



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2017 – 08:36 AM EST

PDB ID : 4IX2
Title : Inosine 5'-monophosphate dehydrogenase from *Vibrio cholerae*, deletion mutant, complexed with IMP
Authors : Osipiuk, J.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : unknown
Resolution : 2.15 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

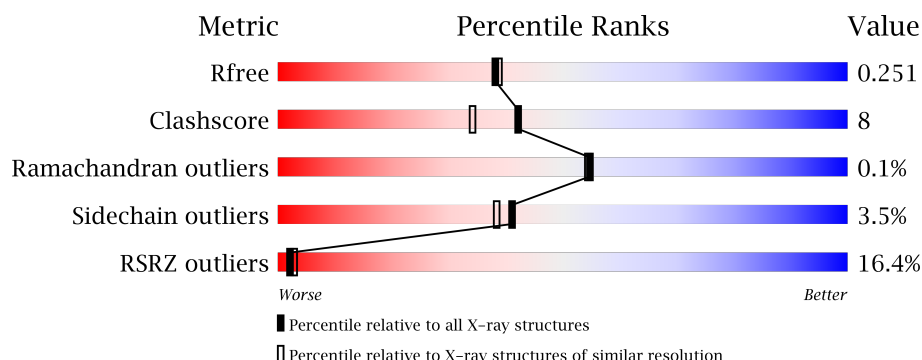
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	366	<div> <div>12%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	B	366	<div> <div>15%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	C	366	<div> <div>17%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	D	366	<div> <div>15%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10714 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	334	Total	C	N	O	S	0	0	0
			2444	1523	444	464	13			
1	B	333	Total	C	N	O	S	0	0	0
			2436	1518	443	463	12			
1	C	332	Total	C	N	O	S	0	0	0
			2425	1512	439	462	12			
1	D	333	Total	C	N	O	S	0	1	0
			2440	1522	442	463	13			

There are 24 discrepancies between the modelled and reference sequences:

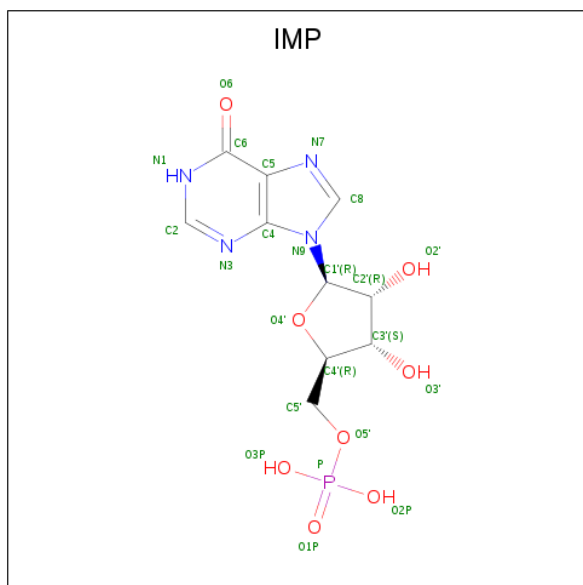
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KTW3
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KTW3
A	0	ALA	-	EXPRESSION TAG	UNP Q9KTW3
A	101	SER	-	LINKER	UNP Q9KTW3
A	102	GLY	-	LINKER	UNP Q9KTW3
A	103	GLY	-	LINKER	UNP Q9KTW3
B	-2	SER	-	EXPRESSION TAG	UNP Q9KTW3
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KTW3
B	0	ALA	-	EXPRESSION TAG	UNP Q9KTW3
B	101	SER	-	LINKER	UNP Q9KTW3
B	102	GLY	-	LINKER	UNP Q9KTW3
B	103	GLY	-	LINKER	UNP Q9KTW3
C	-2	SER	-	EXPRESSION TAG	UNP Q9KTW3
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KTW3
C	0	ALA	-	EXPRESSION TAG	UNP Q9KTW3
C	101	SER	-	LINKER	UNP Q9KTW3
C	102	GLY	-	LINKER	UNP Q9KTW3
C	103	GLY	-	LINKER	UNP Q9KTW3
D	-2	SER	-	EXPRESSION TAG	UNP Q9KTW3
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KTW3
D	0	ALA	-	EXPRESSION TAG	UNP Q9KTW3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	101	SER	-	LINKER	UNP Q9KTW3
D	102	GLY	-	LINKER	UNP Q9KTW3
D	103	GLY	-	LINKER	UNP Q9KTW3

- 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 POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	K	0	0
			2	2		
3	C	2	Total	K	0	0
			2	2		

