



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:11 AM GMT

PDB ID : 3DG8
Title : Quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with RJF670, NADPH, and dUMP
Authors : Dasgupta, T.; Chitnumsub, P.; Maneeruttanarungroj, C.; Kamchonwongpaisan, S.; Nichols, S.; Lyons, T.M.; Tirado-Rives, J.; Jorgensen, W.L.; Yuthavong, Y.; Anderson, K.S.
Deposited on : 2008-06-13
Resolution : 2.58 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 (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

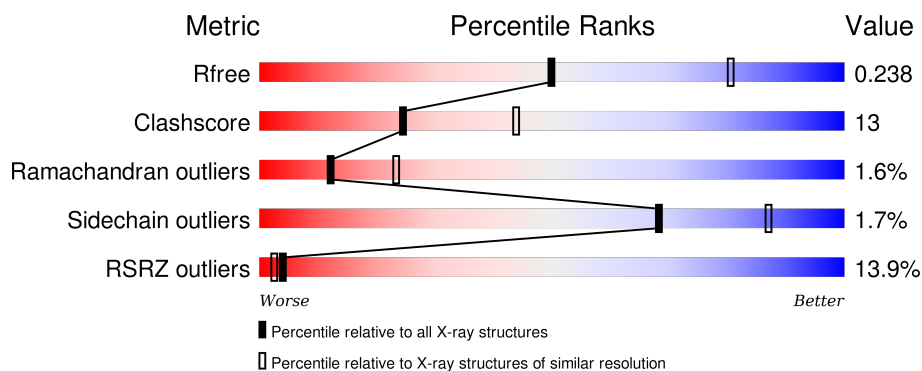
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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	280	<div> <div>10%</div> <div>59%</div> <div>18%</div> <div>21%</div> </div>
1	B	280	<div> <div>30%</div> <div>44%</div> <div>32%</div> <div>21%</div> </div>
2	C	328	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>••</div> </div>
2	D	328	<div> <div>6%</div> <div>81%</div> <div>17%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RJ6	A	609	-	-	-	X
3	RJ6	B	609	-	-	-	X
5	UMP	C	611	-	-	-	X
5	UMP	D	611	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9527 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1837	1190	297	338	12			
1	B	221	Total	C	N	O	S	0	0	0
			1834	1189	297	336	12			

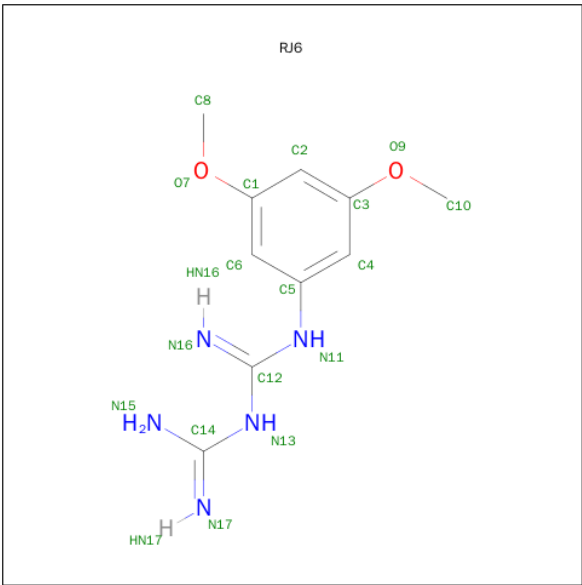
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ILE	ASN	ENGINEERED	UNP Q8I1R6
A	59	ARG	CYS	ENGINEERED	UNP Q8I1R6
A	108	ASN	SER	ENGINEERED	UNP Q8I1R6
A	164	LEU	ILE	ENGINEERED	UNP Q8I1R6
B	51	ILE	ASN	ENGINEERED	UNP Q8I1R6
B	59	ARG	CYS	ENGINEERED	UNP Q8I1R6
B	108	ASN	SER	ENGINEERED	UNP Q8I1R6
B	164	LEU	ILE	ENGINEERED	UNP Q8I1R6

