



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:15 PM UTC

PDB ID : 1AIH / pdb_00001aih
Title : CATALYTIC DOMAIN OF BACTERIOPHAGE HP1 INTEGRASE
Authors : Hickman, A.B.; Waninger, S.; Scocca, J.J.; Dyda, F.
Deposited on : 1997-04-17
Resolution : 2.50 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

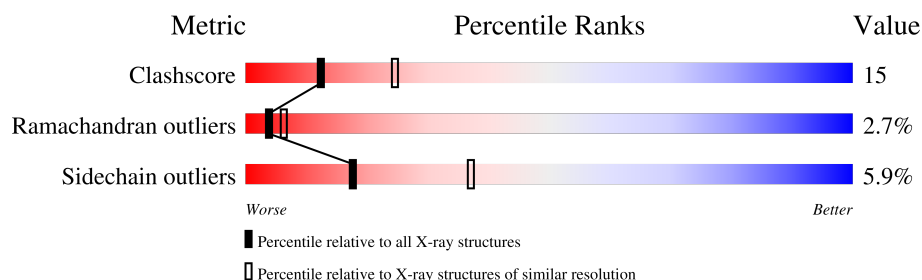
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	170	 65% 31% . .
1	B	170	 64% 31% . .
1	C	170	 55% 41% . .
1	D	170	 59% 38% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	111	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5545 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 HP1 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1349	854	235	252	8			
1	B	168	Total	C	N	O	S	0	0	0
			1330	845	233	244	8			
1	C	168	Total	C	N	O	S	0	0	0
			1330	845	233	244	8			
1	D	170	Total	C	N	O	S	0	0	0
			1339	849	232	250	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	ASP	LYS	conflict	UNP P21442
B	241	ASP	LYS	conflict	UNP P21442
C	241	ASP	LYS	conflict	UNP P21442
D	241	ASP	LYS	conflict	UNP P21442

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

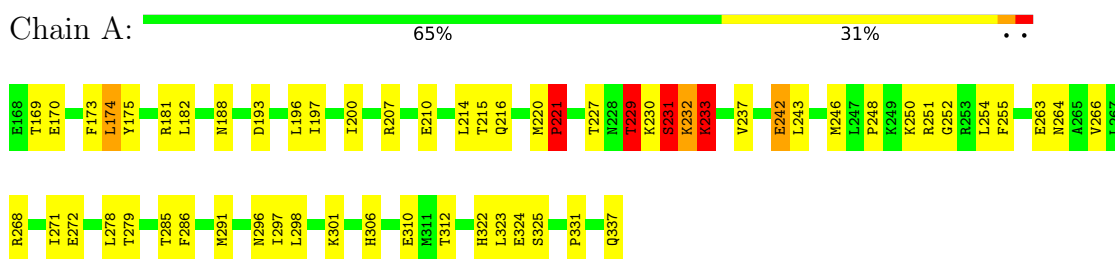
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	33	Total 33	O 33	0	0
4	C	39	Total 39	O 39	0	0
4	D	26	Total 26	O 26	0	0

3 Residue-property plots

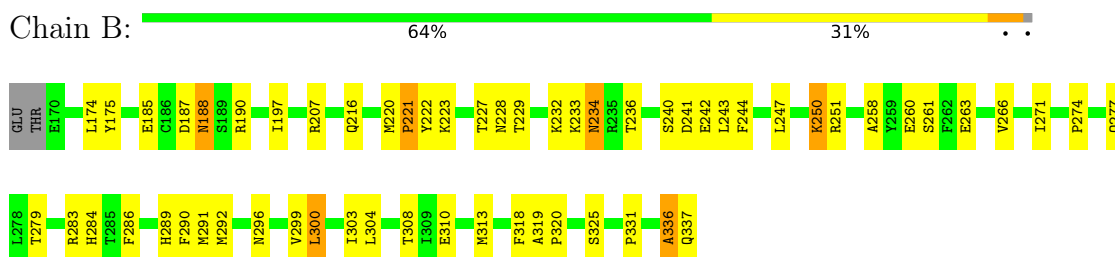
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