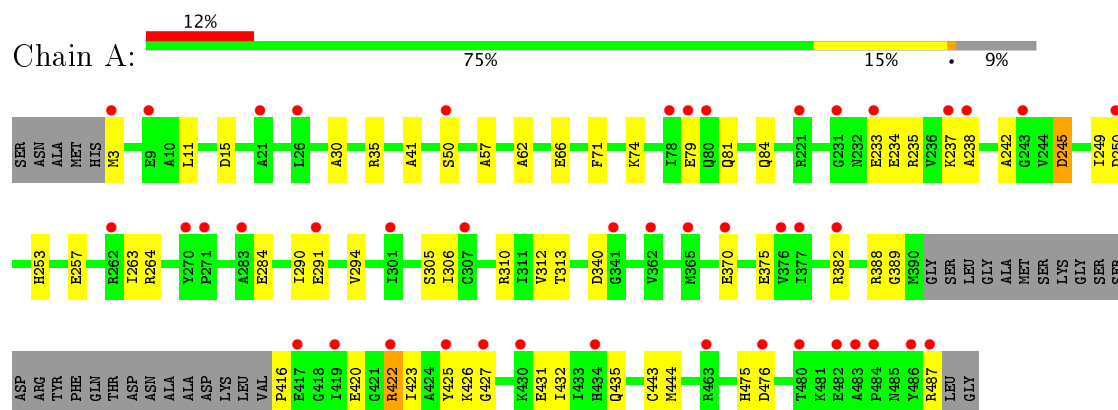
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	240	Total 240	O 240	0	0
4	B	194	Total 194	O 194	0	0
4	C	223	Total 223	O 223	0	0
4	D	216	Total 216	O 216	0	0

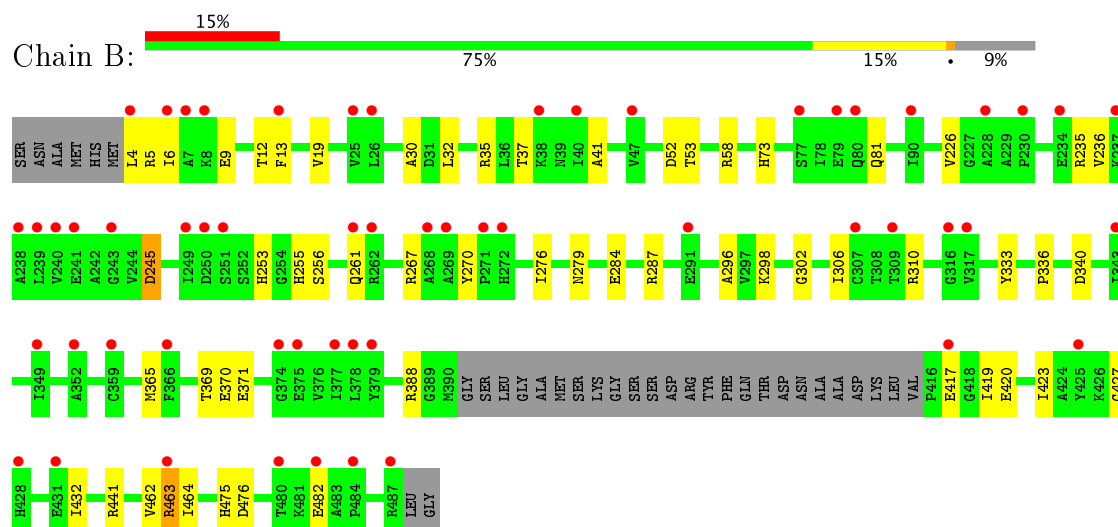
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

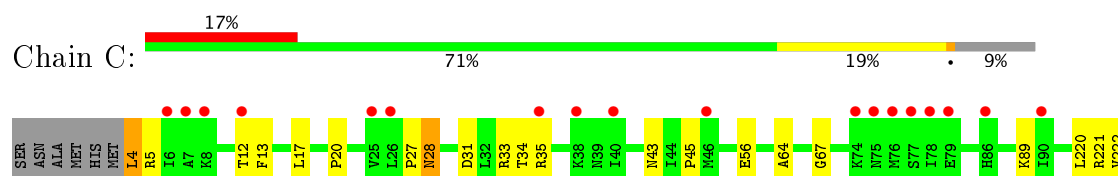
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

