



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 PM GMT

PDB ID : 4QJ1  
Title : Co-crystal structure of the catalytic domain of the inosine monophosphate dehydrogenase from *Cryptosporidium parvum* with inhibitor N109  
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)  
Deposited on : 2014-06-03  
Resolution : 2.42 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

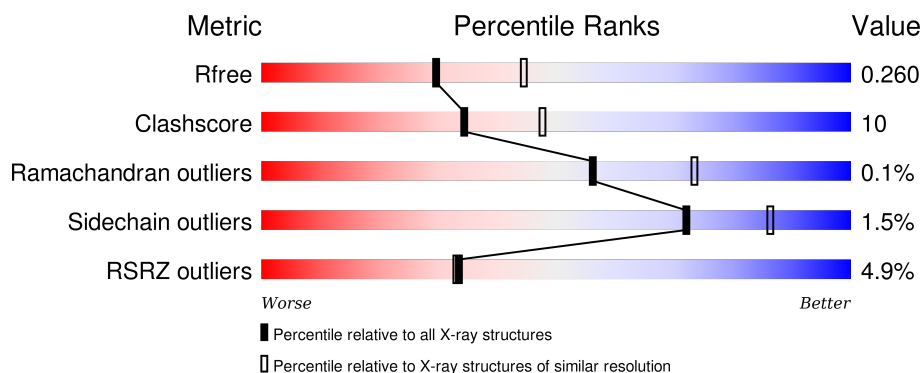
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	361	<div> <div>5%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
1	B	361	<div> <div>5%</div> <div>80%</div> <div>14%</div> <div>• •</div> </div>
1	C	361	<div> <div>4%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	D	361	<div> <div>4%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>

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
3	N09	A	502	-	-	-	X
3	N09	B	502	-	-	-	X
3	N09	B	503	-	-	-	X
4	ACY	B	504	-	-	-	X
5	EDO	C	502	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10616 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.

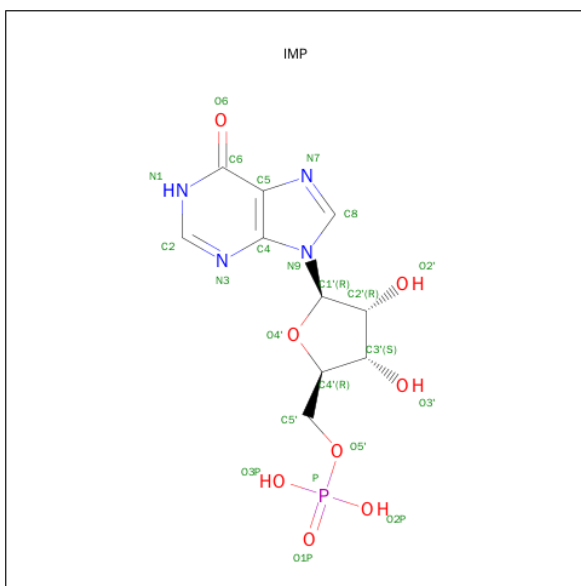
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	2	0
			2554	1606	435	497	16			
1	B	345	Total	C	N	O	S	0	2	0
			2570	1616	437	500	17			
1	C	345	Total	C	N	O	S	0	1	0
			2566	1613	437	499	17			
1	D	346	Total	C	N	O	S	0	1	0
			2574	1617	439	501	17			

There are 20 discrepancies between the modelled and reference sequences:

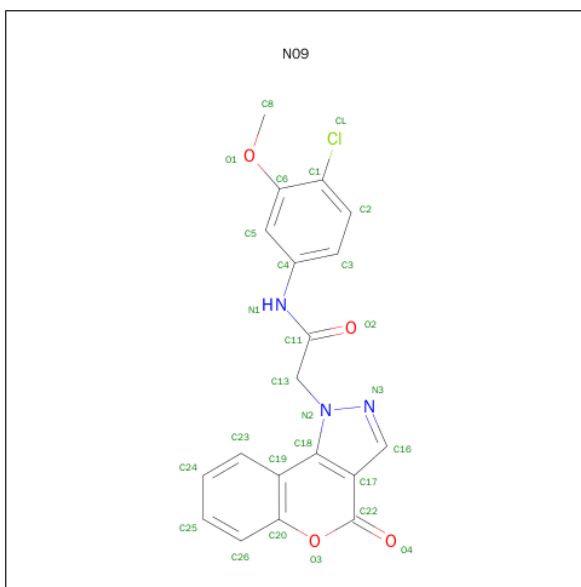
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
A	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
A	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
A	90	SER	LYS	ENGINEERED MUTATION	UNP Q8T6T2
A	92	GLY	ARG	ENGINEERED MUTATION	UNP Q8T6T2
B	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
B	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
B	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
B	90	SER	LYS	ENGINEERED MUTATION	UNP Q8T6T2
B	92	GLY	ARG	ENGINEERED MUTATION	UNP Q8T6T2
C	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
C	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
C	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
C	90	SER	LYS	ENGINEERED MUTATION	UNP Q8T6T2
C	92	GLY	ARG	ENGINEERED MUTATION	UNP Q8T6T2
D	-2	SER	-	EXPRESSION TAG	UNP Q8T6T2
D	-1	ASN	-	EXPRESSION TAG	UNP Q8T6T2
D	0	ALA	-	EXPRESSION TAG	UNP Q8T6T2
D	90	SER	LYS	ENGINEERED MUTATION	UNP Q8T6T2
D	92	GLY	ARG	ENGINEERED MUTATION	UNP Q8T6T2

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula:  $C_{10}H_{13}N_4O_8P$ ).



