	1
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 2-HYDROXYETHYL DISULFIDE (three-letter code: HED) (formula: C₄H₁₀O₂S₂).

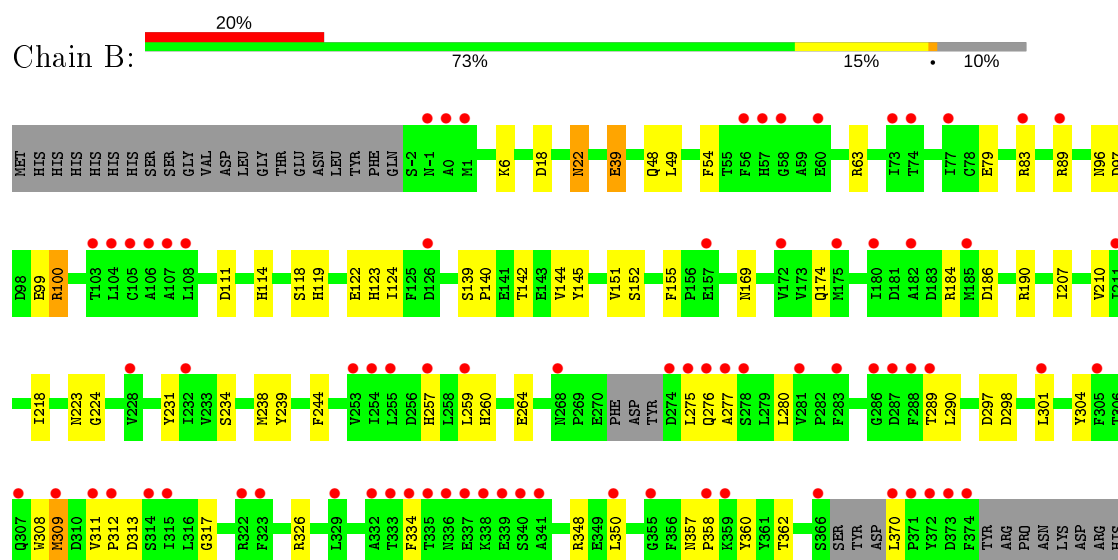


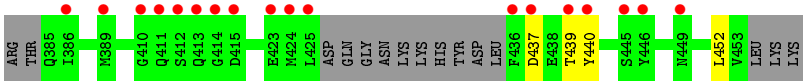
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	169	Total	O	0	2
			170	170		
5	B	128	Total	O	0	4
			132	132		

- Molecule 1: HD domain protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.91Å 109.91Å 182.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.55) 96.3 (29.97-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.317 0.241 , 0.308	Depositor DCC
R_{free} test set	2049 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7556	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HED, ZN, CL

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	0.29	0/3718	0.54	0/5032
1	B	0.28	0/3694	0.53	1/5000 (0.0%)
All	All	0.28	0/7412	0.54	1/10032 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	LEU	CA-CB-CG	5.54	128.03	115.30

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	3632	0	3542	76	0
1	B	3610	0	3512	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	10	1	0
5	A	170	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	132	0	0	0	0
All	All	7556	0	7064	132	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 9.