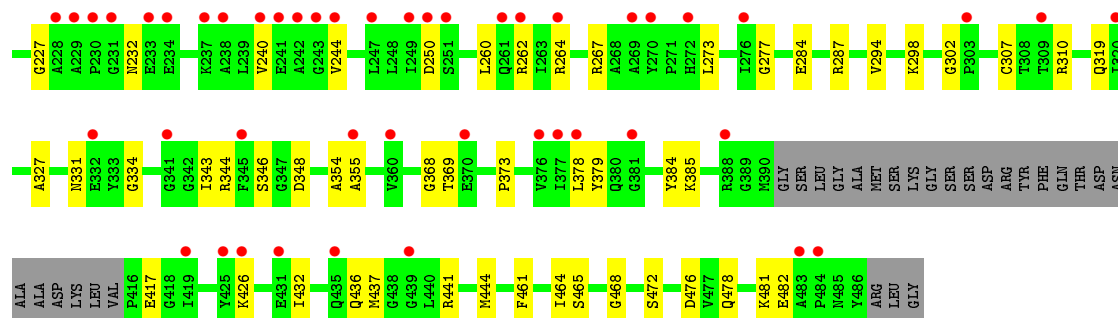


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

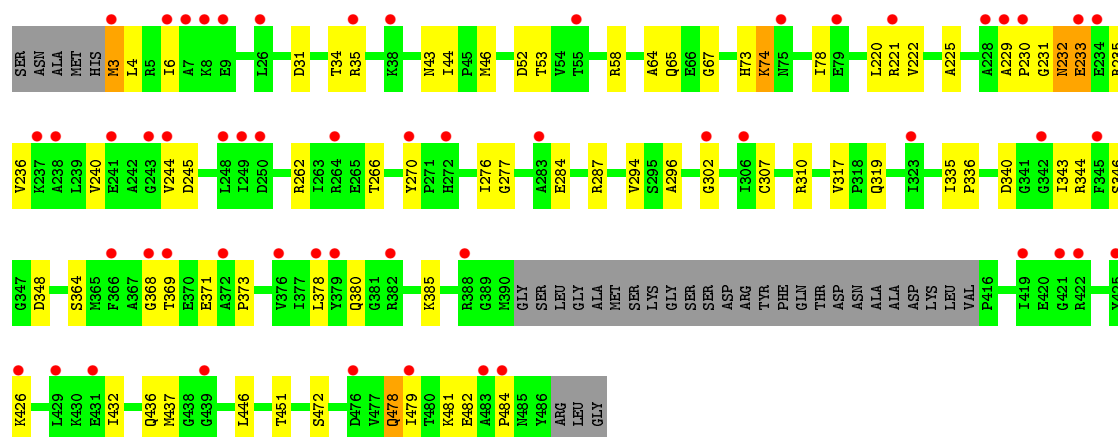


• Molecule 1: Inosine-5'-monophosphate dehydrogenase





• Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.18Å 167.16Å 93.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.10 – 2.15 38.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.10-2.15) 99.7 (38.13-2.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, R_{free}	0.208 , 0.258 0.208 , 0.251	Depositor DCC
R_{free} test set	3602 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
Outliers	5 of 71179 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10714	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2234e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, K

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	0.22	0/2475	0.42	0/3343
1	B	0.22	0/2467	0.42	0/3333
1	C	0.22	0/2456	0.43	0/3319
1	D	0.21	0/2475	0.42	0/3344
All	All	0.22	0/9873	0.42	0/13339

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	2444	0	2498	39	0
1	B	2436	0	2489	36	0
1	C	2425	0	2476	47	0
1	D	2440	0	2492	47	0
2	A	23	0	11	3	0
2	B	23	0	11	3	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
4	A	240	0	0	6	0
4	B	194	0	0	5	0
4	C	223	0	0	8	0
4	D	216	0	0	7	0
All	All	10714	0	9999	156	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 8.