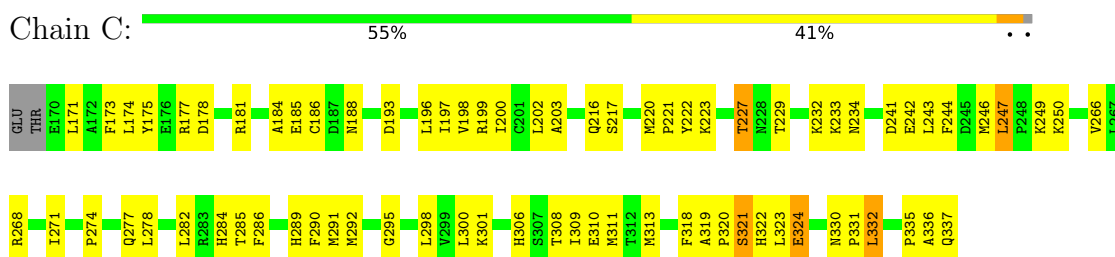
• Molecule 1: HP1 INTEGRASE



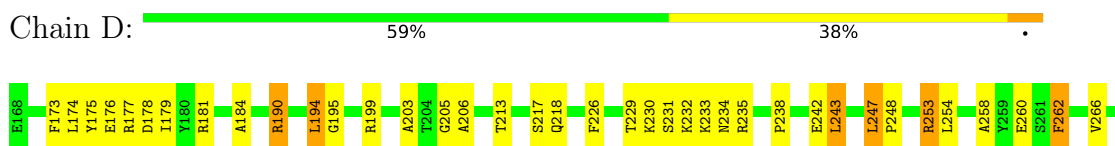
• Molecule 1: HP1 INTEGRASE

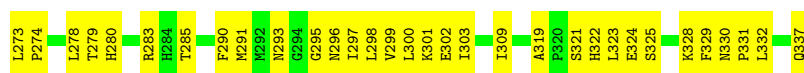


• Molecule 1: HP1 INTEGRASE



• Molecule 1: HP1 INTEGRASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.40Å 129.30Å 234.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.5 (30.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.209 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5545	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: MG, SO4

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	0.54	0/1378	1.00	5/1868 (0.3%)
1	B	0.49	0/1359	1.00	6/1841 (0.3%)
1	C	0.50	0/1359	0.94	2/1841 (0.1%)
1	D	0.47	0/1368	0.96	3/1856 (0.2%)
All	All	0.50	0/5464	0.98	16/7406 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	THR	N-CA-C	8.14	119.01	108.34
1	B	207	ARG	N-CA-C	-7.01	101.25	110.43
1	A	237	VAL	CA-C-N	6.37	126.32	119.76
1	A	237	VAL	C-N-CA	6.37	126.32	119.76
1	C	227	THR	N-CA-C	6.27	116.27	108.19
1	A	233	LYS	N-CA-C	-6.19	97.61	110.80
1	A	229	THR	N-CA-C	-5.91	100.16	109.50
1	D	194	LEU	N-CA-C	5.74	117.23	110.97
1	B	336	ALA	N-CA-C	5.65	117.13	110.97
1	A	170	GLU	N-CA-C	5.59	118.74	109.46
1	B	284	HIS	N-CA-C	-5.51	105.17	111.07
1	C	247	LEU	N-CA-C	5.50	116.75	109.93
1	D	323	LEU	N-CA-C	5.37	119.55	112.89
1	B	229	THR	N-CA-C	-5.29	104.50	111.96
1	B	216	GLN	N-CA-C	5.25	117.68	111.33
1	D	262	PHE	N-CA-C	-5.18	105.53	111.07

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	1349	0	1320	37	7
1	B	1330	0	1310	46	0
1	C	1330	0	1310	51	7
1	D	1339	0	1305	53	0
2	A	15	0	0	1	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	10	0	0	3	3
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	54	0	0	2	3
4	B	33	0	0	4	0
4	C	39	0	0	6	0
4	D	26	0	0	11	0
All	All	5545	0	5245	164	10

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 15.

