



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 2O6I / pdb_00002o6i
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 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

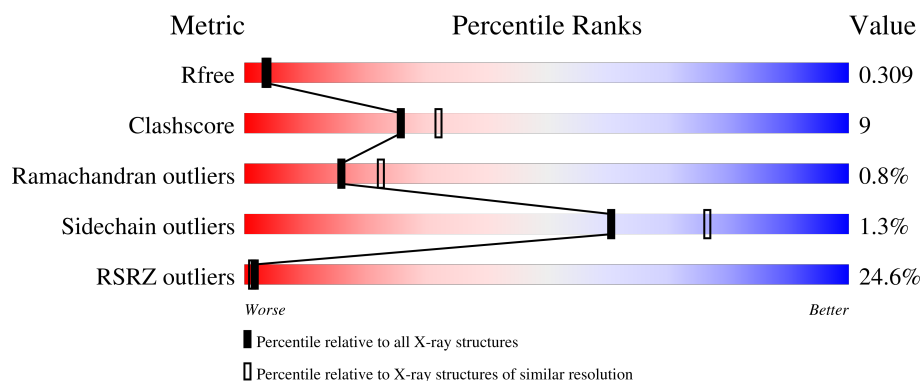
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	480	10% 70% 19% • 9%
1	B	480	35% 72% 17% • 10%

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

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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

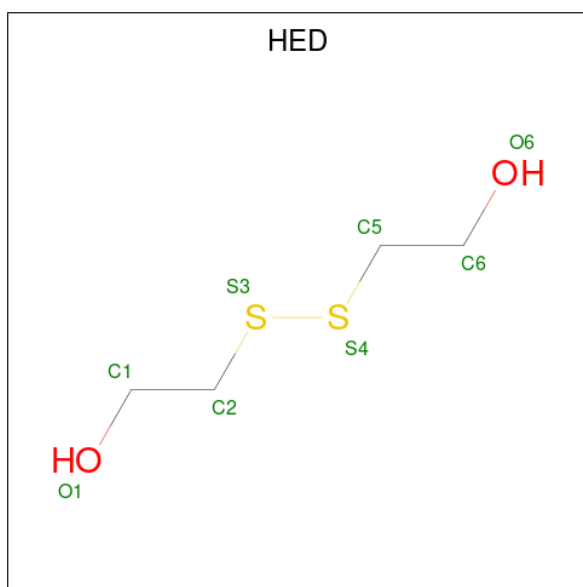
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is 2-HYDROXYETHYL DISULFIDE (CCD ID: HED) (formula: C₄H₁₀O₂S₂).



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

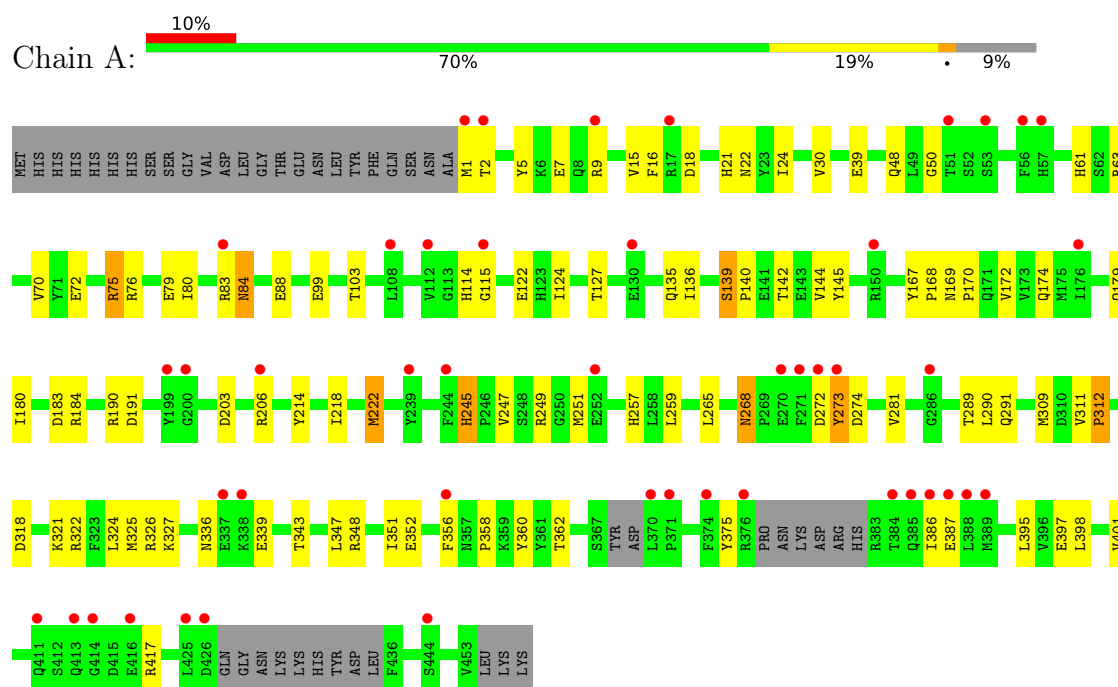
- Molecule 5 is water.

