



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AIH  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

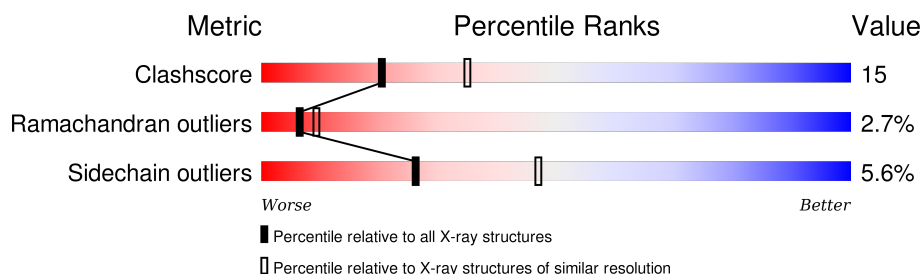
# 1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	C	170	
1	D	170	

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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

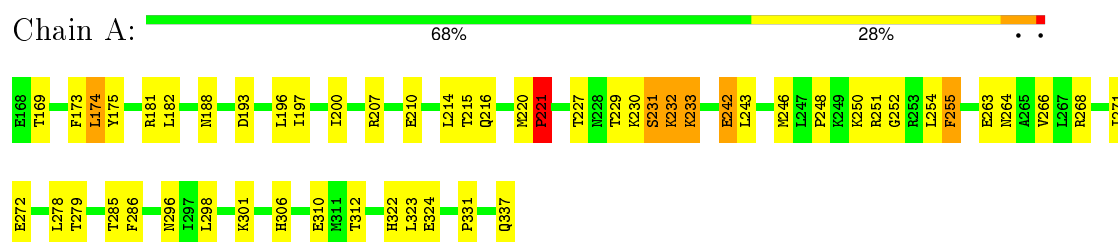
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	33	Total 33	O 33	0	0
4	C	39	Total 39	O 39	0	0
4	D	26	Total 26	O 26	0	0

### 3 Residue-property plots

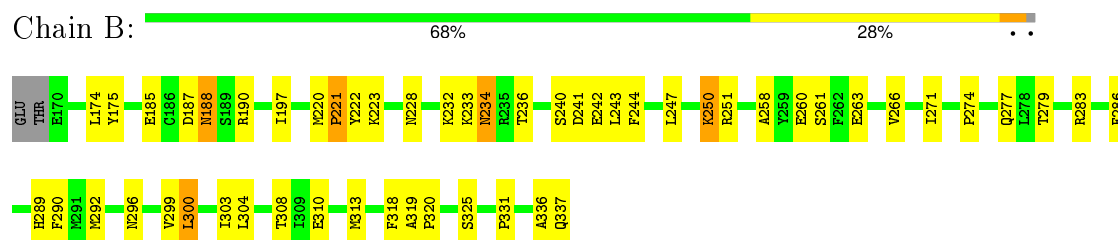
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