All (164) 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:D:194:LEU:HD11	4:D:2120:HOH:O	1.80	0.81
1:A:227:THR:HA	1:A:233:LYS:O	1.82	0.80
1:A:323:LEU:HD12	1:B:299:VAL:HG13	1.67	0.74
1:D:262:PHE:HA	4:D:2120:HOH:O	1.87	0.73
1:A:251:ARG:HD2	2:A:109:SO4:O2	1.89	0.72
1:A:331:PRO:HG3	1:B:289:HIS:HB2	1.69	0.72
1:C:298:LEU:HD11	1:D:297:ILE:HB	1.73	0.68
1:D:285:THR:HG21	4:D:2124:HOH:O	1.94	0.67
1:B:228:ASN:CB	1:B:232:LYS:HA	2.25	0.67
1:D:174:LEU:HB2	4:D:2124:HOH:O	1.94	0.66
1:A:193:ASP:HB3	1:A:255:PHE:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2104:HOH:O	1:D:332:LEU:HD22	1.95	0.65
1:C:309:ILE:O	1:C:313:MET:HG2	1.96	0.65
1:A:337:GLN:HE22	1:B:175:TYR:HB3	1.62	0.65
1:C:324:GLU:HA	1:D:238:PRO:HG3	1.78	0.64
1:D:195:GLY:HA3	4:D:2121:HOH:O	1.98	0.62
1:C:174:LEU:HG	1:C:178:ASP:HB3	1.82	0.62
1:A:291:MET:HE1	1:A:297:ILE:HB	1.82	0.61
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.66	0.61
1:D:290:PHE:CE1	1:D:300:LEU:HB2	2.36	0.60
1:D:280:HIS:HD2	1:D:283:ARG:HD2	1.67	0.60
1:A:216:GLN:HG2	1:A:251:ARG:HD3	1.84	0.59
1:C:244:PHE:HA	1:C:247:LEU:HD12	1.84	0.59
1:D:179:ILE:HG12	4:D:2124:HOH:O	2.01	0.59
1:D:213:THR:HA	1:D:253:ARG:NH1	2.17	0.59
1:B:220:MET:HG2	1:B:221:PRO:HD2	1.83	0.59
1:D:296:ASN:OD1	1:D:298:LEU:HB2	2.03	0.59
1:B:223:LYS:NZ	1:B:236:THR:HG21	2.18	0.58
1:A:263:GLU:O	1:A:266:VAL:HG12	2.04	0.57
1:A:248:PRO:HG2	1:A:254:LEU:HD22	1.86	0.56
1:C:291:MET:HE3	1:C:291:MET:HA	1.88	0.56
1:B:283:ARG:HD3	2:B:106:SO4:O1	2.06	0.55
1:C:175:TYR:HB3	1:D:337:GLN:OE1	2.07	0.55
1:D:194:LEU:HD13	1:D:258:ALA:HB1	1.89	0.55
1:C:193:ASP:HA	1:C:196:LEU:HD23	1.90	0.54
1:D:242:GLU:HB3	4:D:2133:HOH:O	2.06	0.54
1:D:213:THR:HA	1:D:253:ARG:HH11	1.73	0.54
1:D:291:MET:HE3	1:D:319:ALA:HB2	1.89	0.54
1:B:292:MET:HG3	1:B:318:PHE:HB3	1.90	0.53
1:C:331:PRO:O	1:C:335:PRO:HG3	2.08	0.53
1:D:322:HIS:NE2	1:D:324:GLU:HB2	2.24	0.53
1:C:203:ALA:HA	1:D:330:ASN:HB2	1.91	0.52
1:A:286:PHE:HA	1:B:331:PRO:HG3	1.92	0.52
1:A:174:LEU:N	1:A:174:LEU:HD22	2.26	0.51
1:D:248:PRO:HG2	1:D:254:LEU:HD22	1.92	0.51
1:C:249:LYS:HD3	4:C:2098:HOH:O	2.10	0.51
1:A:220:MET:HG2	1:A:221:PRO:HD2	1.92	0.50
1:D:190:ARG:HD3	2:D:111:SO4:O4	2.11	0.50
1:D:260:GLU:HB2	4:D:2119:HOH:O	2.10	0.50
1:B:185:GLU:CD	1:C:268:ARG:HG2	2.35	0.50
1:C:185:GLU:OE1	1:C:268:ARG:HD2	2.11	0.50
1:A:196:LEU:O	1:A:200:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:O	1:C:197:ILE:HG13	2.12	0.50
1:B:337:GLN:HA	1:B:337:GLN:OE1	2.10	0.50
1:C:266:VAL:HG21	1:C:278:LEU:HD11	1.94	0.50
1:D:253:ARG:HG2	4:D:2117:HOH:O	2.11	0.50
1:A:337:GLN:NE2	1:B:175:TYR:HB3	2.26	0.50
1:D:218:GLN:NE2	4:D:2116:HOH:O	2.45	0.50
1:D:301:LYS:HE2	1:D:309:ILE:N	2.27	0.49
1:B:190:ARG:HH11	1:B:190:ARG:HA	1.78	0.49
1:B:336:ALA:O	1:B:337:GLN:HB2	2.13	0.49
1:C:274:PRO:HB2	1:C:277:GLN:HG3	1.94	0.49
1:A:331:PRO:HG2	1:B:286:PHE:HA	1.94	0.49
1:A:193:ASP:CB	1:A:255:PHE:HB3	2.42	0.48
1:A:263:GLU:HA	1:A:278:LEU:HD21	1.95	0.48
1:B:290:PHE:CD2	1:B:300:LEU:HG	2.47	0.48
1:A:296:ASN:OD1	1:A:298:LEU:HB2	2.13	0.48
1:B:266:VAL:HG13	1:B:271:ILE:HB	1.94	0.48
1:A:175:TYR:HB3	1:B:337:GLN:HE22	1.79	0.48
1:A:173:PHE:HB2	1:A:285:THR:HA	1.96	0.47
1:A:230:LYS:O	1:A:232:LYS:N	2.47	0.47
1:C:220:MET:HB2	1:C:223:LYS:HG3	1.95	0.47
1:D:177:ARG:HG3	1:D:178:ASP:N	2.29	0.47
1:D:325:SER:HB2	1:D:329:PHE:CE2	2.50	0.47
1:A:207:ARG:HB2	1:A:210:GLU:HG3	1.97	0.47
1:C:203:ALA:HB2	4:C:2104:HOH:O	2.14	0.47
1:B:260:GLU:HA	1:B:263:GLU:OE1	2.14	0.47
1:B:244:PHE:HA	1:B:247:LEU:HD12	1.97	0.47
1:B:300:LEU:HD22	1:B:304:LEU:HG	1.96	0.47
1:B:187:ASP:HB3	4:B:2071:HOH:O	2.15	0.47
1:C:324:GLU:H	1:C:324:GLU:CD	2.23	0.47
1:D:194:LEU:HA	1:D:194:LEU:HD12	1.53	0.47
1:A:169:THR:HG21	4:A:2010:HOH:O	2.14	0.47
1:C:171:LEU:HD22	1:C:284:HIS:CE1	2.50	0.47
1:C:332:LEU:HD11	1:D:199:ARG:HG2	1.97	0.47
1:D:299:VAL:O	1:D:303:ILE:HG13	2.15	0.47
1:D:266:VAL:HG21	1:D:278:LEU:HD11	1.96	0.47