All (156) 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:368:GLY:HA2	1:D:385:LYS:HB3	1.69	0.75
1:B:420:GLU:HB3	1:C:481:LYS:HB2	1.75	0.69
1:B:5:ARG:NH2	1:C:354:ALA:O	2.26	0.68
1:C:5:ARG:NH2	4:C:812:HOH:O	2.27	0.67
1:A:382:ARG:NH1	4:A:672:HOH:O	2.28	0.66
1:B:340:ASP:OD2	2:B:501:IMP:O2'	2.14	0.66
1:A:340:ASP:OD2	2:A:501:IMP:O2'	2.15	0.65
1:A:420:GLU:HB3	1:D:481:LYS:HB2	1.79	0.65
1:C:35:ARG:NH1	4:C:623:HOH:O	2.30	0.64
1:C:302:GLY:HA3	1:C:310:ARG:HG3	1.81	0.62
1:D:302:GLY:HA3	1:D:310:ARG:HG3	1.81	0.62
1:A:416:PRO:HG2	1:D:484:PRO:HD2	1.83	0.61
1:B:419:ILE:N	4:B:739:HOH:O	2.29	0.61
1:A:81:GLN:OE1	1:A:235:ARG:NH1	2.30	0.61
1:C:4:LEU:N	4:C:794:HOH:O	2.35	0.60
1:B:35:ARG:HA	1:B:41:ALA:HA	1.84	0.59
1:C:378:LEU:HB3	1:D:482:GLU:HB2	1.84	0.59
1:D:302:GLY:HA2	1:D:307:CYS:SG	2.43	0.59
1:C:35:ARG:NH2	1:C:334:GLY:O	2.29	0.59
1:D:3:MET:SD	1:D:3:MET:N	2.76	0.59
1:C:56:GLU:HG3	1:C:373:PRO:HG3	1.84	0.59
1:D:287:ARG:NH2	4:D:788:HOH:O	2.37	0.58
1:D:31:ASP:HB3	1:D:451:THR:HG22	1.86	0.58
1:A:422:ARG:NH2	1:D:479:ILE:O	2.36	0.58
1:D:284:GLU:HG3	1:D:287:ARG:HH12	1.68	0.58
1:C:240:VAL:HA	1:C:244:VAL:HG12	1.85	0.57
1:D:35:ARG:NH1	4:D:749:HOH:O	2.35	0.57
1:B:4:LEU:N	4:B:748:HOH:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:LYS:HB3	1:D:432:ILE:HD11	1.86	0.56
1:B:276:ILE:HG12	1:B:296:ALA:HB3	1.87	0.56
1:C:482:GLU:HB2	1:D:378:LEU:HB3	1.88	0.56
1:B:253:HIS:O	1:B:256:SER:OG	2.25	0.55
1:A:422:ARG:NH2	4:A:609:HOH:O	2.40	0.55
1:D:276:ILE:HG12	1:D:296:ALA:HB3	1.89	0.54
1:A:305:SER:OG	2:A:501:IMP:O2P	2.26	0.54
1:A:257:GLU:OE2	1:A:264:ARG:NH1	2.35	0.54
1:C:468:GLY:N	4:C:768:HOH:O	2.37	0.54
1:A:426:LYS:HB3	1:A:432:ILE:HD11	1.91	0.53
1:C:89:LYS:HD3	1:C:222:VAL:HG12	1.91	0.53
1:A:475:HIS:ND1	1:A:476:ASP:OD2	2.38	0.52
1:C:355:ALA:HB3	4:C:730:HOH:O	2.09	0.52
1:C:346:SER:HB3	1:C:436:GLN:HA	1.89	0.52
1:D:346:SER:HB3	1:D:436:GLN:HA	1.91	0.52
1:A:426:LYS:HE3	1:A:487:ARG:CZ	2.40	0.52
1:C:368:GLY:HA2	1:C:385:LYS:HB3	1.92	0.52
1:A:249:ILE:HD12	1:A:263:ILE:HG12	1.92	0.51
1:B:463:ARG:NH1	1:B:464:ILE:O	2.43	0.51
1:C:344:ARG:NH1	4:C:774:HOH:O	2.42	0.51
1:B:279:ASN:OD1	1:B:298:LYS:NZ	2.35	0.51
1:A:388:ARG:HB3	1:A:420:GLU:HG3	1.92	0.51
1:A:310:ARG:HD2	1:D:472:SER:HA	1.93	0.51
1:B:370:GLU:N	1:B:427:GLY:O	2.39	0.51
1:A:370:GLU:N	1:A:427:GLY:O	2.39	0.50
1:B:417:GLU:OE2	2:B:501:IMP:N1	2.43	0.50
1:D:240:VAL:HA	1:D:244:VAL:HG12	1.93	0.50
1:A:238:ALA:O	1:A:242:ALA:N	2.43	0.50
1:A:35:ARG:HA	1:A:41:ALA:HA	1.93	0.50
1:B:52:ASP:HA	1:B:73:HIS:CE1	2.47	0.50
1:B:310:ARG:HD2	1:C:472:SER:HA	1.93	0.50
1:D:229:ALA:O	1:D:231:GLY:N	2.44	0.50
1:B:245:ASP:OD1	1:B:245:ASP:N	2.44	0.50
1:C:27:PRO:O	1:C:441:ARG:NH1	2.39	0.49
1:B:267:ARG:NH1	1:B:270:TYR:O	2.46	0.49