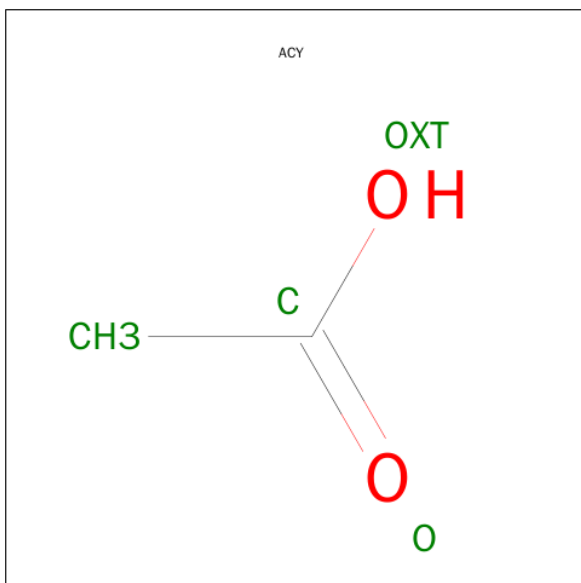
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is N-(4-CHLORO-3-METHOXYPHENYL)-2-(4-OXOCHROMENO[4,3-C]PYR AZOL-1(4H)-YL)ACETAMIDE (three-letter code: N09) (formula:  $C_{19}H_{14}ClN_3O_4$ ).



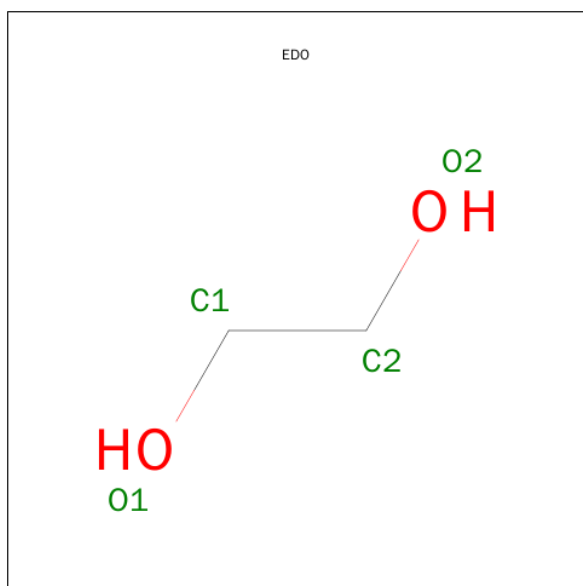
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		
3	D	1	Total	C	Cl	N	O	0	0
			27	19	1	3	4		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



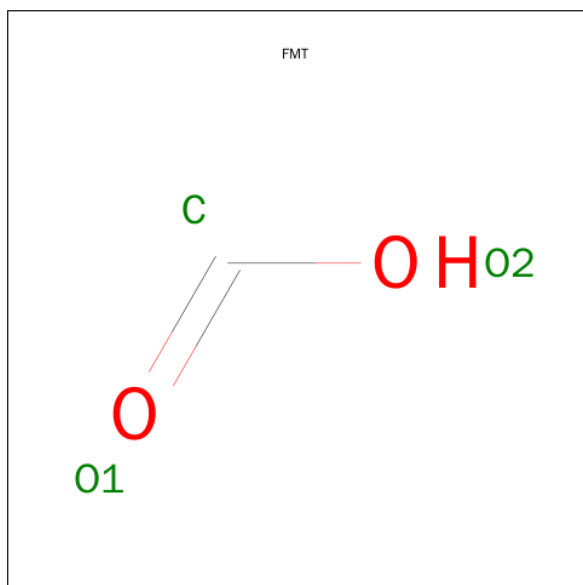
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $CH_2O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			3	1	2		

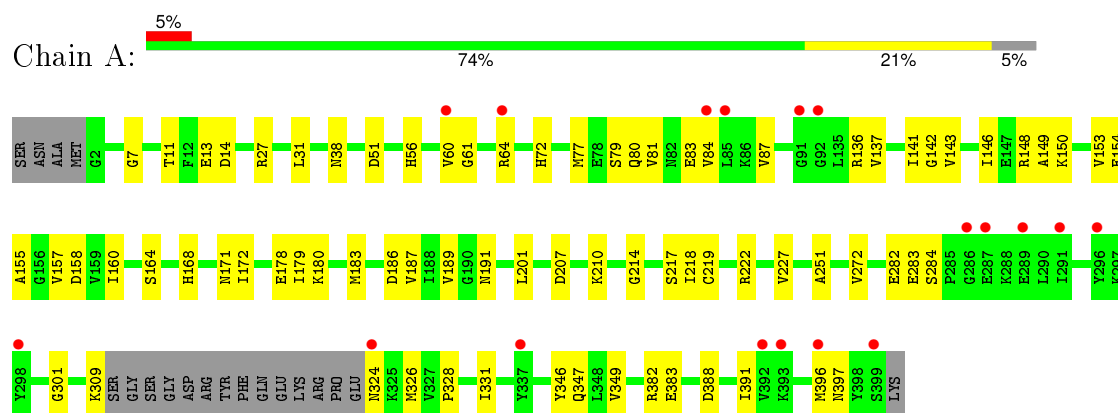
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	34	Total	O	0	0
			34	34		
7	B	31	Total	O	0	0
			31	31		
7	C	26	Total	O	0	0
			26	26		
7	D	42	Total	O	0	0
			42	42		

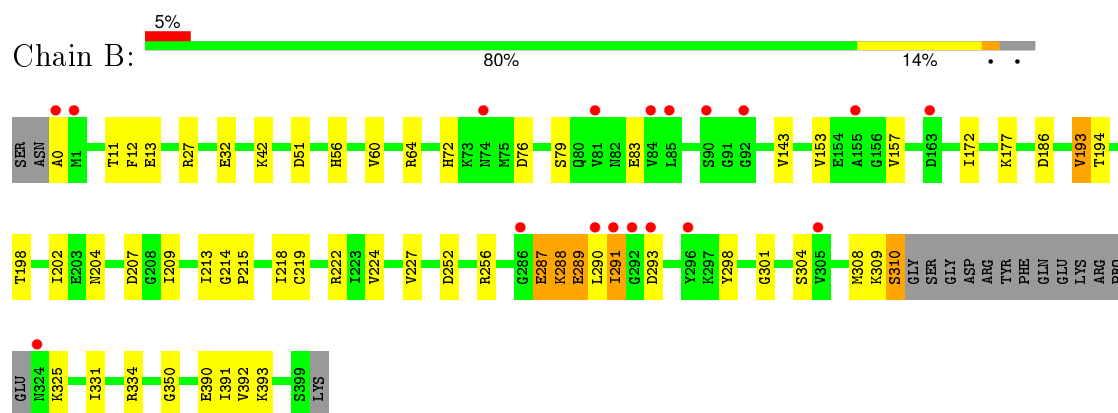
### 3 Residue-property plots

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.