1:A:322:HIS:HB2	1:A:324:GLU:OE1	2.15	0.46
1:D:205:GLY:O	1:D:283:ARG:HB2	2.15	0.46
1:A:331:PRO:CG	1:B:286:PHE:HA	2.45	0.46
1:A:337:GLN:HA	1:A:337:GLN:OE1	2.14	0.46
1:C:323:LEU:HD23	1:C:323:LEU:H	1.80	0.46
1:C:330:ASN:HB2	1:D:203:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LYS:HZ3	1:B:236:THR:HG21	1.80	0.46
1:D:322:HIS:HB3	4:D:2106:HOH:O	2.16	0.46
1:D:181:ARG:O	1:D:184:ALA:HB3	2.16	0.46
1:B:308:THR:HB	1:B:310:GLU:OE1	2.14	0.46
1:A:214:LEU:HD23	1:A:254:LEU:HD12	1.98	0.46
1:C:308:THR:OG1	1:C:311:MET:HG3	2.15	0.46
1:C:220:MET:HE2	4:C:2139:HOH:O	2.16	0.45
4:C:2104:HOH:O	1:D:332:LEU:HB2	2.16	0.45
1:D:290:PHE:CE1	1:D:295:GLY:HA3	2.52	0.45
1:B:197:ILE:HD12	1:B:258:ALA:HB3	1.98	0.45
1:B:242:GLU:CD	1:B:242:GLU:H	2.24	0.45
1:A:193:ASP:O	1:A:197:ILE:HG13	2.15	0.45
1:A:266:VAL:HG22	1:A:271:ILE:HB	1.97	0.45
1:C:216:GLN:OE1	1:C:249:LYS:HA	2.17	0.45
1:C:292:MET:HG3	1:C:318:PHE:HB3	1.99	0.45
1:A:310:GLU:HB2	4:A:2006:HOH:O	2.18	0.44
1:B:240:SER:HB2	4:B:2050:HOH:O	2.17	0.44
1:B:233:LYS:O	1:B:234:ASN:HB2	2.18	0.44
1:C:173:PHE:HB2	1:C:285:THR:HA	2.00	0.44
1:D:206:ALA:HB2	1:D:226:PHE:CZ	2.52	0.44
1:A:215:THR:HA	1:A:252:GLY:O	2.16	0.44
1:D:190:ARG:HB2	2:D:111:SO4:O4	2.18	0.44
1:C:266:VAL:HG13	1:C:271:ILE:HB	2.00	0.44
1:B:291:MET:HE3	1:B:319:ALA:HB2	2.00	0.43
1:B:274:PRO:HG2	4:B:2002:HOH:O	2.19	0.43
1:B:296:ASN:HB3	1:B:299:VAL:HG23	2.00	0.43
1:C:289:HIS:CG	1:D:331:PRO:HB3	2.53	0.43
1:B:277:GLN:NE2	1:B:277:GLN:HA	2.33	0.43
1:C:298:LEU:O	1:C:301:LYS:HB3	2.18	0.43
1:A:242:GLU:O	1:A:246:MET:HG3	2.19	0.43
1:C:202:LEU:HG	1:C:282:LEU:HD22	2.01	0.43
1:D:243:LEU:O	1:D:247:LEU:HD22	2.17	0.43
1:D:273:LEU:HA	1:D:274:PRO:HD3	1.87	0.43
1:A:301:LYS:HG3	1:A:306:HIS:HB2	2.00	0.43
1:C:313:MET:SD	1:D:298:LEU:HD21	2.58	0.43
1:C:321:SER:O	1:C:322:HIS:HB2	2.18	0.43
1:A:323:LEU:C	1:A:325:SER:H	2.26	0.43
1:C:246:MET:HE2	1:C:246:MET:HB3	1.78	0.43
1:D:173:PHE:HB2	1:D:285:THR:HA	2.00	0.42
1:B:319:ALA:HA	1:B:320:PRO:HD3	1.93	0.42
1:C:186:CYS:SG	1:C:198:VAL:HG21	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PHE:CE1	1:C:300:LEU:HB2	2.54	0.42
1:C:306:HIS:HB3	1:C:311:MET:HB2	2.02	0.42
1:C:199:ARG:O	1:C:200:ILE:C	2.62	0.42
1:B:299:VAL:O	1:B:303:ILE:HG13	2.20	0.42
1:B:188:ASN:ND2	1:C:188:ASN:O	2.53	0.42
1:B:290:PHE:HD2	1:B:300:LEU:HG	1.85	0.42
1:C:222:TYR:CE1	1:C:241:ASP:HA	2.54	0.42
1:D:190:ARG:NH1	2:D:111:SO4:O3	2.53	0.42
1:D:253:ARG:HG2	1:D:253:ARG:NH1	2.33	0.42
1:B:228:ASN:HA	1:B:233:LYS:H	1.85	0.42
1:B:222:TYR:CE1	1:B:241:ASP:HA	2.55	0.41
1:B:277:GLN:HA	1:B:277:GLN:HE21	1.85	0.41
1:C:337:GLN:OE1	1:D:175:TYR:HD1	2.02	0.41
1:A:331:PRO:CD	1:B:286:PHE:HA	2.50	0.41
1:C:290:PHE:CE1	1:C:295:GLY:HA3	2.56	0.41
1:D:280:HIS:CD2	1:D:283:ARG:HD2	2.51	0.41
1:B:310:GLU:O	1:B:313:MET:HB2	2.20	0.41
1:D:176:GLU:HA	1:D:179:ILE:HD12	2.02	0.41
1:B:185:GLU:OE2	1:C:268:ARG:HG2	2.21	0.41
1:C:336:ALA:HB2	1:D:293:ASN:OD1	2.21	0.41
1:C:337:GLN:OE1	1:C:337:GLN:HA	2.21	0.41
1:B:325:SER:HB3	4:B:2046:HOH:O	2.20	0.41
1:B:274:PRO:HD2	1:B:277:GLN:HG3	2.04	0.40
1:A:229:THR:C	1:A:231:SER:N	2.75	0.40
1:B:250:LYS:HE2	1:B:251:ARG:O	2.21	0.40
1:C:319:ALA:C	1:C:321:SER:H	2.29	0.40
1:C:321:SER:HB3	4:C:2109:HOH:O	2.21	0.40
1:C:286:PHE:HA	1:D:331:PRO:HG3	2.02	0.40
1:C:310:GLU:O	1:C:313:MET:HB2	2.22	0.40
1:C:227:THR:HG22	1:C:234:ASN:CG	2.46	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:SO4:O2	4:A:2008:HOH:O[2_465]	1.23	0.97
1:A:188:ASN:O	1:C:188:ASN:OD1[3_555]	1.57	0.63
1:A:188:ASN:OD1	1:C:188:ASN:ND2[3_555]	1.64	0.56
1:A:181:ARG:NH2	1:C:181:ARG:NH2[3_555]	1.84	0.36
1:A:272:GLU:OE1	1:C:177:ARG:NH2[3_555]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:OE2	1:C:177:ARG:NE[3_555]	1.93	0.27
2:D:111:SO4:S	4:A:2008:HOH:O[2_465]	2.00	0.20
1:A:268:ARG:CG	1:C:184:ALA:CB[3_555]	2.03	0.17
2:D:111:SO4:O1	4:A:2008:HOH:O[2_465]	2.12	0.08
1:A:268:ARG:CD	1:C:184:ALA:O[3_555]	2.19	0.01