1:A:312:VAL:HG13	1:A:313:THR:HG23	1.95	0.49
1:D:319:GLN:NE2	4:D:606:HOH:O	2.45	0.49
1:D:343:ILE:HG23	1:D:348:ASP:HB2	1.93	0.49
1:C:227:GLY:O	1:C:232:ASN:ND2	2.46	0.48
1:A:306:ILE:HD13	1:A:389:GLY:HA2	1.95	0.48
1:A:3:MET:N	4:A:729:HOH:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLU:HA	1:A:237:LYS:HB3	1.95	0.48
1:B:81:GLN:OE1	1:B:235:ARG:NH1	2.47	0.48
1:C:465:SER:OG	4:C:768:HOH:O	2.20	0.48
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.49	0.48
1:D:78:ILE:HG23	1:D:235:ARG:HA	1.95	0.48
1:C:277:GLY:HA3	1:C:294:VAL:HG11	1.96	0.48
1:D:364:SER:O	4:D:723:HOH:O	2.20	0.48
1:A:245:ASP:OD1	1:A:245:ASP:N	2.46	0.48
1:A:3:MET:N	4:A:829:HOH:O	2.46	0.47
1:D:64:ALA:HB3	1:D:220:LEU:HD13	1.96	0.47
1:D:74:LYS:HB2	1:D:74:LYS:HE2	1.74	0.47
1:B:306:ILE:HB	4:B:739:HOH:O	2.14	0.47
1:A:57:ALA:HB2	1:A:84:GLN:HB3	1.97	0.47
1:C:34:THR:OG1	1:C:35:ARG:N	2.46	0.47
1:C:43:ASN:HB2	1:C:67:GLY:HA3	1.95	0.47
1:D:232:ASN:ND2	4:D:644:HOH:O	2.48	0.47
1:B:302:GLY:HA3	1:B:310:ARG:HG3	1.97	0.47
1:B:287:ARG:NH1	1:B:333:TYR:OH	2.47	0.47
1:D:43:ASN:HB2	1:D:67:GLY:HA3	1.95	0.47
1:D:65:GLN:HG3	1:D:220:LEU:HD11	1.96	0.47
1:A:431:GLU:O	1:A:435:GLN:HG2	2.16	0.46
1:C:4:LEU:N	4:C:717:HOH:O	2.48	0.46
1:A:375:GLU:O	4:A:708:HOH:O	2.20	0.46
1:C:284:GLU:HG3	1:C:287:ARG:HH22	1.79	0.46
1:B:6:ILE:HD13	1:C:461:PHE:HB2	1.98	0.46
1:C:17:LEU:HD12	1:C:464:ILE:HG21	1.97	0.46
1:D:222:VAL:N	1:D:245:ASP:OD1	2.39	0.46
1:B:388:ARG:HB3	1:B:420:GLU:HG3	1.97	0.46
1:D:266:THR:O	1:D:270:TYR:N	2.48	0.46
1:C:64:ALA:HB3	1:C:220:LEU:HD13	1.97	0.46
1:C:250:ASP:OD2	1:C:298:LYS:NZ	2.39	0.46
1:D:34:THR:OG1	1:D:35:ARG:N	2.48	0.46
1:A:290:ILE:HA	1:A:294:VAL:HG22	1.97	0.46
1:C:343:ILE:HG23	1:C:348:ASP:HB2	1.98	0.46
1:D:4:LEU:HD23	1:D:6:ILE:HD11	1.98	0.45
1:A:62:ALA:O	1:A:66:GLU:HG2	2.15	0.45
1:A:30:ALA:HB1	1:A:444:MET:HE2	1.98	0.45
1:A:425:TYR:CZ	1:A:427:GLY:HA2	2.51	0.45
1:D:317:VAL:O	4:D:617:HOH:O	2.21	0.45
1:B:12:THR:OG1	1:B:13:PHE:N	2.47	0.45
1:C:417:GLU:HG3	2:C:502:IMP:HN1	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:GLN:OE1	1:C:478:GLN:N	2.49	0.45
1:C:426:LYS:HB3	1:C:432:ILE:HD11	1.97	0.45
1:B:253:HIS:CE1	1:C:20:PRO:HB2	2.52	0.45
1:C:302:GLY:HA2	1:C:307:CYS:SG	2.57	0.45
1:B:30:ALA:O	1:B:441:ARG:NH2	2.51	0.44
1:B:253:HIS:CE1	1:B:255:HIS:HB3	2.52	0.44
1:A:50:SER:HB3	1:A:71:PHE:HB3	1.98	0.44
1:D:74:LYS:HB3	1:D:225:ALA:O	2.18	0.44
1:B:19:VAL:HG22	1:B:462:VAL:HG13	2.00	0.44
1:D:369:THR:O	1:D:385:LYS:NZ	2.36	0.44
1:D:380:GLN:NE2	4:D:687:HOH:O	2.40	0.44
1:C:45:PRO:HD2	1:C:437:MET:HE1	1.99	0.44
1:B:226:VAL:HG11	1:B:236:VAL:HG22	2.00	0.43
1:D:335:ILE:HA	1:D:336:PRO:HD3	1.89	0.43
1:A:388:ARG:NH2	4:A:820:HOH:O	2.52	0.43
1:B:58:ARG:NH2	4:B:611:HOH:O	2.51	0.43
1:D:44:ILE:HB	1:D:437:MET:HE3	2.01	0.42