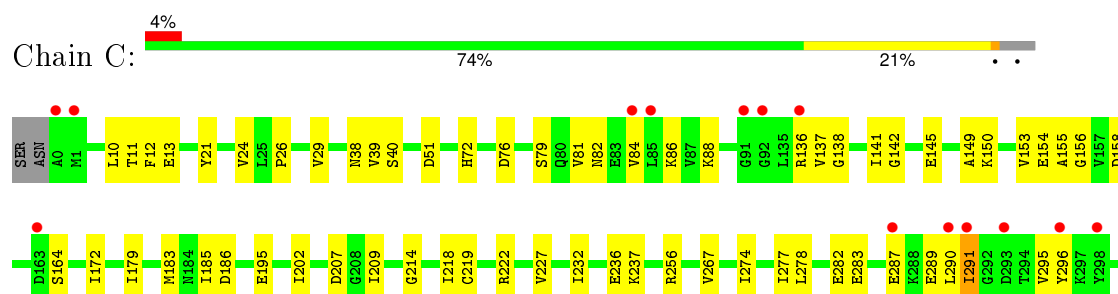
#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase



#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase



#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.41Å 92.34Å 91.91Å 90.00° 104.24° 90.00°	Depositor
Resolution (Å)	39.59 – 2.42 46.17 – 2.42	Depositor EDS
% Data completeness (in resolution range)	88.6 (39.59-2.42) 88.7 (46.17-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, $R_{free}$	0.202 , 0.258 0.211 , 0.260	Depositor DCC
$R_{free}$ test set	2555 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.9	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49988 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ACY, IMP, FMT, N09, EDO

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	0.49	0/2580	0.69	0/3472
1	B	0.45	0/2599	0.67	0/3497
1	C	0.50	0/2592	0.69	1/3487 (0.0%)
1	D	0.51	1/2600 (0.0%)	0.71	1/3498 (0.0%)
All	All	0.49	1/10371 (0.0%)	0.69	2/13954 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	215	PRO	N-CD	5.18	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	GLY	C-N-CD	5.40	139.74	128.40
1	C	334	ARG	CA-CB-CG	-5.11	102.16	113.40

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	2554	0	2654	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2570	0	2677	48	0
1	C	2566	0	2670	58	0
1	D	2574	0	2676	63	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	27	0	14	0	0
3	B	54	0	28	1	0
3	D	27	0	14	2	0
4	B	4	0	3	0	0
5	C	4	0	6	2	0
5	D	8	0	12	2	0
6	D	3	0	1	0	0
7	A	34	0	0	1	0
7	B	31	0	0	2	0
7	C	26	0	0	0	0
7	D	42	0	0	4	0
All	All	10616	0	10799	212	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 10.