All (132) 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:75:ARG:HG3	1:A:75:ARG:HH11	1.25	1.01
1:A:75:ARG:CG	1:A:75:ARG:HH11	1.85	0.88
1:B:18:ASP:O	1:B:22:ASN:HA	1.75	0.86
1:B:257:HIS:HD2	1:B:360:TYR:HA	1.46	0.81
1:A:265:LEU:HD13	1:A:272:ASP:OD2	1.81	0.80
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.01	0.73
1:A:16:PHE:HB2	1:A:24:ILE:HB	1.72	0.71
1:A:75:ARG:HG3	1:A:75:ARG:NH1	1.94	0.69
1:A:124:ILE:HD13	1:A:259:LEU:HB2	1.72	0.69
1:B:111:ASP:HB2	1:B:114:HIS:ND1	2.08	0.68
1:A:249:ARG:NH2	1:A:417:ARG:HG3	2.10	0.66
1:A:80:ILE:O	1:A:84:ASN:ND2	2.29	0.66
1:A:1:MET:N	1:A:2:THR:HA	2.12	0.65
1:B:39:GLU:CD	1:B:39:GLU:H	2.01	0.64
1:A:375:TYR:HB3	1:A:386:ILE:HD11	1.81	0.63
1:B:297:ASP:OD2	1:B:298:ASP:N	2.33	0.61
1:A:140:PRO:HA	1:A:145:TYR:CD2	2.35	0.61
1:B:118:SER:O	1:B:122:GLU:HB2	2.02	0.60
1:A:124:ILE:CD1	1:A:259:LEU:HB2	2.31	0.60
1:A:79:GLU:O	1:A:83:ARG:HG2	2.02	0.59
1:A:257:HIS:HD2	1:A:360:TYR:HA	1.66	0.59
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.68	0.59
1:A:351:ILE:HG22	1:A:356:PHE:HB2	1.86	0.58
1:A:245:HIS:CD2	1:A:247:VAL:HG22	2.39	0.58
1:A:88:GLU:OE2	1:A:88:GLU:N	2.36	0.57
1:B:99:GLU:OE2	1:B:169:ASN:ND2	2.38	0.57
1:B:18:ASP:O	1:B:22:ASN:CA	2.49	0.57
1:B:275:LEU:O	1:B:277:ALA:N	2.37	0.57
1:A:386:ILE:CG2	1:A:397:GLU:HB2	2.35	0.57
1:A:21:HIS:O	1:A:22:ASN:HB2	2.05	0.56
1:B:111:ASP:HB2	1:B:114:HIS:CE1	2.40	0.56
1:B:152:SER:HB3	1:B:155:PHE:HB2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASP:O	1:A:322:ARG:HG3	2.06	0.56
1:A:142:THR:HG22	1:A:144:VAL:H	1.71	0.56
1:A:7:GLU:O	1:A:9[B]:ARG:HD2	2.06	0.55
1:A:18:ASP:OD1	1:A:190:ARG:NH2	2.39	0.55
1:B:54:PHE:HD1	1:B:326:ARG:HG2	1.71	0.55
1:A:103:THR:HB	1:A:172:VAL:HG13	1.88	0.55
1:A:214:TYR:CE1	1:A:395:LEU:HD11	2.42	0.55
1:A:358:PRO:O	1:A:362:THR:HB	2.07	0.55
1:B:184:ARG:HH22	1:B:370:LEU:HD13	1.70	0.55
1:A:72:GLU:O	1:A:76:ARG:HG2	2.07	0.54
1:B:239:TYR:HD2	1:B:244:PHE:CE2	2.25	0.54
1:B:210[B]:VAL:HG11	1:B:224:GLY:HA3	1.90	0.53
1:A:251:MET:HE3	1:A:326:ARG:HA	1.91	0.52
1:A:251:MET:HE1	1:A:326:ARG:C	2.30	0.52
1:B:124:ILE:CD1	1:B:259:LEU:HB2	2.39	0.52
1:B:124:ILE:HD13	1:B:259:LEU:HB2	1.91	0.51
1:A:122:GLU:HA	1:A:127[A]:THR:HG23	1.93	0.51
1:A:84:ASN:HD22	1:A:84:ASN:H	1.60	0.50
1:B:234:SER:O	1:B:238:MET:HB2	2.11	0.50
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.68	0.50
1:A:84:ASN:HD22	1:A:84:ASN:N	2.08	0.50
1:B:6:LYS:HB3	1:B:151:VAL:HG13	1.94	0.50