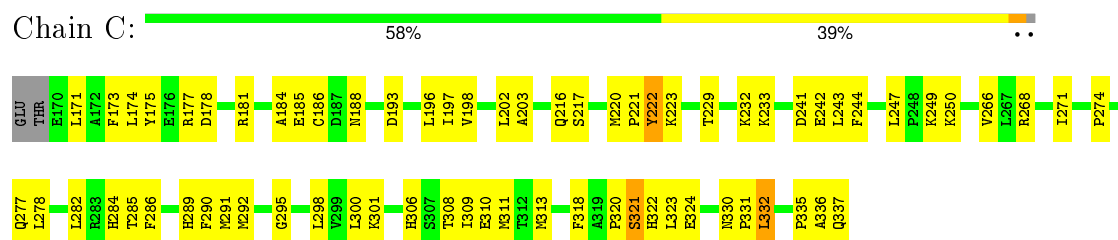
#### • Molecule 1: HP1 INTEGRASE



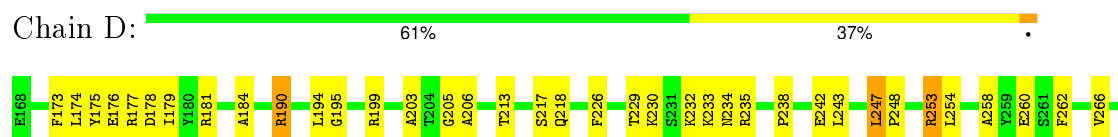
#### • Molecule 1: HP1 INTEGRASE



#### • Molecule 1: HP1 INTEGRASE



#### • Molecule 1: HP1 INTEGRASE



L273	F274		L278	T279	H280		H283	H284	T285		F290	H291	H292	H293	H294	G295	H296	L297	L298	V299	L300	K301	E302	L303		T309		S321	H322	L323	E324	S325		F329	H330	P331	L332		Q337
------	------	--	------	------	------	--	------	------	------	--	------	------	------	------	------	------	------	------	------	------	------	------	------	------	--	------	--	------	------	------	------	------	--	------	------	------	------	--	------



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.40 Å   129.30 Å   234.20 Å 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 <sup>2</sup> )	48.0	wwPDB-VP

## 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: 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	0.45	0/1378	0.66	0/1868
1	B	0.42	0/1359	0.64	0/1841
1	C	0.41	0/1359	0.61	0/1841
1	D	0.38	0/1368	0.61	0/1856
All	All	0.42	0/5464	0.63	0/7406

There are no bond length outliers.

There are no bond angle outliers.

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	1349	0	1320	34	7
1	B	1330	0	1310	45	0
1	C	1330	0	1310	47	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
4	D	26	0	0	11	0
All	All	5545	0	5245	155	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 (155) 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
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: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:D:296:ASN:OD1	1:D:298:LEU:HB2	2.03	0.59
1:B:220:MET:HG2	1:B:221:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:283:ARG:HD3	2:B:106:SO4:O1	2.06	0.55
1:D:194:LEU:HD13	1:D:258:ALA:HB1	1.89	0.55
1:C:175:TYR:HB3	1:D:337:GLN:OE1	2.07	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: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:HD22	1:A:174:LEU:N	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:D:260:GLU:HB2	4:D:2119:HOH:O	2.10	0.50
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:C:185:GLU:OE1	1:C:268:ARG:HD2	2.11	0.50
1:C:193:ASP:O	1:C:197:ILE:HG13	2.12	0.50
1:A:196:LEU:O	1:A:200:ILE:HG13	2.12	0.50
1:B:337:GLN:OE1	1:B:337:GLN:HA	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:337:GLN:OE1	1:A:337:GLN:HA	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:203:ALA:HB2	4:C:2104:HOH:O	2.14	0.47
1:A:207:ARG:HB2	1:A:210:GLU:HG3	1.97	0.47
1:B:260:GLU:HA	1:B:263:GLU:OE1	2.14	0.47
1:B:300:LEU:HD22	1:B:304:LEU:HG	1.96	0.47
1:B:244:PHE:HA	1:B:247:LEU:HD12	1.97	0.47
1:D:194:LEU:HD12	1:D:194:LEU:HA	1.53	0.47
1:B:187:ASP:HB3	4:B:2071:HOH:O	2.15	0.47
1:C:332:LEU:HD11	1:D:199:ARG:HG2	1.97	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: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:D:205:GLY:O	1:D:283:ARG:HB2	2.15	0.46
1:A:322:HIS:HB2	1:A:324:GLU:OE1	2.15	0.46
1:A:331:PRO:CG	1:B:286:PHE:HA	2.45	0.46
1:C:330:ASN:HB2	1:D:203:ALA:HA	1.96	0.46
1:C:323:LEU:HD23	1:C:323:LEU:H	1.80	0.46
1:C:291:MET:HE3	1:C:291:MET:HA	1.97	0.46
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:B:185:GLU:CD	1:C:268:ARG:HG2	2.35	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
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: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:D:206:ALA:HB2	1:D:226:PHE:CZ	2.52	0.44
1:C:173:PHE:HB2	1:C:285:THR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HA	1:A:252:GLY:O	2.16	0.44
1:C:336:ALA:CB	1:D:292:MET:HE2	2.48	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: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:274:PRO:HG2	4:B:2002:HOH:O	2.19	0.43
1:C:298:LEU:O	1:C:301:LYS:HB3	2.18	0.43
1:B:277:GLN:HA	1:B:277:GLN:NE2	2.33	0.43
1:D:273:LEU:HA	1:D:274:PRO:HD3	1.87	0.43
1:C:202:LEU:HG	1:C:282:LEU:HD22	2.01	0.43
1:A:242:GLU:O	1:A:246:MET:HG3	2.19	0.43
1:D:243:LEU:O	1:D:247:LEU:HD22	2.17	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:301:LYS:HG3	1:A:306:HIS:HB2	2.00	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:306:HIS:HB3	1:C:311:MET:HB2	2.02	0.42
1:C:290:PHE:CE1	1:C:300:LEU:HB2	2.54	0.42
1:C:186:CYS:SG	1:C:198:VAL:HG21	2.60	0.42
1:C:324:GLU:H	1:C:324:GLU:CD	2.23	0.42
1:B:299:VAL:O	1:B:303:ILE:HG13	2.20	0.42
1:D:253:ARG:HG2	1:D:253:ARG:NH1	2.33	0.42
1:D:190:ARG:NH1	2:D:111:SO4:O3	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:B:188:ASN:ND2	1:C:188:ASN:O	2.53	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:HE21	1:B:277:GLN:HA	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:D:280:HIS:CD2	1:D:283:ARG:HD2	2.51	0.41
1:C:290:PHE:CE1	1:C:295:GLY:HA3	2.56	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:HA	1:C:337:GLN:OE1	2.21	0.41
1:B:325:SER:HB3	4:B:2046:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:PRO:HD2	1:B:277:GLN:HG3	2.04	0.40
1:B:242:GLU:CD	1:B:242:GLU:H	2.24	0.40
1:C:321:SER:HB3	4:C:2109:HOH:O	2.21	0.40
1:B:250:LYS:HE2	1:B:251:ARG:O	2.21	0.40
1:C:310:GLU:O	1:C:313:MET:HB2	2.22	0.40
1:C:286:PHE:HA	1:D:331:PRO:HG3	2.02	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
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%)	7	11
1	B	166/170 (98%)	151 (91%)	11 (7%)	4 (2%)	7	11
1	C	166/170 (98%)	150 (90%)	12 (7%)	4 (2%)	7	11
1	D	168/170 (99%)	147 (88%)	15 (9%)	6 (4%)	4	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	668/680 (98%)	603 (90%)	47 (7%)	18 (3%)	6 9