All (212) 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:B:304:SER:O	1:B:308:MET:HG3	1.82	0.80
1:A:331:ILE:HD13	1:D:391:ILE:HG12	1.63	0.78
1:A:391:ILE:HG12	1:B:331:ILE:HD13	1.65	0.76
1:D:291:ILE:HD12	1:D:334:ARG:NH1	1.99	0.76
1:A:347:GLN:HG3	1:A:396:MET:HG2	1.68	0.75
1:A:141:ILE:HG12	1:A:160:ILE:HD11	1.69	0.74
1:C:11:THR:HG22	1:C:12:PHE:H	1.52	0.74
1:D:291:ILE:HD12	1:D:334:ARG:HH11	1.51	0.73
1:D:13:GLU:OE2	1:D:256:ARG:NH1	2.21	0.73
1:B:287:GLU:HG3	1:B:288:LYS:N	2.06	0.70
1:D:295:VAL:HG23	1:D:337:TYR:HB3	1.75	0.69
1:C:391:ILE:HG12	1:D:331:ILE:HD13	1.76	0.68
1:B:291:ILE:HG13	1:B:334:ARG:NH1	2.09	0.67
1:B:391:ILE:HG12	1:C:331:ILE:HD13	1.75	0.67
1:A:309:LYS:HE2	1:A:324:ASN:OD1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:OE2	1:C:256:ARG:NH1	2.28	0.66
1:A:219:CYS:SG	2:A:501:IMP:H2	2.35	0.66
1:A:186:ASP:HA	1:A:207:ASP:OD2	1.96	0.65
1:A:56:HIS:O	1:A:60:VAL:HG23	1.96	0.64
1:D:219:CYS:SG	2:D:501:IMP:H2	2.37	0.64
1:B:350:GLY:HA3	1:C:327:VAL:HG21	1.79	0.64
1:C:218:ILE:HD13	1:C:301:GLY:HA2	1.79	0.64
1:D:218:ILE:HD13	1:D:301:GLY:HA2	1.80	0.63
1:B:219:CYS:SG	2:B:501:IMP:H2	2.39	0.63
1:D:306:GLY:HA2	1:D:309:LYS:HE2	1.80	0.63
1:B:153:VAL:HA	1:B:157:VAL:HG12	1.81	0.63
1:A:13:GLU:OE1	1:D:382:ARG:NH2	2.32	0.62
1:A:143:VAL:HG21	1:A:171:ASN:HB3	1.80	0.62
1:D:71:ILE:HD13	1:D:84:VAL:HG12	1.82	0.62
1:B:193:VAL:HG13	1:B:213:ILE:HG12	1.80	0.62
1:C:274:ILE:HD11	1:C:278:LEU:HG	1.80	0.62
1:D:27[A]:ARG:HG3	7:D:603:HOH:O	1.98	0.62
5:C:502:EDO:H21	1:D:14:ASP:OD1	1.99	0.62
1:C:219:CYS:SG	2:C:501:IMP:H2	2.40	0.62
1:C:295:VAL:HG13	1:C:337:TYR:HB3	1.82	0.61
1:D:214:GLY:HA2	1:D:219:CYS:SG	2.40	0.61
1:B:218:ILE:HD13	1:B:301:GLY:CA	2.32	0.60
1:C:11:THR:HG22	1:C:12:PHE:N	2.16	0.59
1:C:39:VAL:HG13	1:C:136:ARG:HD3	1.84	0.59
1:A:328:PRO:O	1:D:397:ASN:ND2	2.36	0.59
1:A:222:ARG:HG2	1:A:227:VAL:O	2.03	0.59
1:D:338:LYS:NZ	5:D:503:EDO:H21	2.19	0.58
1:D:186:ASP:HA	1:D:207:ASP:OD2	2.03	0.58
1:C:202:ILE:HG13	1:C:209:ILE:HD11	1.87	0.57
1:D:27[B]:ARG:HD3	1:D:28:GLU:HG3	1.88	0.56
1:D:51:ASP:HA	1:D:72:HIS:CD2	2.40	0.56
1:C:218:ILE:HD13	1:C:301:GLY:CA	2.36	0.56
1:A:324:ASN:HA	1:A:326:MET:HG2	1.88	0.56
1:B:390:GLU:OE1	1:C:334:ARG:HD2	2.06	0.55
1:A:283:GLU:OE1	1:A:283:GLU:N	2.40	0.55
1:B:218:ILE:HD13	1:B:301:GLY:HA2	1.88	0.55
1:D:26:PRO:O	1:D:29:VAL:HG12	2.06	0.55
1:A:150:LYS:HB3	1:A:183:MET:SD	2.46	0.55
1:C:214:GLY:HA2	1:C:219:CYS:SG	2.47	0.54
1:C:186:ASP:HA	1:C:207:ASP:OD2	2.07	0.54
1:A:80:GLN:OE1	1:A:148:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG22	1:A:87:VAL:HG13	1.90	0.54
1:C:51:ASP:HA	1:C:72:HIS:CD2	2.43	0.54
1:C:397:ASN:ND2	1:D:328:PRO:O	2.41	0.54
1:A:179:ILE:HA	1:A:183:MET:HE3	1.89	0.54
1:A:61:GLY:HA2	1:A:64:ARG:NE	2.23	0.54
1:C:291:ILE:CD1	1:C:296:TYR:CD2	2.92	0.53
1:A:218:ILE:HD13	1:A:301:GLY:HA2	1.89	0.53
1:D:261:ILE:HD12	1:D:272:VAL:HG21	1.91	0.53
1:B:56:HIS:O	1:B:60:VAL:HG22	2.09	0.53
1:D:289:GLU:OE1	1:D:298:TYR:OH	2.25	0.53
1:D:364:ILE:HG12	7:D:629:HOH:O	2.08	0.53
1:C:76:ASP:OD1	1:C:79:SER:HB3	2.08	0.53
1:C:393:LYS:HD3	1:D:332:GLU:OE1	2.09	0.53
1:A:79:SER:O	1:A:83:GLU:HG2	2.08	0.53
1:B:309:LYS:O	1:B:310:SER:CB	2.57	0.53