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

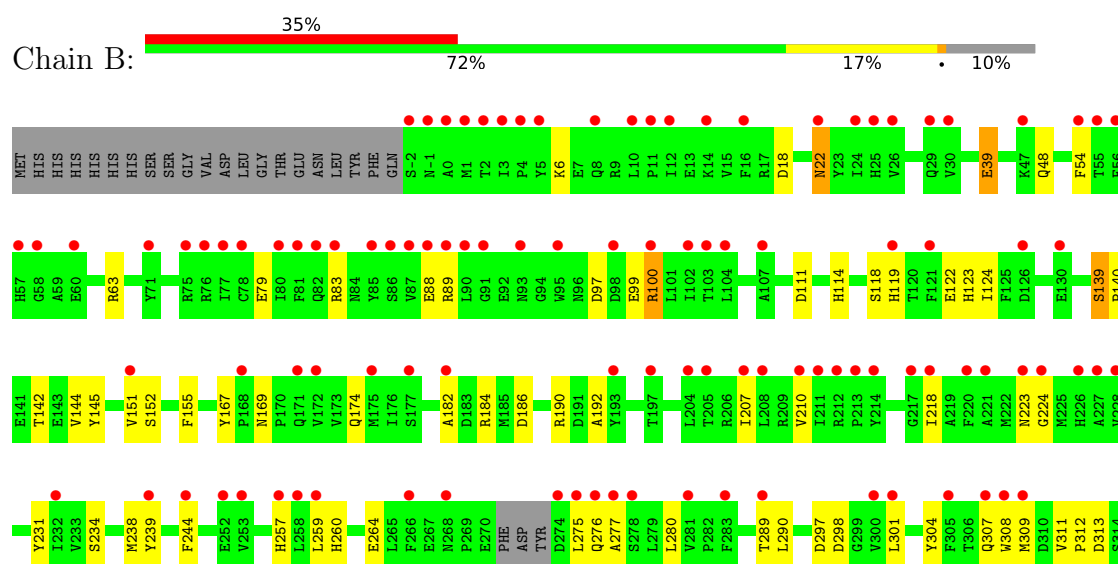
3 Residue-property plots [i](#)

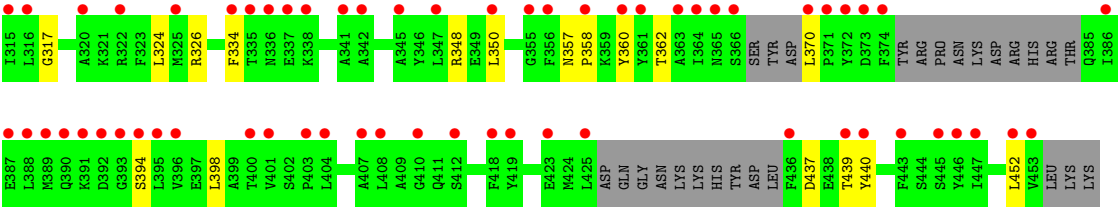
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• 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 30.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.55) 96.2 (30.00-2.55)	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 , 0.309	Depositor DCC
R_{free} test set	2049 reflections (4.86%)	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)	0.31 , 63.4	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	0.90	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

5.1 Standard geometry

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	0.38	1/3718 (0.0%)	0.90	8/5032 (0.2%)
1	B	0.37	0/3694	0.88	7/5000 (0.1%)
All	All	0.38	1/7412 (0.0%)	0.89	15/10032 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CA-CB	5.62	1.56	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	HIS	N-CA-C	8.50	121.39	111.02
1	A	139	SER	CA-C-N	8.00	129.84	119.84
1	A	139	SER	C-N-CA	8.00	129.84	119.84
1	B	139	SER	CA-C-N	6.62	126.32	119.56
1	B	139	SER	C-N-CA	6.62	126.32	119.56
1	B	167	TYR	CA-C-N	6.30	127.71	119.84
1	B	167	TYR	C-N-CA	6.30	127.71	119.84
1	A	245	HIS	CA-C-N	6.00	125.48	119.24
1	A	245	HIS	C-N-CA	6.00	125.48	119.24
1	B	394	SER	N-CA-C	5.55	117.08	110.19
1	A	398	LEU	N-CA-C	5.53	117.76	111.02
1	B	398	LEU	N-CA-C	5.49	117.70	111.11
1	B	182	ALA	N-CA-C	-5.49	105.40	111.71
1	A	115	GLY	CA-C-N	5.20	125.45	119.83
1	A	115	GLY	C-N-CA	5.20	125.45	119.83