1:C:260:LEU:O	1:C:264:ARG:HG2	2.19	0.42
1:C:369:THR:O	1:C:385:LYS:NZ	2.35	0.42
1:A:306:ILE:HD11	2:A:501:IMP:H8	2.01	0.42
1:C:28:ASN:OD1	1:C:28:ASN:N	2.53	0.42
1:B:475:HIS:ND1	1:B:476:ASP:OD2	2.50	0.42
1:D:310:ARG:NH2	1:D:317:VAL:O	2.53	0.42
1:D:58:ARG:HD3	1:D:371:GLU:HA	2.01	0.42
1:D:233:GLU:HA	1:D:236:VAL:HB	2.01	0.41
1:C:31:ASP:OD2	1:C:33:ARG:NH2	2.51	0.41
1:D:277:GLY:HA3	1:D:294:VAL:HG11	2.02	0.41
1:B:369:THR:HG22	1:B:432:ILE:HG13	2.02	0.41
1:D:53:THR:HA	1:D:373:PRO:HG2	2.03	0.41
1:A:422:ARG:HG2	1:D:478:GLN:HB2	2.02	0.41
1:B:32:LEU:HD21	1:B:441:ARG:HG2	2.02	0.41
1:C:227:GLY:H	1:C:232:ASN:HD21	1.68	0.41
1:A:370:GLU:OE2	1:A:425:TYR:OH	2.30	0.41
1:B:306:ILE:O	4:B:739:HOH:O	2.22	0.41
1:C:379:TYR:HB3	1:C:384:TYR:CE1	2.56	0.41
1:B:371:GLU:OE1	1:B:371:GLU:N	2.53	0.40
1:C:13:PHE:HB2	1:C:344:ARG:HH22	1.86	0.40
1:D:340:ASP:OD2	2:D:502:IMP:O2'	2.32	0.40
1:A:11:LEU:HD22	1:A:15:ASP:HB3	2.04	0.40
1:A:253:HIS:CD2	1:D:446:LEU:HA	2.57	0.40
1:A:233:GLU:HG2	1:A:233:GLU:H	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ILE:HD11	2:B:501:IMP:H8	2.04	0.40
1:B:37:THR:C	1:B:336:PRO:HG2	2.42	0.40
1:C:267:ARG:NH1	1:C:273:LEU:O	2.48	0.40
1:C:327:ALA:O	1:C:331:ASN:N	2.43	0.40
1:C:432:ILE:O	1:C:436:GLN:HG2	2.22	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	330/366 (90%)	322 (98%)	8 (2%)	0	100	100
1	B	329/366 (90%)	319 (97%)	10 (3%)	0	100	100
1	C	328/366 (90%)	307 (94%)	21 (6%)	0	100	100
1	D	330/366 (90%)	309 (94%)	20 (6%)	1 (0%)	44	39
All	All	1317/1464 (90%)	1257 (95%)	59 (4%)	1 (0%)	55	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	230	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	250/274 (91%)	241 (96%)	9 (4%)	40	37
1	B	249/274 (91%)	240 (96%)	9 (4%)	40	37
1	C	248/274 (90%)	240 (97%)	8 (3%)	44	42
1	D	250/274 (91%)	241 (96%)	9 (4%)	40	37
All	All	997/1096 (91%)	962 (96%)	35 (4%)	41	38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	79	GLU
1	A	245	ASP
1	A	250	ASP
1	A	284	GLU
1	A	291	GLU
1	A	422	ARG
1	A	423	ILE
1	A	443	CYS
1	B	9	GLU
1	B	53	THR
1	B	245	ASP
1	B	261	GLN
1	B	284	GLU
1	B	365	MET
1	B	423	ILE
1	B	463	ARG
1	B	482	GLU
1	C	4	LEU
1	C	12	THR
1	C	28	ASN
1	C	221	ARG
1	C	262	ARG
1	C	319	GLN
1	C	444	MET
1	C	476	ASP
1	D	3	MET
1	D	46	MET
1	D	74	LYS
1	D	221	ARG
1	D	232	ASN
1	D	233	GLU
1	D	262	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	344	ARG
1	D	478	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	232	ASN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	IMP	A	501	-	21,25,25	1.25	3 (14%)	22,38,38	2.44	3 (13%)
2	IMP	B	501	-	21,25,25	1.26	3 (14%)	22,38,38	2.42	2 (9%)
2	IMP	C	502	-	21,25,25	1.27	3 (14%)	22,38,38	2.38	2 (9%)
2	IMP	D	502	-	21,25,25	1.23	3 (14%)	22,38,38	2.27	2 (9%)