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	168/170 (99%)	155 (92%)	9 (5%)	4 (2%)	4	8
1	B	166/170 (98%)	151 (91%)	11 (7%)	4 (2%)	4	8
1	C	166/170 (98%)	150 (90%)	12 (7%)	4 (2%)	4	8
1	D	168/170 (99%)	147 (88%)	15 (9%)	6 (4%)	2	3
All	All	668/680 (98%)	603 (90%)	47 (7%)	18 (3%)	4	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	SER
1	C	233	LYS
1	D	321	SER
1	A	232	LYS
1	B	188	ASN
1	B	234	ASN
1	B	250	LYS
1	D	230	LYS
1	D	232	LYS
1	A	221	PRO
1	C	229	THR
1	D	229	THR

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Mol	Chain	Res	Type
1	D	233	LYS
1	C	321	SER
1	D	234	ASN
1	A	233	LYS
1	B	221	PRO
1	C	320	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	146/150 (97%)	135 (92%)	11 (8%)	12	26
1	B	143/150 (95%)	138 (96%)	5 (4%)	32	58
1	C	143/150 (95%)	135 (94%)	8 (6%)	19	39
1	D	144/150 (96%)	134 (93%)	10 (7%)	14	30
All	All	576/600 (96%)	542 (94%)	34 (6%)	18	37