- Molecule 2 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

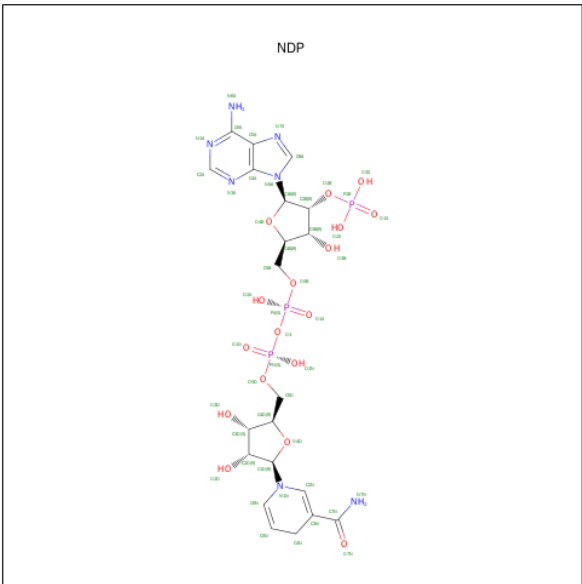
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			
2	D	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			

- Molecule 3 is N-(3,5-DIMETHOXYPHENYL)IMIDODICARBONIMIDIC DIAMIDE (three-letter code: RJ6) (formula: C₁₀H₁₅N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	10	5	2		
3	B	1	Total	C	N	O	0	0
			17	10	5	2		

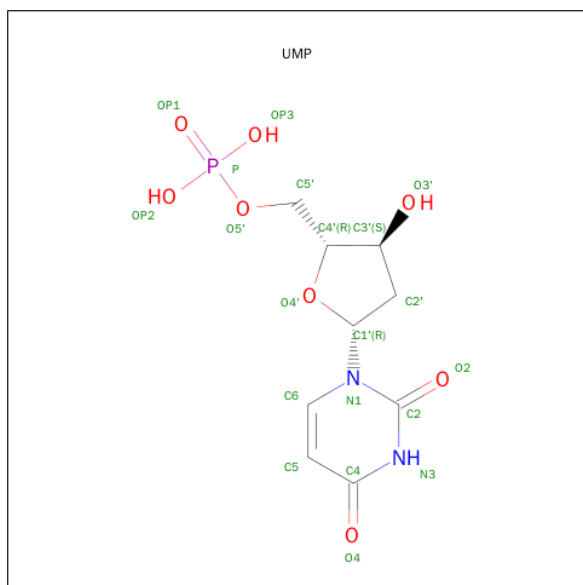
- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
5	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

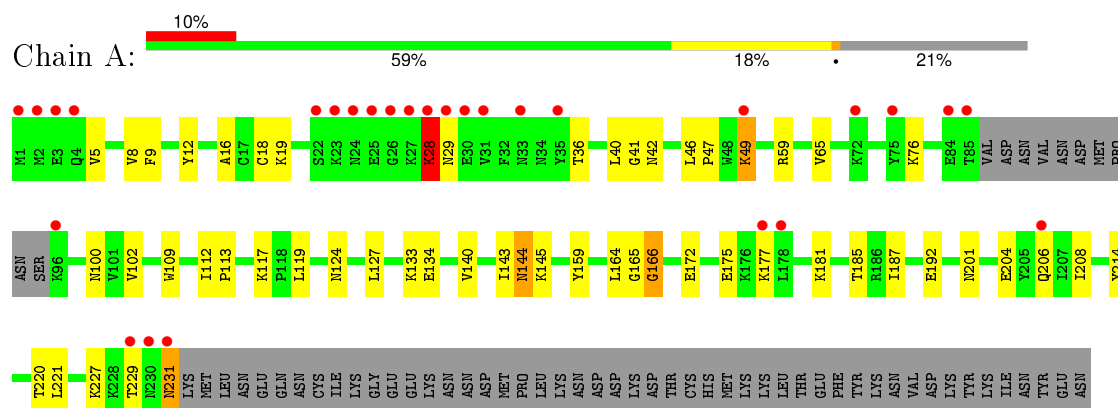
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total	O	0	0
			40	40		
6	B	7	Total	O	0	0
			7	7		
6	C	93	Total	O	0	0
			93	93		
6	D	120	Total	O	0	0
			120	120		