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	3632	0	3542	77	0
1	B	3610	0	3512	59	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
5	B	132	0	0	0	0
All	All	7556	0	7064	136	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 (136) 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:HH11	1:A:75:ARG:HG3	1.25	1.01
1:A:75:ARG:HH11	1:A:75:ARG:CG	1.85	0.88
1:B:18:ASP:O	1:B:22:ASN:HA	1.75	0.86
1:A:251:MET:HE1	1:A:326:ARG:HA	1.56	0.85
1:A:309:MET:HE3	1:A:324:LEU:HD12	1.58	0.83
1:B:257:HIS:HD2	1:B:360:TYR:HA	1.46	0.81
1:A:222:MET:HE1	1:A:401:VAL:HG11	1.61	0.81
1:A:265:LEU:HD13	1:A:272:ASP:OD2	1.81	0.80
1:A:309:MET:HE2	1:A:321:LYS:HA	1.64	0.79
1:B:100:ARG:CG	1:B:100:ARG:HH11	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:39:GLU:H	1:B:39:GLU:CD	2.01	0.69
1:B:111:ASP:HB2	1:B:114:HIS:ND1	2.08	0.68
1:A:1:MET:H3	1:A:2:THR:HA	1.58	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:2:THR:HA	2.12	0.63
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:251:MET:HE1	1:A:326:ARG:CA	2.28	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:18:ASP:O	1:B:22:ASN:CA	2.49	0.57
1:B:99:GLU:OE2	1:B:169:ASN:ND2	2.38	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
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:B:309:MET:HE1	1:B:324:LEU:HD12	1.90	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:LEU:C	1:B:277:ALA:H	2.24	0.46
1:B:260:HIS:O	1:B:264:GLU:HG3	2.15	0.45
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:99:GLU:O	1:A:103:THR:HG22	2.17	0.45
1:A:289:THR:HG22	1:A:290:LEU:N	2.30	0.45
1:A:122:GLU:HG3	1:A:127[B]:THR:O	2.17	0.44
1:A:39:GLU:CD	1:A:142:THR:HG23	2.41	0.44
1:A:48:GLN:HG2	5:A:569:HOH:O	2.18	0.44
1:A:84:ASN:ND2	1:A:84:ASN:N	2.65	0.44
1:A:347:LEU:O	1:A:351:ILE:HG13	2.18	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:325:MET:HE2	1:A:325:MET:HB3	1.84	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:48:GLN:HE21	1:B:63:ARG:HA	1.83	0.44
1:B:142:THR:CG2	1:B:144:VAL:HG22	2.48	0.44
1:B:18:ASP:O	1:B:22:ASN:N	2.51	0.43
1:B:348:ARG:HG2	1:B:362:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:HA	1:B:358:PRO:HD2	1.90	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: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:257:HIS:CD2	1:A:360:TYR:HA	2.50	0.42
1:A:343:THR:O	1:A:347:LEU:HG	2.18	0.42
1:B:79:GLU:HG3	1:B:83[B]:ARG:HE	1.83	0.42
1:B:119[B]:HIS:O	1:B:123[B]:HIS:ND1	2.49	0.42
1:A:61:HIS:HE1	1:A:191:ASP:OD1	2.01	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:B:88[B]:GLU:N	1:B:88[B]:GLU:CD	2.78	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
1:B:79:GLU:OE1	1:B:100:ARG:NH2	2.53	0.42
1:B:304:TYR:O	1:B:308:TRP:CD1	2.73	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: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:B:192:ALA:HA	1:B:238:MET:HE1	2.03	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:A:122:GLU:HG3	1:A:127[A]:THR:O	2.21	0.41
1:A:401:VAL:HG12	1:A:401:VAL:O	2.20	0.41
1:A:268:ASN:HD22	1:A:268:ASN:C	2.29	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%)	14	20
1	B	432/480 (90%)	406 (94%)	23 (5%)	3 (1%)	18	25
All	All	866/960 (90%)	811 (94%)	48 (6%)	7 (1%)	16	22