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
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%)	134 (92%)	12 (8%)	14 27
1	B	143/150 (95%)	138 (96%)	5 (4%)	43 70
1	C	143/150 (95%)	135 (94%)	8 (6%)	26 47
1	D	144/150 (96%)	137 (95%)	7 (5%)	31 55
All	All	576/600 (96%)	544 (94%)	32 (6%)	26 47



All (32) 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	255	PHE
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
1	B	300	LEU
1	C	217	SER
1	C	221	PRO
1	C	222	TYR
1	C	232	LYS
1	C	242	GLU
1	C	243	LEU
1	C	250	LYS
1	C	332	LEU
1	D	190	ARG
1	D	217	SER
1	D	235	ARG
1	D	247	LEU
1	D	253	ARG
1	D	279	THR
1	D	302	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	C	188	ASN
1	D	188	ASN
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 ⓘ

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 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	A	105	-	4,4,4	1.10	0	6,6,6	0.14	0
2	SO4	A	109	-	4,4,4	0.97	0	6,6,6	0.10	0
2	SO4	A	112	-	4,4,4	1.00	0	6,6,6	0.13	0
2	SO4	B	106	-	4,4,4	1.21	0	6,6,6	0.08	0
2	SO4	B	110	-	4,4,4	1.04	0	6,6,6	0.12	0
2	SO4	C	107	-	4,4,4	1.15	0	6,6,6	0.07	0
2	SO4	D	108	-	4,4,4	1.15	0	6,6,6	0.10	0
2	SO4	D	111	-	4,4,4	0.97	0	6,6,6	0.19	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
2	SO4	A	105	-	-	0/0/0/0	0/0/0/0
2	SO4	A	109	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	112	-	-	0/0/0/0	0/0/0/0
2	SO4	B	106	-	-	0/0/0/0	0/0/0/0
2	SO4	B	110	-	-	0/0/0/0	0/0/0/0
2	SO4	C	107	-	-	0/0/0/0	0/0/0/0
2	SO4	D	108	-	-	0/0/0/0	0/0/0/0
2	SO4	D	111	-	-	0/0/0/0	0/0/0/0

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	A	109	SO4	1	0
2	B	106	SO4	1	0
2	D	111	SO4	3	3

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.