1:A:5:TYR:CE2	1:A:30:VAL:HG22	2.47	0.49
1:A:348:ARG:HE	1:A:362:THR:HG21	1.77	0.49
1:B:142:THR:HG22	1:B:144:VAL:H	1.77	0.49
1:A:135:GLN:OE1	4:A:505:HED:H21	2.12	0.49
1:A:142:THR:HG22	1:A:144:VAL:N	2.28	0.48
1:A:48:GLN:HE21	1:A:63:ARG:HA	1.79	0.48
1:B:100:ARG:HH11	1:B:100:ARG:HG3	1.79	0.48
1:A:386:ILE:HG21	1:A:397:GLU:HB2	1.96	0.47
1:B:275:LEU:HD23	1:B:277:ALA:H	1.79	0.47
1:B:79:GLU:HG3	1:B:83[A]:ARG:HE	1.79	0.47
1:B:97:ASP:OD1	1:B:100:ARG:NH1	2.47	0.47
1:A:61:HIS:CD2	1:A:61:HIS:H	2.32	0.46
1:B:309:MET:HA	1:B:317:GLY:HA2	1.97	0.46
1:B:48:GLN:NE2	1:B:63:ARG:HG2	2.31	0.46
1:A:289:THR:HG22	1:A:291:GLN:H	1.81	0.46
1:B:257:HIS:CD2	1:B:360:TYR:HA	2.36	0.46
1:A:352:GLU:HG2	1:A:358:PRO:HD3	1.98	0.46
1:A:174:GLN:NE2	1:A:218:ILE:H	2.14	0.46
1:B:260:HIS:O	1:B:264:GLU:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:TYR:CG	1:A:274:ASP:N	2.84	0.45
1:B:142:THR:HG21	1:B:144:VAL:HG22	1.98	0.45
1:A:139:SER:HA	1:A:140:PRO:HD3	1.75	0.45
1:A:289:THR:HG22	1:A:290:LEU:N	2.30	0.45
1:A:99:GLU:O	1:A:103:THR:HG22	2.17	0.45
1:A:309:MET:CE	1:A:324:LEU:HD12	2.47	0.45
1:A:122:GLU:HG3	1:A:127[B]:THR:O	2.17	0.44
1:A:48:GLN:HG2	5:A:569:HOH:O	2.18	0.44
1:A:347:LEU:O	1:A:351:ILE:HG13	2.18	0.44
1:A:84:ASN:N	1:A:84:ASN:ND2	2.65	0.44
1:B:139:SER:HA	1:B:140:PRO:HD3	1.84	0.44
1:A:311:VAL:HA	1:A:312:PRO:HD2	1.85	0.44
1:A:336:ASN:HB3	1:A:339:GLU:HB2	1.98	0.44
1:B:39:GLU:OE2	1:B:142:THR:HG23	2.17	0.44
1:B:140:PRO:HA	1:B:145:TYR:CD2	2.53	0.44
1:B:334:PHE:HB3	1:B:452:LEU:HD12	1.99	0.44
1:B:142:THR:CG2	1:B:144:VAL:HG22	2.48	0.44
1:B:48:GLN:HE21	1:B:63:ARG:HA	1.83	0.44
1:B:18:ASP:O	1:B:22:ASN:N	2.51	0.43
1:B:357:ASN:HA	1:B:358:PRO:HD2	1.90	0.43
1:B:348:ARG:HG2	1:B:362:THR:HG21	2.00	0.43
1:A:251:MET:CE	1:A:326:ARG:HA	2.47	0.43
1:A:75:ARG:CG	1:A:75:ARG:NH1	2.55	0.43
1:B:289:THR:HG22	1:B:290:LEU:N	2.32	0.43
1:B:437:ASP:HA	1:B:440:TYR:HD1	1.83	0.43
1:A:263:LYS:NZ	1:A:267:GLU:OE2	2.42	0.43
1:A:124:ILE:HD13	1:A:259:LEU:CB	2.45	0.43
1:A:136:ILE:HG23	1:A:142:THR:HG21	2.01	0.43
1:B:174:GLN:NE2	1:B:218:ILE:H	2.16	0.43
1:B:207:ILE:HD11	1:B:231:TYR:HB2	2.01	0.43
1:A:169:ASN:HA	1:A:170:PRO:HD2	1.88	0.43
1:A:343:THR:O	1:A:347:LEU:HG	2.18	0.42
1:A:257:HIS:CD2	1:A:360:TYR:HA	2.50	0.42
1:B:119[B]:HIS:O	1:B:123[B]:HIS:ND1	2.49	0.42
1:B:79:GLU:HG3	1:B:83[B]:ARG:HE	1.83	0.42
1:A:61:HIS:HE1	1:A:191:ASP:OD1	2.01	0.42
1:A:309:MET:HE3	1:A:324:LEU:HD12	2.00	0.42
1:B:280:LEU:HD21	1:B:301:LEU:HD21	2.00	0.42