1:A:11[B]:THR:O	1:A:14:ASP:HB2	2.09	0.53
1:A:141:ILE:HD12	1:A:142:GLY:O	2.08	0.53
1:C:195:GLU:OE2	1:C:237:LYS:HD2	2.08	0.53
1:B:51:ASP:HA	1:B:72:HIS:CD2	2.44	0.52
1:D:87:VAL:HG11	1:D:137:VAL:HB	1.92	0.52
1:D:37:LYS:HE2	7:D:616:HOH:O	2.08	0.52
1:A:383:GLU:OE2	1:B:215:PRO:HB3	2.08	0.52
1:C:164:SER:HB2	1:C:172:ILE:HD11	1.92	0.52
1:D:76:ASP:N	1:D:76:ASP:OD1	2.43	0.52
1:C:82:ASN:O	1:C:86:LYS:HG3	2.10	0.51
1:B:186:ASP:HA	1:B:207:ASP:OD2	2.09	0.51
1:A:51:ASP:HA	1:A:72:HIS:CD2	2.45	0.51
1:A:61:GLY:HA2	1:A:64:ARG:HE	1.77	0.50
1:C:153:VAL:HG22	1:C:185:ILE:HD13	1.93	0.50
1:C:274:ILE:CD1	1:C:278:LEU:HG	2.40	0.50
1:C:81:VAL:HG13	1:C:155:ALA:HB2	1.93	0.50
1:D:236:GLU:OE2	1:D:373:TYR:OH	2.24	0.50
1:C:40:SER:H	1:C:136:ARG:NH2	2.09	0.50
1:A:346:TYR:CZ	1:B:325:LYS:HG2	2.47	0.50
1:B:11[B]:THR:HG22	1:B:12:PHE:N	2.27	0.50
1:D:218:ILE:HD13	1:D:301:GLY:CA	2.40	0.50
1:B:393:LYS:HE2	1:C:332:GLU:CD	2.33	0.50
1:C:29:VAL:O	1:C:353:ARG:NH1	2.41	0.49
1:A:168:HIS:CE1	1:D:21:TYR:HB2	2.47	0.49
1:A:214:GLY:HA2	1:A:219:CYS:SG	2.52	0.49
1:C:10:LEU:O	1:C:232:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:O	1:A:153:VAL:HG23	2.12	0.49
1:D:282:GLU:HG2	1:D:337:TYR:OH	2.12	0.49
1:C:26:PRO:O	1:C:353:ARG:HD3	2.13	0.49
1:D:283:GLU:N	1:D:283:GLU:OE1	2.43	0.49
1:C:142:GLY:H	1:C:145:GLU:CD	2.15	0.49
1:B:143:VAL:HG12	1:B:172:ILE:HG13	1.94	0.49
1:D:76:ASP:OD1	1:D:79:SER:HB3	2.12	0.49
1:A:189:VAL:HG11	1:A:201:LEU:HD22	1.93	0.49
1:C:397:ASN:ND2	1:D:328:PRO:HD2	2.28	0.49
1:D:141:ILE:HG22	1:D:148:ARG:HD2	1.95	0.49
1:D:56:HIS:ND1	1:D:83:GLU:OE2	2.42	0.49
1:D:136:ARG:HA	1:D:158:ASP:OD2	2.13	0.48
1:D:191:ASN:OD1	1:D:210:LYS:HD2	2.14	0.48
1:B:289:GLU:OE1	1:B:298:TYR:OH	2.24	0.48
1:D:366:GLU:CG	1:D:370:LYS:HE2	2.44	0.48
1:A:77:MET:O	1:A:81:VAL:HG23	2.14	0.48
1:A:150:LYS:O	1:A:154:GLU:HG3	2.14	0.48
1:B:11[A]:THR:OG1	1:B:12:PHE:N	2.46	0.48
1:A:397:ASN:HB3	1:B:224:VAL:HG22	1.96	0.47
1:A:38:ASN:HB2	1:A:186:ASP:OD2	2.14	0.47
1:A:346:TYR:OH	1:B:325:LYS:HG2	2.13	0.47
1:B:202:ILE:HG13	1:B:209:ILE:HD11	1.95	0.47
1:D:81:VAL:O	1:D:84:VAL:HG22	2.14	0.47
1:A:347:GLN:HG3	1:A:396:MET:CG	2.42	0.47
1:B:32:GLU:HA	1:B:42:LYS:HA	1.97	0.47
1:C:218:ILE:H	1:C:218:ILE:HG13	1.56	0.47
1:D:164:SER:HB2	1:D:172:ILE:HD11	1.97	0.47
1:D:82:ASN:HA	1:D:85:LEU:HD12	1.96	0.47
1:A:217:SER:HB2	1:D:387:HIS:O	2.15	0.47
1:A:218:ILE:HG13	1:A:218:ILE:H	1.46	0.47
1:A:153:VAL:HA	1:A:157:VAL:HG12	1.97	0.46
1:C:214:GLY:HA3	1:C:222:ARG:NE	2.29	0.46
1:C:291:ILE:HD13	1:C:334:ARG:NH2	2.30	0.46
1:A:60:VAL:O	1:A:64:ARG:HG3	2.16	0.46
1:A:388:ASP:OD2	1:B:256:ARG:NE	2.46	0.46
1:C:21:TYR:HB2	1:D:168:HIS:CE1	2.51	0.46
1:C:24:VAL:HG21	1:C:362:ALA:HB2	1.98	0.46
1:A:81:VAL:HG13	1:A:155:ALA:HB2	1.97	0.45
1:A:7:GLY:HA3	1:B:0:ALA:N	2.32	0.45
1:B:27:ARG:HG2	7:B:624:HOH:O	2.16	0.45
1:D:338:LYS:HZ1	5:D:503:EDO:H21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLY:O	1:A:64:ARG:HB2	2.17	0.45
1:B:252:ASP:OD2	2:B:501:IMP:O2'	2.33	0.45
1:A:31:LEU:CD1	1:A:349:VAL:HG13	2.47	0.45
1:A:61:GLY:HA2	1:A:64:ARG:NH2	2.32	0.45
1:A:11[A]:THR:O	1:A:14:ASP:HB2	2.17	0.44
1:D:397:ASN:OD1	7:D:631:HOH:O	2.20	0.44
1:A:150:LYS:HB2	1:A:150:LYS:HE3	1.66	0.44