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/430 (92%)	390 (98%)	6 (2%)	57	74
1	B	395/430 (92%)	391 (99%)	4 (1%)	68	80
All	All	791/860 (92%)	781 (99%)	10 (1%)	61	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	75	ARG
1	A	84	ASN
1	A	222	MET
1	A	268	ASN
1	A	387	GLU
1	B	39	GLU
1	B	89	ARG
1	B	100	ARG
1	B	307	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	25	HIS
1	A	27	GLN
1	A	29	GLN
1	A	48	GLN
1	A	61	HIS
1	A	84	ASN
1	A	119	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	146	GLN
1	B	149	ASN
1	B	174	GLN
1	B	237	GLN
1	B	241	GLN

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Mol	Chain	Res	Type
1	B	268	ASN
1	B	385	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 oligosaccharides 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	0.76	0	6,6,6	1.26	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
4	HED	A	505	-	-	2/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	505	HED	C2-S3-S4	2.03	112.39	103.46

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.06	46 (10%)	11 11	32, 67, 78, 96	6 (1%)
1	B	430/480 (89%)	1.87	167 (38%)	1 0	31, 68, 81, 101	12 (2%)
All	All	866/960 (90%)	1.46	213 (24%)	2 1	31, 67, 79, 101	18 (2%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	MET	5.0
1	B	423	GLU	4.9
1	B	-2	SER	4.8
1	A	271	PHE	4.5
1	A	387	GLU	4.5
1	B	14[A]	LYS	4.4
1	B	259	LEU	4.4
1	B	387	GLU	4.3
1	A	374	PHE	4.3
1	B	275	LEU	4.2
1	B	0	ALA	4.2
1	B	82[A]	GLN	4.1
1	B	388	LEU	4.1
1	B	81	PHE	4.0
1	B	446	TYR	4.0
1	B	268	ASN	4.0
1	B	277	ALA	3.9
1	B	370	LEU	3.9
1	A	370	LEU	3.8
1	B	90	LEU	3.8
1	A	337	GLU	3.8
1	B	119[A]	HIS	3.8
1	B	130[A]	GLU	3.8
1	B	86	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	210[A]	VAL	3.7
1	B	355	GLY	3.6
1	B	342	ALA	3.6
1	B	393	GLY	3.6
1	B	3	ILE	3.6
1	B	253	VAL	3.6
1	A	150[A]	ARG	3.6
1	B	88[A]	GLU	3.6
1	B	373	ASP	3.6
1	B	316	LEU	3.5
1	B	266	PHE	3.5
1	B	391	LYS	3.5
1	B	350	LEU	3.5
1	B	11	PRO	3.5
1	B	356	PHE	3.5
1	A	384	THR	3.5
1	B	309	MET	3.4
1	B	335	THR	3.4
1	A	414	GLY	3.4
1	B	58	GLY	3.4
1	B	211	ILE	3.4
1	B	440	TYR	3.4
1	B	390	GLN	3.4
1	B	443	PHE	3.3
1	B	87	VAL	3.3
1	B	372	TYR	3.3
1	B	54	PHE	3.3
1	A	272	ASP	3.3
1	B	204	LEU	3.3
1	B	208	LEU	3.3
1	B	371	PRO	3.3
1	B	396	VAL	3.3
1	B	172	VAL	3.3
1	A	389	MET	3.2
1	A	9[A]	ARG	3.2
1	B	365	ASN	3.2
1	B	102	ILE	3.2
1	B	436	PHE	3.2
1	B	403	PRO	3.2
1	B	412	SER	3.1
1	B	5	TYR	3.1
1	A	376	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	3.1
1	B	83[A]	ARG	3.1
1	B	85	TYR	3.1
1	A	1	MET	3.1
1	A	371	PRO	3.1
1	A	56	PHE	3.1
1	B	374	PHE	3.1
1	B	80	ILE	3.1
1	B	360	TYR	3.0
1	B	78	CYS	3.0
1	A	386	ILE	3.0
1	A	53	SER	3.0
1	B	410	GLY	3.0
1	B	401	VAL	3.0