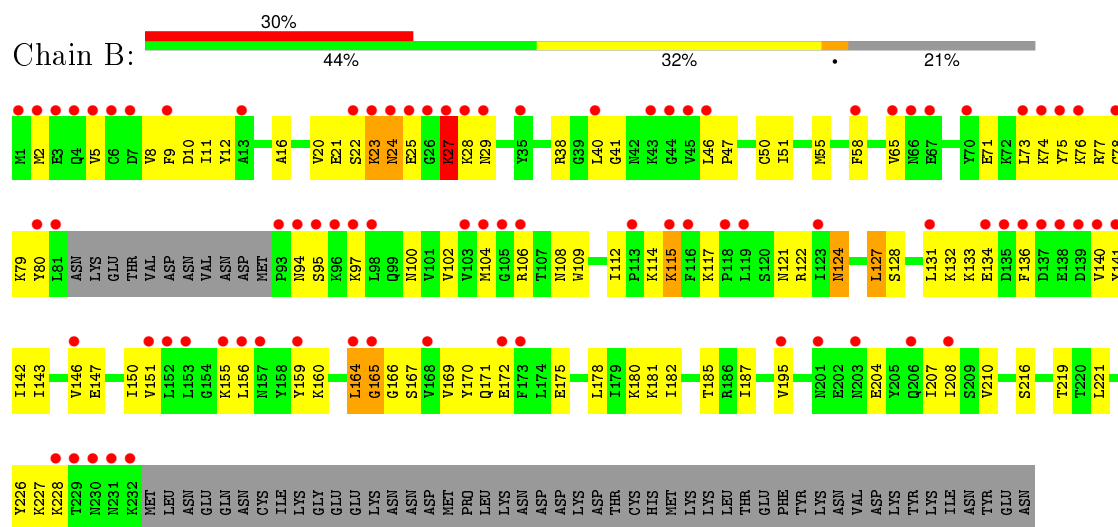
3 Residue-property plots

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.

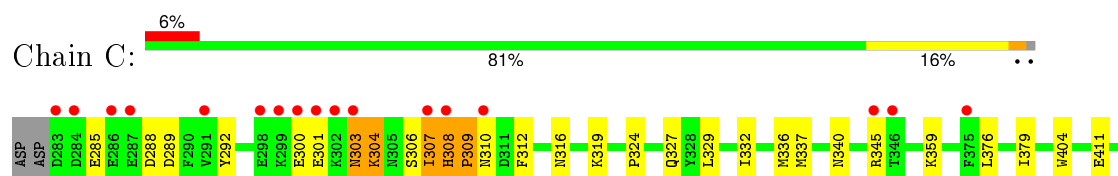
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

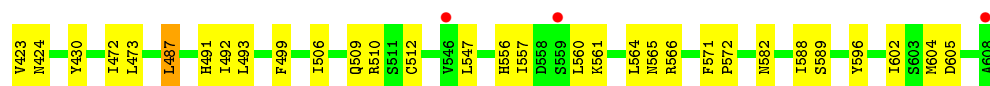


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

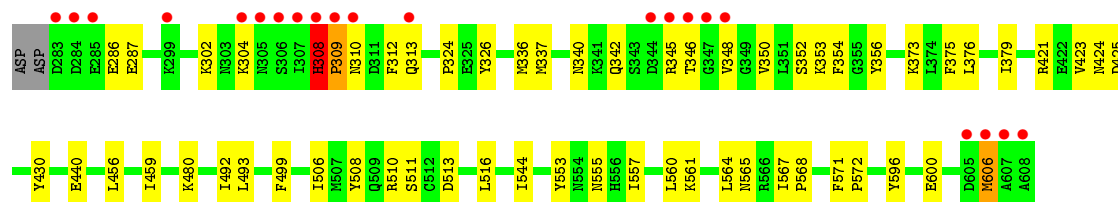
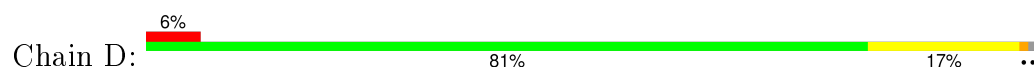


- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase





- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.52Å 155.40Å 165.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.58 49.43 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.43-2.58) 97.3 (49.43-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.86 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.239 0.199 , 0.238	Depositor DCC
R_{free} test set	2321 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45637 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9527	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: RJ6, UMP, NDP

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	0.39	0/1871	0.66	3/2515 (0.1%)
1	B	0.35	0/1869	0.62	1/2512 (0.0%)
2	C	0.38	0/2784	0.64	0/3766
2	D	0.38	0/2784	0.65	1/3766 (0.0%)
All	All	0.38	0/9308	0.64	5/12559 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLY	N-CA-C	-8.11	92.82	113.10
1	B	27	LYS	N-CA-C	6.12	127.52	111.00
1	A	165	GLY	N-CA-C	5.59	127.07	113.10
1	A	28	LYS	N-CA-C	5.54	125.96	111.00
2	D	308	HIS	N-CA-C	5.02	124.57	111.00

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	1837	0	1873	46	0
1	B	1834	0	1873	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2713	0	2638	52	0
2	D	2713	0	2638	49	0
3	A	17	0	13	6	0
3	B	17	0	13	3	0
4	A	48	0	26	7	0
4	B	48	0	26	6	0
5	C	20	0	11	0	0
5	D	20	0	11	1	0
6	A	40	0	0	0	0
6	B	7	0	0	0	0
6	C	93	0	0	1	0
6	D	120	0	0	4	0
All	All	9527	0	9122	237	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 13.