1:B:392:VAL:HG22	1:C:332:GLU:O	2.17	0.44
1:A:191:ASN:OD1	1:A:210:LYS:HE2	2.17	0.44
1:B:177:LYS:HD3	1:B:204:ASN:OD1	2.17	0.44
1:A:218:ILE:HD13	1:A:301:GLY:CA	2.48	0.44
1:D:210:LYS:HD3	1:D:252:ASP:OD2	2.18	0.44
1:D:32:GLU:OE2	1:D:42:LYS:NZ	2.40	0.44
1:A:11[A]:THR:HG21	1:D:380:GLY:HA2	2.00	0.44
1:B:214:GLY:HA3	1:B:222:ARG:HE	1.83	0.43
1:C:76:ASP:OD1	1:C:76:ASP:N	2.50	0.43
1:A:136:ARG:HA	1:A:158:ASP:OD2	2.17	0.43
1:A:382:ARG:NH1	1:B:13:GLU:OE1	2.38	0.43
1:C:88:LYS:HE3	1:C:156:GLY:O	2.18	0.43
1:A:164:SER:HB2	1:A:172:ILE:HD11	2.00	0.43
1:C:326:MET:HB2	1:C:326:MET:HE2	1.89	0.43
1:A:309:LYS:HE2	1:A:324:ASN:CG	2.38	0.43
1:B:56:HIS:HB3	1:B:83:GLU:OE1	2.19	0.43
1:C:236:GLU:HG3	1:C:267:VAL:HG13	2.01	0.43
3:D:502:N09:H11	3:D:502:N09:O2	2.19	0.43
1:C:282:GLU:HG2	1:C:283:GLU:CD	2.38	0.43
1:C:179:ILE:HA	1:C:183:MET:HE3	2.01	0.42
1:D:306:GLY:HA2	1:D:309:LYS:CE	2.49	0.42
1:D:43:ILE:HA	1:D:44:PRO:HD3	1.76	0.42
1:A:61:GLY:CA	1:A:64:ARG:NH2	2.83	0.42
1:B:214:GLY:HA3	1:B:222:ARG:NE	2.35	0.42
1:C:149:ALA:O	1:C:153:VAL:HG23	2.20	0.42
1:A:251:ALA:HB3	1:A:272:VAL:HG12	2.02	0.42
1:A:160:ILE:CG2	1:A:187:VAL:HG22	2.50	0.42
1:D:218:ILE:H	1:D:218:ILE:HG13	1.43	0.42
1:D:78:GLU:HA	1:D:81:VAL:HB	2.01	0.42
1:D:366:GLU:HG2	1:D:370:LYS:HE2	2.02	0.42
1:C:137:VAL:HG22	1:C:138:GLY:N	2.35	0.42
1:C:150:LYS:O	1:C:154:GLU:HG3	2.20	0.42
1:D:305:VAL:O	1:D:309:LYS:HG3	2.20	0.41
1:C:274:ILE:HD13	1:C:277:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG23	1:A:137:VAL:HG11	2.00	0.41
1:B:222:ARG:HG2	1:B:227:VAL:O	2.20	0.41
1:C:136:ARG:HA	1:C:158:ASP:OD2	2.20	0.41
1:B:79:SER:O	1:B:83:GLU:HG2	2.20	0.41
3:D:502:N09:H7	3:D:502:N09:H5	2.01	0.41
1:D:283:GLU:OE1	1:D:341:MET:HB2	2.21	0.41
1:A:282:GLU:C	1:A:284:SER:H	2.23	0.41
1:D:150:LYS:O	1:D:154:GLU:HG3	2.20	0.41
1:C:389:VAL:HG12	1:D:335:VAL:HG22	2.02	0.41
1:A:81:VAL:HA	1:A:84:VAL:HG12	2.01	0.41
1:B:214:GLY:HA2	1:B:219:CYS:SG	2.60	0.41
1:C:141:ILE:HD12	1:C:142:GLY:O	2.20	0.41
1:B:293:ASP:N	7:B:623:HOH:O	2.53	0.41
1:B:309:LYS:O	1:B:310:SER:OG	2.37	0.41
1:A:383:GLU:CD	1:B:222:ARG:HH12	2.24	0.41
1:C:214:GLY:HA3	1:C:222:ARG:HG3	2.02	0.41
1:C:222:ARG:HG2	1:C:227:VAL:O	2.21	0.41
1:D:277:ILE:HG23	1:D:338:LYS:HZ1	1.86	0.41
1:C:81:VAL:HA	1:C:84:VAL:HG12	2.03	0.41
1:A:83:GLU:O	1:A:87:VAL:HG23	2.21	0.41
1:B:393:LYS:HE2	1:C:332:GLU:OE1	2.20	0.41
1:D:222:ARG:HG2	1:D:227:VAL:O	2.20	0.41
1:A:61:GLY:CA	1:A:64:ARG:HH21	2.34	0.40
1:D:82:ASN:HD22	1:D:85:LEU:HD12	1.86	0.40
3:B:503:N09:O2	3:B:503:N09:H11	2.20	0.40
1:A:146:ILE:HD13	1:A:178:GLU:OE1	2.21	0.40
1:B:288:LYS:H	1:B:288:LYS:HG3	1.73	0.40
5:C:502:EDO:H12	1:D:378:THR:N	2.36	0.40
1:B:76:ASP:OD1	1:B:76:ASP:N	2.52	0.40
1:C:38:ASN:HB2	1:C:186:ASP:OD2	2.22	0.40
1:B:194:THR:O	1:B:198:THR:HG23	2.21	0.40
1:A:180:LYS:NZ	7:A:612:HOH:O	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/361 (94%)	323 (95%)	17 (5%)	0	100	100
1	B	343/361 (95%)	330 (96%)	12 (4%)	1 (0%)	46	62
1	C	342/361 (95%)	327 (96%)	15 (4%)	0	100	100
1	D	343/361 (95%)	330 (96%)	12 (4%)	1 (0%)	46	62
All	All	1368/1444 (95%)	1310 (96%)	56 (4%)	2 (0%)	56	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	VAL
1	D	193	VAL