1:A:179:GLN:HA	1:A:184:ARG:NH1	2.34	0.42
1:A:351:ILE:CG2	1:A:356:PHE:HB2	2.48	0.42
1:B:350:LEU:HB3	1:B:439:THR:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:TYR:O	1:B:308:TRP:CD1	2.73	0.42
1:B:79:GLU:OE1	1:B:100:ARG:NH2	2.53	0.42
1:A:203:ASP:OD2	1:A:206:ARG:HG3	2.21	0.41
1:B:311:VAL:HG12	1:B:313:ASP:H	1.85	0.41
1:A:70:VAL:HG22	1:A:183:ASP:HA	2.02	0.41
1:A:222:MET:HE1	1:A:401:VAL:HG11	2.03	0.41
1:A:48:GLN:HA	1:A:63:ARG:HG2	2.03	0.41
1:B:223[A]:ASN:H	1:B:223[A]:ASN:HD22	1.69	0.41
1:A:336:ASN:CB	1:A:339:GLU:HB2	2.51	0.41
1:B:142:THR:HG22	1:B:144:VAL:N	2.35	0.41
1:B:275:LEU:C	1:B:277:ALA:H	2.24	0.41
1:A:122:GLU:HG3	1:A:127[A]:THR:O	2.21	0.41
1:A:401:VAL:O	1:A:401:VAL:HG12	2.20	0.41
1:A:39:GLU:CD	1:A:142:THR:HG23	2.41	0.40
1:A:322:ARG:HG2	1:A:327:LYS:HE3	2.04	0.40
1:A:167:TYR:HA	1:A:168:PRO:HD3	1.91	0.40
1:A:249:ARG:NH2	1:A:417:ARG:CG	2.81	0.40
1:B:186:ASP:OD1	1:B:190:ARG:NH1	2.54	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	434/480 (90%)	405 (93%)	25 (6%)	4 (1%)	17	24
1	B	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	22	30
All	All	866/960 (90%)	811 (94%)	48 (6%)	7 (1%)	19	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	276	GLN
1	A	50	GLY
1	A	273	TYR
1	B	22	ASN
1	A	180	ILE
1	B	312	PRO
1	A	312	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	396/430 (92%)	389 (98%)	7 (2%)	59	74
1	B	395/430 (92%)	390 (99%)	5 (1%)	69	80
All	All	791/860 (92%)	779 (98%)	12 (2%)	62	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	84	ASN
1	A	222	MET
1	A	268	ASN
1	A	275	LEU
1	A	347	LEU
1	A	387	GLU
1	B	39	GLU
1	B	89	ARG
1	B	96	ASN
1	B	100	ARG
1	B	309	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	25	HIS
1	A	27	GLN
1	A	48	GLN
1	A	61	HIS
1	A	84	ASN
1	A	114	HIS
1	A	149	ASN
1	A	174	GLN
1	A	223	ASN
1	A	245	HIS
1	A	257	HIS
1	A	268	ASN
1	A	276	GLN
1	A	307	GLN
1	A	336	ASN
1	A	390	GLN
1	A	411	GLN
1	A	413	GLN
1	B	8	GLN
1	B	48	GLN
1	B	61	HIS
1	B	96	ASN
1	B	128	ASN
1	B	146	GLN
1	B	149	ASN
1	B	174	GLN
1	B	237	GLN
1	B	241	GLN
1	B	268	ASN
1	B	385	GLN
1	B	413	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
4	HED	A	505	-	7,7,7	0.75	0	6,6,6	1.21	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
4	HED	A	505	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	HED	O1-C1-C2-S3
4	A	505	HED	S4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	HED	1	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