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
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3
2	IMP	D	502	-	-	0/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IMP	C2-N1	2.27	1.38	1.33
2	D	502	IMP	C2-N1	2.33	1.38	1.33
2	B	501	IMP	C2-N1	2.35	1.38	1.33
2	C	502	IMP	C2-N1	2.45	1.38	1.33
2	C	502	IMP	C6-N1	2.89	1.38	1.33
2	B	501	IMP	C6-N1	2.93	1.38	1.33
2	D	502	IMP	C6-N1	2.96	1.38	1.33
2	A	501	IMP	C6-N1	3.05	1.38	1.33
2	A	501	IMP	C2-N3	3.68	1.38	1.32
2	D	502	IMP	C2-N3	3.70	1.38	1.32
2	B	501	IMP	C2-N3	3.79	1.38	1.32
2	C	502	IMP	C2-N3	3.83	1.38	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	IMP	N3-C2-N1	-10.34	119.85	128.86
2	A	501	IMP	N3-C2-N1	-10.23	119.95	128.86
2	C	502	IMP	N3-C2-N1	-10.09	120.07	128.86
2	D	502	IMP	N3-C2-N1	-9.71	120.40	128.86
2	A	501	IMP	O2P-P-O1P	2.20	119.11	110.50
2	D	502	IMP	C2-N1-C6	2.45	120.00	115.91
2	C	502	IMP	C2-N1-C6	2.54	120.14	115.91
2	A	501	IMP	C2-N1-C6	2.81	120.60	115.91
2	B	501	IMP	C2-N1-C6	2.87	120.70	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMP	3	0
2	B	501	IMP	3	0
2	C	502	IMP	1	0
2	D	502	IMP	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	334/366 (91%)	1.11	44 (13%) 4 5	8, 25, 43, 55	0
1	B	333/366 (90%)	1.25	56 (16%) 2 2	9, 25, 44, 65	0
1	C	332/366 (90%)	1.32	64 (19%) 1 2	11, 24, 49, 70	0
1	D	333/366 (90%)	1.21	55 (16%) 2 3	10, 25, 48, 69	0
All	All	1332/1464 (90%)	1.22	219 (16%) 2 3	8, 25, 46, 70	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	ILE	6.8
1	D	230	PRO	6.0
1	B	4	LEU	5.9
1	D	229	ALA	5.9
1	B	240	VAL	5.8
1	C	228	ALA	5.5
1	B	249	ILE	5.4
1	C	238	ALA	5.3
1	C	426	LYS	5.1
1	C	241	GLU	5.1
1	B	262	ARG	5.0
1	B	228	ALA	4.9
1	B	484	PRO	4.9
1	C	230	PRO	4.9
1	D	221	ARG	4.6
1	B	374	GLY	4.4
1	D	234	GLU	4.3
1	D	228	ALA	4.3
1	D	345	PHE	4.3
1	B	272	HIS	4.3
1	C	378	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	377	ILE	4.2
1	D	388	ARG	4.2
1	C	345	PHE	4.2
1	A	419	ILE	4.0
1	D	3	MET	4.0
1	C	332	GLU	3.9
1	B	487	ARG	3.8
1	C	8	LYS	3.8
1	D	7	ALA	3.8
1	D	483	ALA	3.8
1	C	231	GLY	3.7
1	C	376	VAL	3.7
1	A	480	THR	3.7
1	B	375	GLU	3.6
1	C	38	LYS	3.6
1	D	272[A]	HIS	3.6
1	B	271	PRO	3.6
1	C	79	GLU	3.6
1	C	250	ASP	3.6
1	A	270	TYR	3.6
1	A	484	PRO	3.5
1	A	483	ALA	3.5
1	C	244	VAL	3.5
1	A	79	GLU	3.4
1	B	359	CYS	3.4
1	C	377	ILE	3.4
1	B	77	SER	3.3
1	D	249	ILE	3.3
1	D	79	GLU	3.3
1	C	262	ARG	3.3
1	D	421	GLY	3.3
1	A	463	ARG	3.3
1	C	261	GLN	3.3
1	A	271	PRO	3.3
1	C	90	ILE	3.3
1	D	241	GLU	3.2
1	D	484	PRO	3.2
1	A	3	MET	3.2
1	A	26	LEU	3.2
1	A	417	GLU	3.2
1	C	234	GLU	3.1
1	C	77	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	26	LEU	3.1
1	A	262	ARG	3.1
1	B	482	GLU	3.0
1	D	250	ASP	3.0
1	C	7	ALA	3.0
1	C	435	GLN	3.0
1	B	80	GLN	3.0
1	B	349	ILE	3.0
1	C	86	HIS	3.0
1	C	381	GLY	3.0
1	A	307	CYS	2.9
1	B	40	ILE	2.9
1	B	238	ALA	2.9
1	B	317	VAL	2.9
1	B	268	ALA	2.9
1	A	422	ARG	2.9