### 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	281/295 (95%)	279 (99%)	2 (1%)	88	95
1	B	283/295 (96%)	276 (98%)	7 (2%)	55	75
1	C	282/295 (96%)	276 (98%)	6 (2%)	61	79
1	D	283/295 (96%)	280 (99%)	3 (1%)	80	91
All	All	1129/1180 (96%)	1111 (98%)	18 (2%)	72	85

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

Mol	Chain	Res	Type
1	A	27[A]	ARG
1	A	27[B]	ARG
1	B	64	ARG
1	B	287	GLU

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Mol	Chain	Res	Type
1	B	288	LYS
1	B	289	GLU
1	B	290	LEU
1	B	291	ILE
1	B	310	SER
1	C	287	GLU
1	C	289	GLU
1	C	290	LEU
1	C	291	ILE
1	C	324	ASN
1	C	325	LYS
1	D	287	GLU
1	D	289	GLU
1	D	291	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	347	GLN
1	D	82	ASN
1	D	166	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 ⓘ

13 ligands are modelled in this entry.

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	IMP	A	501	-	20,25,25	1.36	3 (15%)	22,38,38	2.24	3 (13%)
3	N09	A	502	-	25,30,30	1.62	4 (16%)	31,43,43	2.41	13 (41%)
2	IMP	B	501	-	20,25,25	1.25	2 (10%)	22,38,38	2.43	4 (18%)
3	N09	B	502	-	25,30,30	1.66	4 (16%)	31,43,43	2.25	12 (38%)
3	N09	B	503	-	25,30,30	1.64	4 (16%)	31,43,43	2.34	12 (38%)
4	ACY	B	504	-	1,3,3	1.14	0	0,3,3	0.00	-
2	IMP	C	501	-	20,25,25	1.19	2 (10%)	22,38,38	2.47	4 (18%)
5	EDO	C	502	-	3,3,3	0.53	0	2,2,2	0.06	0
2	IMP	D	501	-	20,25,25	1.21	3 (15%)	22,38,38	2.39	3 (13%)
3	N09	D	502	-	25,30,30	1.52	4 (16%)	31,43,43	2.05	9 (29%)
5	EDO	D	503	-	3,3,3	0.63	0	2,2,2	0.10	0
6	FMT	D	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	EDO	D	505	-	3,3,3	0.58	0	2,2,2	0.27	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	IMP	A	501	-	-	0/6/26/26	0/3/3/3
3	N09	A	502	-	-	0/10/10/10	0/4/4/4
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
3	N09	B	502	-	-	0/10/10/10	0/4/4/4
3	N09	B	503	-	-	0/10/10/10	0/4/4/4
4	ACY	B	504	-	-	0/0/0/0	0/0/0/0
2	IMP	C	501	-	-	0/6/26/26	0/3/3/3
5	EDO	C	502	-	-	0/1/1/1	0/0/0/0
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
3	N09	D	502	-	-	0/10/10/10	0/4/4/4
5	EDO	D	503	-	-	0/1/1/1	0/0/0/0
6	FMT	D	504	-	-	0/0/0/0	0/0/0/0
5	EDO	D	505	-	-	0/1/1/1	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	N09	C4-N1	-3.06	1.35	1.41
3	B	503	N09	C4-N1	-2.78	1.36	1.41
3	D	502	N09	C4-N1	-2.58	1.36	1.41
3	B	502	N09	C4-N1	-2.32	1.37	1.41
2	A	501	IMP	C2-N1	2.05	1.37	1.33
2	D	501	IMP	C2-N1	2.38	1.38	1.33
3	D	502	N09	C1-CL	2.57	1.79	1.73
2	B	501	IMP	C6-N1	2.80	1.38	1.33
3	B	502	N09	C1-CL	2.83	1.80	1.73
2	C	501	IMP	C6-N1	2.92	1.38	1.33
3	B	503	N09	C1-CL	2.94	1.80	1.73
3	A	502	N09	C1-CL	2.95	1.80	1.73
2	D	501	IMP	C6-N1	3.06	1.38	1.33
2	A	501	IMP	C6-N1	3.27	1.39	1.33
2	D	501	IMP	C2-N3	3.33	1.38	1.32
3	D	502	N09	C17-C18	3.34	1.46	1.41
2	B	501	IMP	C2-N3	3.43	1.38	1.32
3	A	502	N09	C17-C18	3.47	1.47	1.41
3	B	503	N09	C17-C18	3.50	1.47	1.41
3	B	502	N09	C17-C18	3.54	1.47	1.41
2	C	501	IMP	C2-N3	3.61	1.38	1.32
2	A	501	IMP	C2-N3	4.03	1.39	1.32
3	D	502	N09	C6-C1	4.66	1.48	1.39
3	A	502	N09	C6-C1	4.80	1.48	1.39
3	B	503	N09	C6-C1	5.18	1.49	1.39
3	B	502	N09	C6-C1	5.23	1.49	1.39