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	182	LEU
1	A	221	PRO
1	A	229	THR
1	A	231	SER
1	A	242	GLU
1	A	243	LEU
1	A	250	LYS
1	A	264	ASN
1	A	279	THR
1	A	312	THR
1	B	174	LEU
1	B	243	LEU
1	B	261	SER
1	B	279	THR

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Mol	Chain	Res	Type
1	B	300	LEU
1	C	217	SER
1	C	221	PRO
1	C	232	LYS
1	C	242	GLU
1	C	243	LEU
1	C	250	LYS
1	C	324	GLU
1	C	332	LEU
1	D	190	ARG
1	D	217	SER
1	D	231	SER
1	D	235	ARG
1	D	243	LEU
1	D	247	LEU
1	D	253	ARG
1	D	279	THR
1	D	302	GLU
1	D	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	B	188	ASN
1	B	216	GLN
1	B	218	GLN
1	B	280	HIS
1	B	306	HIS
1	C	188	ASN
1	D	188	ASN
1	D	216	GLN
1	D	234	ASN
1	D	280	HIS

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 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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	$\# Z > 2$
2	SO4	B	106	-	4,4,4	0.83	0	6,6,6	0.08	0
2	SO4	C	107	-	4,4,4	0.81	0	6,6,6	0.06	0
2	SO4	D	111	-	4,4,4	0.72	0	6,6,6	0.18	0
2	SO4	D	108	-	4,4,4	0.81	0	6,6,6	0.10	0
2	SO4	A	112	-	4,4,4	0.77	0	6,6,6	0.12	0
2	SO4	A	105	-	4,4,4	0.75	0	6,6,6	0.13	0
2	SO4	A	109	-	4,4,4	0.71	0	6,6,6	0.10	0
2	SO4	B	110	-	4,4,4	0.73	0	6,6,6	0.13	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	106	SO4	1	0
2	D	111	SO4	3	3
2	A	109	SO4	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

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.