All (237) 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:114:LYS:H	1:B:114:LYS:HD2	1.09	1.12
1:B:133:LYS:HD2	1:B:133:LYS:H	1.36	0.90
2:D:376:LEU:HD22	2:D:379:ILE:HD11	1.56	0.86
2:C:308:HIS:O	2:C:310:ASN:N	2.08	0.86
2:C:332:ILE:HD13	2:C:560:LEU:HD22	1.58	0.85
1:B:12:TYR:HE2	1:B:160:LYS:HD3	1.44	0.80
2:D:309:PRO:HG3	2:D:337:MET:HE1	1.62	0.79
1:A:28:LYS:HD2	1:A:29:ASN:HD22	1.45	0.78
2:C:376:LEU:HD22	2:C:379:ILE:HD11	1.65	0.78
1:B:114:LYS:H	1:B:114:LYS:CD	1.91	0.77
1:B:8:VAL:HA	1:B:76:LYS:HD3	1.65	0.77
1:B:5:VAL:HG11	1:B:150:ILE:HD12	1.67	0.77
1:B:104:MET:HA	1:B:165:GLY:HA2	1.68	0.76
2:C:306:SER:C	2:C:308:HIS:H	1.88	0.75
1:A:164:LEU:HD13	3:A:609:RJ6:H8A	1.69	0.75
2:D:308:HIS:O	2:D:310:ASN:N	2.20	0.74
2:C:306:SER:O	2:C:308:HIS:N	2.19	0.74
2:D:336:MET:HE2	2:D:557:ILE:HG23	1.70	0.74
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.70	0.73
1:B:112:ILE:HB	1:B:117:LYS:HD3	1.71	0.72
1:B:124:ASN:N	1:B:124:ASN:HD22	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:N	1:B:114:LYS:HD2	1.95	0.71
1:A:28:LYS:HD2	1:A:29:ASN:ND2	2.07	0.70
1:B:22:SER:O	1:B:23:LYS:HB2	1.91	0.70
3:A:609:RJ6:HN11	3:A:609:RJ6:HN15	1.41	0.69
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.75	0.69
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.74	0.68
2:D:312:PHE:HA	2:D:565:ASN:HD21	1.59	0.67
1:B:127:LEU:HD23	1:B:143:ILE:HG13	1.75	0.67
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.77	0.67
3:A:609:RJ6:H10	4:A:610:NDP:O2D	1.97	0.65
1:B:106:ARG:HG3	1:B:131:LEU:HD11	1.77	0.65
1:B:46:LEU:HG	3:B:609:RJ6:H10A	1.77	0.65
1:A:124:ASN:HB2	1:A:140:VAL:HG12	1.78	0.64
2:C:307:ILE:HG23	2:C:561:LYS:HE2	1.80	0.63
1:B:171:GLN:O	1:B:175:GLU:HG3	1.98	0.63
1:B:133:LYS:CD	1:B:133:LYS:H	2.11	0.63
1:A:28:LYS:CD	1:A:29:ASN:HD22	2.12	0.63
1:A:166:GLY:HA3	4:A:610:NDP:PA	2.38	0.63
2:C:303:ASN:HD22	2:C:303:ASN:C	2.02	0.63
1:B:25:GLU:C	1:B:27:LYS:H	2.01	0.63
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.34	0.63
2:D:376:LEU:HD22	2:D:379:ILE:CD1	2.26	0.62
2:D:310:ASN:O	2:D:313:GLN:HG3	1.98	0.62
1:B:167:SER:HB3	4:B:610:NDP:O2N	2.00	0.62
2:D:308:HIS:N	2:D:309:PRO:HD2	2.15	0.62
1:B:208:ILE:HD13	1:B:227:LYS:HD2	1.82	0.62
2:D:480:LYS:HE2	6:D:1167:HOH:O	2.01	0.61
2:C:512:CYS:SG	2:C:547:LEU:HD22	2.40	0.61
2:C:336:MET:HE2	2:C:557:ILE:HG23	1.81	0.61
1:B:151:VAL:HG12	1:B:155:LYS:HE2	1.83	0.61
2:D:423:VAL:O	2:D:424:ASN:HB2	2.00	0.60
1:A:46:LEU:HG	3:A:609:RJ6:H10A	1.82	0.60
2:C:303:ASN:O	2:C:304:LYS:HB2	2.00	0.60
2:D:309:PRO:HA	2:D:312:PHE:CD2	2.37	0.59
1:A:201:ASN:HB3	1:A:204:GLU:HG3	1.84	0.59
1:B:21:GLU:C	1:B:23:LYS:H	2.04	0.59
2:D:421:ARG:HH11	2:D:421:ARG:HG2	1.68	0.59
2:C:376:LEU:HD22	2:C:379:ILE:CD1	2.32	0.59
2:D:312:PHE:CE1	2:D:561:LYS:HG2	2.37	0.58
2:D:324:PRO:HB2	2:D:571:PHE:HE2	1.68	0.58
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:LEU:C	2:C:493:LEU:HD12	2.23	0.58
1:B:133:LYS:N	1:B:133:LYS:HD2	2.15	0.58
2:C:319:LYS:HG2	2:D:286:GLU:HG2	1.84	0.58
2:C:306:SER:O	2:C:309:PRO:HD2	2.03	0.57
2:C:491:HIS:HD2	2:C:509:GLN:HG3	1.69	0.57