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	IMP	N3-C2-N1	-10.41	120.92	128.89
2	D	501	IMP	N3-C2-N1	-9.92	121.30	128.89
2	B	501	IMP	N3-C2-N1	-9.76	121.42	128.89
2	A	501	IMP	N3-C2-N1	-9.22	121.84	128.89
3	B	502	N09	C26-C20-C19	-3.82	118.96	123.11
3	A	502	N09	C11-C13-N2	-3.72	105.85	110.68
3	D	502	N09	C11-C13-N2	-3.59	106.02	110.68
3	A	502	N09	C26-C20-C19	-3.45	119.36	123.11
3	B	503	N09	C17-C16-N3	-3.39	103.86	110.71
3	A	502	N09	O1-C6-C5	-3.37	118.46	124.21
3	B	502	N09	C17-C16-N3	-3.20	104.25	110.71
3	B	503	N09	O1-C6-C5	-3.16	118.82	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	N09	C17-C16-N3	-3.10	104.44	110.71
3	A	502	N09	C17-C16-N3	-3.07	104.50	110.71
3	B	503	N09	O2-C11-C13	-2.98	116.40	120.30
3	A	502	N09	O2-C11-C13	-2.79	116.65	120.30
3	B	503	N09	C26-C20-C19	-2.74	120.13	123.11
3	D	502	N09	C26-C20-C19	-2.67	120.20	123.11
2	C	501	IMP	C4-C5-N7	-2.66	107.03	109.48
3	B	502	N09	O3-C22-C17	-2.63	118.43	121.21
3	A	502	N09	C2-C1-C6	-2.58	117.09	120.84
3	B	503	N09	O3-C22-C17	-2.44	118.63	121.21
2	A	501	IMP	C4-C5-N7	-2.36	107.31	109.48
3	B	503	N09	C2-C1-C6	-2.34	117.44	120.84
3	B	502	N09	C13-N2-N3	-2.30	112.96	118.19
3	B	503	N09	C11-C13-N2	-2.17	107.86	110.68
3	B	502	N09	O1-C6-C5	-2.15	120.54	124.21
3	A	502	N09	O3-C22-C17	-2.14	118.95	121.21
3	D	502	N09	O3-C22-C17	-2.12	118.98	121.21
3	B	503	N09	C13-N2-N3	-2.11	113.39	118.19
3	B	502	N09	O2-C11-C13	-2.11	117.55	120.30
2	B	501	IMP	O3P-P-O1P	-2.02	104.09	110.58
3	A	502	N09	O3-C20-C26	2.03	118.62	116.10
3	D	502	N09	O1-C6-C1	2.03	118.98	116.76
2	C	501	IMP	C2-N1-C6	2.03	119.12	116.04
2	B	501	IMP	C2-N1-C6	2.10	119.22	116.04
3	B	502	N09	O3-C20-C26	2.29	118.95	116.10
3	B	502	N09	C2-C3-C4	2.30	122.87	120.28
2	D	501	IMP	C2-N1-C6	2.36	119.62	116.04
2	A	501	IMP	O2P-P-O1P	2.41	118.34	110.58
3	A	502	N09	C6-C1-CL	2.49	122.48	119.42
2	C	501	IMP	O3P-P-O2P	2.70	117.64	107.38
3	D	502	N09	C8-O1-C6	2.75	121.71	117.54
3	B	502	N09	O1-C6-C1	2.95	119.98	116.76
2	D	501	IMP	O2P-P-O1P	3.08	120.51	110.58
3	D	502	N09	C13-N2-C18	3.27	134.68	126.19
3	A	502	N09	C13-N2-C18	3.46	135.16	126.19
3	A	502	N09	C13-C11-N1	3.55	116.98	112.80
2	B	501	IMP	O3P-P-O2P	3.57	120.98	107.38
3	B	503	N09	C13-C11-N1	3.67	117.12	112.80
3	B	503	N09	C13-N2-C18	3.87	136.22	126.19
3	B	502	N09	C13-N2-C18	4.01	136.60	126.19
3	D	502	N09	C13-C11-N1	4.04	117.56	112.80
3	B	502	N09	C13-C11-N1	4.35	117.92	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	N09	O1-C6-C1	4.38	121.55	116.76
3	A	502	N09	O1-C6-C1	5.20	122.44	116.76
3	A	502	N09	C16-N3-N2	5.88	110.33	104.24
3	D	502	N09	C16-N3-N2	5.92	110.37	104.24
3	B	502	N09	C16-N3-N2	6.48	110.96	104.24
3	B	503	N09	C16-N3-N2	6.82	111.30	104.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	1	0
2	B	501	IMP	2	0
3	B	503	N09	1	0
2	C	501	IMP	1	0
5	C	502	EDO	2	0
2	D	501	IMP	1	0
3	D	502	N09	2	0
5	D	503	EDO	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	342/361 (94%)	0.33	18 (5%) 30 29	24, 51, 87, 128	0
1	B	345/361 (95%)	0.31	18 (5%) 31 30	25, 50, 82, 142	0
1	C	345/361 (95%)	0.26	16 (4%) 36 36	24, 49, 88, 115	0
1	D	346/361 (95%)	0.26	16 (4%) 36 36	24, 49, 85, 123	0
All	All	1378/1444 (95%)	0.29	68 (4%) 33 33	24, 50, 88, 142	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	ILE	5.3
1	A	287	GLU	4.7
1	A	291	ILE	4.5
1	C	91	GLY	4.4
1	C	1	MET	4.3
1	B	291	ILE	4.2
1	B	293	ASP	4.1
1	D	298	TYR	4.1
1	C	92	GLY	3.9
1	A	92	GLY	3.9
1	A	298	TYR	3.6
1	D	0	ALA	3.6
1	C	290	LEU	3.6
1	C	0	ALA	3.5
1	A	324	ASN	3.5
1	B	84	VAL	3.5
1	A	60	VAL	3.5
1	B	292	GLY	3.2
1	C	163	ASP	3.1
1	A	64	ARG	3.1
1	C	296	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	392	VAL	3.1
1	D	-1	ASN	3.0
1	A	91	GLY	3.0
1	D	163	ASP	3.0
1	A	84	VAL	2.8
1	D	92	GLY	2.8
1	A	337	TYR	2.8
1	D	296	TYR	2.8
1	D	84	VAL	2.8
1	C	293	ASP	2.8
1	B	92	GLY	2.7
1	B	90	SER	2.7
1	A	392	VAL	2.7
1	D	90	SER	2.6
1	C	85	LEU	2.5
1	B	155	ALA	2.5
1	B	286	GLY	2.5
1	A	85	LEU	2.5
1	B	296	TYR	2.5
1	B	324	ASN	2.5
1	C	84	VAL	2.4
1	B	0	ALA	2.4
1	B	1	MET	2.4
1	B	163	ASP	2.4
1	B	305	VAL	2.3
1	C	287	GLU	2.3
1	D	291	ILE	2.3
1	A	296	TYR	2.3
1	B	81	VAL	2.3
1	A	289	GLU	2.3
1	A	393	LYS	2.3
1	B	74	ASN	2.3
1	C	298	TYR	2.3
1	D	1	MET	2.2
1	A	286	GLY	2.2
1	A	396	MET	2.2
1	D	186	ASP	2.2
1	B	85	LEU	2.2
1	C	393	LYS	2.2
1	C	310	SER	2.1
1	C	136	ARG	2.1
1	D	88	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	LEU	2.1
1	A	399	SER	2.1
1	D	324	ASN	2.0
1	B	290	LEU	2.0
1	D	305	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACY	B	504	4/4	0.94	0.26	6.49	67,68,68,68	0
5	EDO	C	502	4/4	0.95	0.27	6.29	46,47,48,48	0
3	N09	B	503	27/27	0.90	0.21	3.64	53,65,70,71	0
3	N09	B	502	27/27	0.93	0.22	2.60	51,59,62,82	0
3	N09	A	502	27/27	0.91	0.18	2.36	58,68,69,70	0
3	N09	D	502	27/27	0.95	0.18	0.85	46,55,58,65	0
5	EDO	D	503	4/4	0.66	0.19	0.25	59,60,61,61	0
2	IMP	C	501	23/23	0.96	0.14	-0.45	35,37,41,43	0
5	EDO	D	505	4/4	0.95	0.15	-0.56	48,49,50,50	0
2	IMP	B	501	23/23	0.98	0.13	-0.69	28,33,38,41	0
2	IMP	A	501	23/23	0.96	0.14	-0.75	33,37,45,47	0
2	IMP	D	501	23/23	0.97	0.12	-0.82	29,35,39,40	0
6	FMT	D	504	3/3	0.93	0.18	-	52,52,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.