1	B	395	LEU	3.0
1	B	453	VAL	2.9
1	A	17[A]	ARG	2.9
1	B	358	PRO	2.9
1	A	270	GLU	2.9
1	B	289	THR	2.9
1	B	56	PHE	2.9
1	B	419	TYR	2.9
1	B	207	ILE	2.8
1	A	199	TYR	2.8
1	B	77	ILE	2.8
1	B	1	MET	2.8
1	B	95	TRP	2.8
1	B	232	ILE	2.8
1	B	439	THR	2.8
1	B	283	PHE	2.8
1	B	175	MET	2.7
1	B	337	GLU	2.7
1	B	315	ILE	2.7
1	B	300	VAL	2.7
1	A	130[A]	GLU	2.7
1	B	244	PHE	2.7
1	B	223[A]	ASN	2.7
1	A	273	TYR	2.7
1	B	71	TYR	2.7
1	B	301	LEU	2.7
1	B	221	ALA	2.7
1	A	413	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	10	LEU	2.7
1	B	392	ASP	2.6
1	A	252[A]	GLU	2.6
1	A	338	LYS	2.6
1	B	98	ASP	2.6
1	B	24	ILE	2.6
1	B	408	LEU	2.6
1	B	8	GLN	2.6
1	B	325	MET	2.6
1	B	308	TRP	2.5
1	A	426	ASP	2.5
1	B	91	GLY	2.5
1	B	205	THR	2.5
1	B	12	ILE	2.5
1	A	385	GLN	2.5
1	B	30	VAL	2.5
1	B	345	ALA	2.5
1	B	239	TYR	2.5
1	B	126	ASP	2.5
1	B	338	LYS	2.5
1	B	228	VAL	2.5
1	B	220	PHE	2.5
1	A	57	HIS	2.5
1	B	217	GLY	2.4
1	B	364	ILE	2.4
1	B	121	PHE	2.4
1	B	452	LEU	2.4
1	B	57	HIS	2.4
1	B	2	THR	2.4
1	B	197	THR	2.4
1	B	224	GLY	2.4
1	A	425	LEU	2.4
1	B	445	SER	2.4
1	B	447	ILE	2.4
1	B	89	ARG	2.4
1	B	104	LEU	2.4
1	B	26	VAL	2.4
1	B	151	VAL	2.4
1	A	2	THR	2.3
1	B	16	PHE	2.3
1	B	193	TYR	2.3
1	A	444	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	404	LEU	2.3
1	A	416	GLU	2.3
1	B	213	PRO	2.3
1	B	103	THR	2.3
1	B	75	ARG	2.3
1	B	76	ARG	2.3
1	B	418	PHE	2.3
1	A	239	TYR	2.3
1	B	320	ALA	2.3
1	B	336	ASN	2.3
1	B	341	ALA	2.3
1	A	206	ARG	2.3
1	B	400	THR	2.3
1	B	366	SER	2.3
1	B	386	ILE	2.3
1	B	425	LEU	2.3
1	B	60	GLU	2.3
1	B	407	ALA	2.2
1	B	29	GLN	2.2
1	B	307	GLN	2.2
1	B	218	ILE	2.2
1	B	278	SER	2.2
1	B	305	PHE	2.2
1	B	281	VAL	2.2
1	B	-1	ASN	2.2
1	B	227	ALA	2.2
1	B	361	TYR	2.2
1	B	25	HIS	2.2
1	A	176	ILE	2.2
1	B	334	PHE	2.2
1	B	107	ALA	2.2
1	B	182	ALA	2.2
1	B	363	ALA	2.2
1	A	115	GLY	2.2
1	B	258	LEU	2.2
1	B	177	SER	2.2
1	B	322	ARG	2.2
1	B	22	ASN	2.2
1	B	171	GLN	2.2
1	A	83	ARG	2.2
1	B	93	ASN	2.1
1	B	4	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLN	2.1
1	B	55	THR	2.1
1	B	347	LEU	2.1
1	B	252	GLU	2.1
1	B	276	GLN	2.1
1	A	108	LEU	2.1
1	A	51	THR	2.1
1	B	394	SER	2.1
1	A	112	VAL	2.1
1	A	244	PHE	2.1
1	B	100	ARG	2.1
1	B	226	HIS	2.1
1	B	257	HIS	2.1
1	B	212	ARG	2.0
1	A	286	GLY	2.0
1	B	168	PRO	2.0
1	B	214	TYR	2.0
1	A	356	PHE	2.0
1	A	200	GLY	2.0
1	B	47	LYS	2.0
1	B	274	ASP	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	CL	A	503	1/1	0.81	0.34	84,84,84,84	1
3	CL	B	504[A]	1/1	0.89	0.11	63,63,63,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HED	A	505	8/8	0.89	0.19	63,64,66,67	0
2	ZN	B	502	1/1	0.95	0.07	74,74,74,74	1
2	ZN	A	501	1/1	0.95	0.06	68,68,68,68	1

6.5 Other polymers [i](#)

There are no such residues in this entry.