1	B	269	ALA	2.9
1	C	229	ALA	2.9
1	C	264	ARG	2.9
1	D	26	LEU	2.9
1	B	417	GLU	2.8
1	A	476	ASP	2.8
1	C	251	SER	2.8
1	D	379	TYR	2.8
1	C	233	GLU	2.8
1	C	242	ALA	2.8
1	B	79	GLU	2.8
1	C	320	ILE	2.7
1	C	237	LYS	2.7
1	C	270	TYR	2.7
1	D	270	TYR	2.7
1	A	231	GLY	2.7
1	B	234	GLU	2.7
1	A	487	ARG	2.7
1	C	269	ALA	2.7
1	D	372	ALA	2.7
1	C	26	LEU	2.7
1	C	483	ALA	2.7
1	B	480	THR	2.7
1	A	365	MET	2.7
1	A	9	GLU	2.6
1	B	251	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	376	VAL	2.6
1	A	382	ARG	2.6
1	A	377	ILE	2.6
1	B	241	GLU	2.6
1	B	230	PRO	2.6
1	A	362	VAL	2.6
1	A	425	TYR	2.6
1	D	75	ASN	2.6
1	A	250	ASP	2.5
1	A	243	GLY	2.5
1	A	238	ALA	2.5
1	A	291	GLU	2.5
1	C	75	ASN	2.5
1	C	243	GLY	2.5
1	C	309	THR	2.5
1	B	261	GLN	2.5
1	A	78	ILE	2.5
1	C	431	GLU	2.5
1	A	482	GLU	2.5
1	A	427	GLY	2.5
1	C	360	VAL	2.5
1	A	237	LYS	2.5
1	C	276	ILE	2.5
1	B	378	LEU	2.5
1	D	238	ALA	2.5
1	B	38	LYS	2.5
1	C	76	MET	2.5
1	B	47	VAL	2.5
1	D	425	TYR	2.5
1	D	366	PHE	2.5
1	B	239	LEU	2.4
1	A	233	GLU	2.4
1	D	237	LYS	2.4
1	D	342	GLY	2.4
1	C	272	HIS	2.4
1	C	74	LYS	2.4
1	B	6	ILE	2.4
1	D	302	GLY	2.4
1	C	240	VAL	2.4
1	B	8	LYS	2.4
1	D	426	LYS	2.4
1	C	25	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	237	LYS	2.3
1	B	243	GLY	2.3
1	B	250	ASP	2.3
1	C	370	GLU	2.3
1	B	463	ARG	2.3
1	C	388	ARG	2.3
1	C	484	PRO	2.3
1	D	368	GLY	2.3
1	A	370	GLU	2.3
1	A	50	SER	2.3
1	C	247	LEU	2.3
1	D	429	LEU	2.3
1	D	35	ARG	2.3
1	D	38	LYS	2.3
1	D	323	ILE	2.3
1	C	439	GLY	2.3
1	B	425	TYR	2.3
1	C	35	ARG	2.3
1	A	21	ALA	2.3
1	A	283	ALA	2.3
1	B	352	ALA	2.3
1	A	221	ARG	2.3
1	C	341	GLY	2.3
1	D	431	GLU	2.3
1	B	428	HIS	2.2
1	D	264	ARG	2.2
1	A	434	HIS	2.2
1	B	291	GLU	2.2
1	C	425	TYR	2.2
1	D	233	GLU	2.2
1	D	283	ALA	2.2
1	D	243	GLY	2.2
1	D	439	GLY	2.2
1	D	382	ARG	2.2
1	D	422	ARG	2.2
1	A	301	ILE	2.2
1	B	90	ILE	2.2
1	C	78	ILE	2.2
1	C	12	THR	2.2
1	C	355	ALA	2.2
1	C	419	ILE	2.1
1	D	419	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	8	LYS	2.1
1	B	316	GLY	2.1
1	D	369	THR	2.1
1	B	343	ILE	2.1
1	D	6	ILE	2.1
1	B	13	PHE	2.1
1	B	7	ALA	2.1
1	B	379	TYR	2.1
1	C	40	ILE	2.1
1	D	306	ILE	2.1
1	D	479	ILE	2.1
1	A	376	VAL	2.1
1	B	25	VAL	2.1
1	B	309	THR	2.1
1	D	476	ASP	2.1
1	C	6	ILE	2.1
1	C	46	MET	2.1
1	C	303	PRO	2.1
1	B	366	PHE	2.1
1	A	486	TYR	2.1
1	B	431	GLU	2.0
1	A	430	LYS	2.0
1	D	248	LEU	2.0
1	D	378	LEU	2.0
1	D	55	THR	2.0
1	D	9	GLU	2.0
1	A	341	GLY	2.0
1	B	307	CYS	2.0
1	A	80	GLN	2.0
1	D	244	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	IMP	B	501	23/23	0.86	0.25	1.11	15,35,56,67	0
2	IMP	A	501	23/23	0.84	0.24	0.82	10,27,62,70	0
2	IMP	D	502	23/23	0.87	0.19	-0.17	4,23,29,30	0
3	K	C	503	1/1	0.86	0.17	-0.32	26,26,26,26	0
2	IMP	C	502	23/23	0.91	0.15	-0.87	7,19,26,28	0
3	K	C	501	1/1	0.92	0.09	-1.97	16,16,16,16	0
3	K	D	503	1/1	0.93	0.12	-2.79	19,19,19,19	0
3	K	D	501	1/1	0.98	0.10	-3.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.