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	436/480 (90%)	0.93	63 (14%) 2 3	57, 67, 78, 96	0
1	B	430/480 (89%)	1.21	94 (21%) 0 0	57, 69, 81, 101	0
All	All	866/960 (90%)	1.07	157 (18%) 1 1	57, 68, 79, 101	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ARG	7.8
1	A	414	GLY	7.4
1	B	58	GLY	6.9
1	B	371	PRO	6.9
1	A	271	PHE	6.8
1	A	374	PHE	6.6
1	B	412	SER	6.3
1	B	312	PRO	6.3
1	A	337	GLU	6.1
1	B	335	THR	6.0
1	B	338	LYS	5.8
1	B	374	PHE	5.6
1	A	338	LYS	5.5
1	A	335	THR	5.4
1	B	423	GLU	5.4
1	B	370	LEU	5.4
1	B	287	ASP	5.3
1	B	289	THR	5.2
1	A	273	TYR	5.2
1	B	337	GLU	5.2
1	B	355	GLY	5.2
1	A	270	GLU	5.2
1	B	275	LEU	5.0
1	B	336	ASN	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	373	ASP	4.7
1	B	413	GLN	4.5
1	B	386	ILE	4.4
1	A	411	GLN	4.4
1	B	410	GLY	4.3
1	A	336	ASN	4.3
1	A	126	ASP	4.2
1	B	411	GLN	4.1
1	B	274	ASP	4.0
1	A	108	LEU	4.0
1	B	439	THR	4.0
1	A	441	ARG	4.0
1	B	126	ASP	3.9
1	A	413	GLN	3.8
1	A	410	GLY	3.8
1	B	255	LEU	3.8
1	A	272	ASP	3.7
1	B	414	GLY	3.7
1	A	370	LEU	3.7
1	B	449	ASN	3.7
1	B	268	ASN	3.6
1	B	440	TYR	3.6
1	B	366	SER	3.6
1	B	175	MET	3.5
1	B	57	HIS	3.5
1	B	286	GLY	3.4
1	B	334	PHE	3.4
1	B	276	GLN	3.4
1	A	423	GLU	3.3
1	B	446	TYR	3.3
1	A	176	ILE	3.3
1	B	283	PHE	3.3
1	A	74	THR	3.3
1	A	57	HIS	3.3
1	A	104	LEU	3.3
1	A	107	ALA	3.3
1	B	372	TYR	3.3
1	A	371	PRO	3.2
1	A	2	THR	3.1
1	A	89	ARG	3.0
1	B	415	ASP	3.0
1	B	389	MET	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	309	MET	3.0
1	B	339	GLU	3.0
1	A	1	MET	3.0
1	A	367	SER	3.0
1	B	60	GLU	2.9
1	B	107	ALA	2.9
1	A	175	MET	2.9
1	A	182	ALA	2.9
1	A	70	VAL	2.9
1	A	180	ILE	2.9
1	B	323	PHE	2.9
1	B	182	ALA	2.8
1	A	103	THR	2.8
1	B	277	ALA	2.8
1	B	301	LEU	2.8
1	B	288	PHE	2.8
1	B	333	THR	2.8
1	B	305	PHE	2.7
1	A	269	PRO	2.7
1	B	74	THR	2.7
1	B	1	MET	2.7
1	B	311	VAL	2.7
1	A	314	SER	2.7
1	B	104	LEU	2.6
1	B	232	ILE	2.6
1	A	88	GLU	2.6
1	B	253	VAL	2.6
1	A	73	ILE	2.6
1	B	329	LEU	2.6
1	A	375	TYR	2.6
1	A	440	TYR	2.6
1	B	89	ARG	2.6
1	A	56	PHE	2.6
1	B	185	MET	2.6
1	A	422	LYS	2.6
1	A	362	THR	2.5
1	B	-1	ASN	2.5
1	A	115	GLY	2.5
1	B	315	ILE	2.5
1	B	314	SER	2.5
1	B	278	SER	2.5
1	B	259	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	252[A]	GLU	2.5
1	B	108	LEU	2.4
1	B	322	ARG	2.4
1	A	244	PHE	2.4
1	A	363	ALA	2.4
1	B	341	ALA	2.4
1	A	112	VAL	2.4
1	B	445	SER	2.4
1	A	53	SER	2.4
1	B	56	PHE	2.4
1	A	385	GLN	2.4
1	A	412	SER	2.4
1	A	209	ARG	2.4
1	B	228	VAL	2.4
1	A	109	LEU	2.4
1	B	358	PRO	2.3
1	A	343	THR	2.3
1	B	425	LEU	2.3
1	B	254	ILE	2.3
1	B	436	PHE	2.3
1	A	90	LEU	2.3
1	B	257	HIS	2.3
1	B	157	GLU	2.3
1	A	71	TYR	2.2
1	A	105	CYS	2.2
1	A	83	ARG	2.2
1	B	307	GLN	2.2
1	B	437	ASP	2.2
1	A	340	SER	2.2
1	B	281	VAL	2.2
1	B	340	SER	2.2
1	B	105	CYS	2.2
1	B	211	ILE	2.2
1	B	350	LEU	2.2
1	A	426	ASP	2.1
1	B	180	ILE	2.1
1	A	436	PHE	2.1
1	B	172	VAL	2.1
1	B	103	THR	2.1
1	B	424	MET	2.1
1	B	106	ALA	2.1
1	A	198	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	73	ILE	2.1
1	B	83[A]	ARG	2.1
1	B	0	ALA	2.0
1	B	332	ALA	2.0
1	B	359	LYS	2.0
1	A	231	TYR	2.0
1	B	77	ILE	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, 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(Å ²)	Q<0.9
3	CL	A	503	1/1	0.81	0.41	84,84,84,84	1
4	HED	A	505	8/8	0.91	0.18	63,64,66,67	0
2	ZN	A	501	1/1	0.92	0.11	68,68,68,68	1
3	CL	B	504[A]	1/1	0.96	0.17	63,63,63,63	1
2	ZN	B	502	1/1	0.98	0.09	74,74,74,74	1

6.5 Other polymers [i](#)

There are no such residues in this entry.