1:B:78:CYS:C	1:B:80:TYR:H	2.06	0.57
1:B:210:VAL:HG21	2:D:326:TYR:HE2	1.69	0.57
2:C:301:GLU:OE1	2:C:301:GLU:HA	2.05	0.57
1:B:58:PHE:HZ	1:B:164:LEU:HD13	1.69	0.57
1:B:12:TYR:CE2	1:B:160:LYS:HD3	2.34	0.57
2:D:506:ILE:HG12	2:D:544:ILE:HB	1.86	0.57
1:A:144:ASN:ND2	1:A:145:LYS:HG3	2.21	0.55
1:B:131:LEU:HB3	1:B:136:PHE:HE2	1.69	0.55
2:C:404:TRP:CZ3	2:C:487:LEU:HD21	2.41	0.55
2:C:300:GLU:HA	2:C:303:ASN:HB2	1.89	0.55
1:B:65:VAL:HG13	1:B:159:TYR:HB2	1.88	0.55
1:A:102:VAL:HB	1:A:164:LEU:HD11	1.88	0.55
2:C:582:ASN:HB3	6:C:1037:HOH:O	2.06	0.55
2:C:492:ILE:HD11	2:C:510:ARG:HD3	1.88	0.54
2:C:306:SER:C	2:C:308:HIS:N	2.59	0.54
1:A:177:LYS:NZ	1:A:204:GLU:OE1	2.41	0.54
1:A:49:LYS:H	1:A:49:LYS:HD3	1.71	0.54
1:B:95:SER:C	1:B:97:LYS:H	2.11	0.54
2:D:572:PRO:HB3	2:D:596:TYR:HA	1.88	0.54
1:A:201:ASN:CG	1:A:204:GLU:HG3	2.28	0.53
2:D:304:LYS:HB3	6:D:1189:HOH:O	2.07	0.53
2:C:312:PHE:HA	2:C:565:ASN:HD21	1.74	0.53
1:B:166:GLY:H	1:B:169:VAL:HB	1.73	0.53
1:B:102:VAL:HG11	1:B:122:ARG:HD2	1.91	0.53
2:D:302:LYS:HB2	6:D:1182:HOH:O	2.08	0.53
1:A:164:LEU:CD1	3:A:609:RJ6:H8A	2.39	0.53
1:A:16:ALA:HA	1:A:185:THR:HB	1.91	0.53
1:B:171:GLN:HE21	1:B:175:GLU:CD	2.13	0.52
1:B:132:LYS:HD2	1:B:134:GLU:CD	2.30	0.52
1:B:146:VAL:HG22	1:B:172:GLU:OE2	2.08	0.52
1:A:112:ILE:HB	1:A:117:LYS:HD3	1.90	0.52
1:B:169:VAL:HG23	4:B:610:NDP:O1A	2.10	0.52
1:B:95:SER:C	1:B:97:LYS:N	2.62	0.52
2:C:308:HIS:N	2:C:309:PRO:HD2	2.24	0.51
1:A:214:TYR:O	1:A:220:THR:HA	2.10	0.51
1:B:164:LEU:HD12	3:B:609:RJ6:H8A	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:309:PRO:HG3	2:C:337:MET:CE	2.41	0.51
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.93	0.51
1:B:124:ASN:N	1:B:124:ASN:ND2	2.57	0.50
2:C:566:ARG:NH1	2:C:602:ILE:HD11	2.27	0.50
1:B:216:SER:O	1:B:219:THR:HG22	2.12	0.50
1:B:171:GLN:HG3	1:B:175:GLU:OE2	2.12	0.50
2:D:302:LYS:HZ1	2:D:340:ASN:HA	1.77	0.50
1:B:71:GLU:OE2	1:B:74:LYS:HD3	2.11	0.50
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.11	0.50
2:D:373:LYS:HE2	2:D:375:PHE:CE1	2.46	0.50
1:A:172:GLU:HA	1:A:175:GLU:HG2	1.93	0.50
1:A:59:ARG:HH11	1:A:59:ARG:HG2	1.77	0.50
1:B:204:GLU:O	1:B:228:LYS:HD2	2.11	0.50
2:C:572:PRO:HB3	2:C:596:TYR:HA	1.93	0.49
2:D:302:LYS:NZ	2:D:340:ASN:HA	2.26	0.49
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.46	0.49
2:C:329:LEU:HD22	2:C:564:LEU:HD12	1.95	0.49
1:B:8:VAL:HG13	1:B:76:LYS:HG2	1.94	0.48
2:C:345:ARG:HG2	2:C:345:ARG:HH11	1.79	0.48
2:D:421:ARG:HD2	2:D:425:ASP:CG	2.34	0.48
1:A:49:LYS:N	1:A:49:LYS:HD3	2.28	0.48
2:C:506:ILE:HG13	2:D:354:PHE:CE2	2.49	0.48
2:D:309:PRO:HG3	2:D:337:MET:CE	2.38	0.48
1:A:119:LEU:HD11	3:A:609:RJ6:C8	2.44	0.48
2:D:492:ILE:HD11	2:D:510:ARG:HD3	1.96	0.48
1:B:136:PHE:HD2	1:B:142:ILE:HD11	1.78	0.47
1:B:127:LEU:HG	1:B:143:ILE:HD11	1.95	0.47
1:A:201:ASN:CB	1:A:204:GLU:HG3	2.43	0.47
2:D:493:LEU:C	2:D:493:LEU:HD12	2.35	0.47
1:B:78:CYS:C	1:B:80:TYR:N	2.68	0.47
2:C:404:TRP:HZ3	2:C:487:LEU:HD21	1.80	0.47
2:D:511:SER:OG	5:D:611:UMP:H3'	2.15	0.47
1:B:40:LEU:O	4:B:610:NDP:H2N	2.15	0.47
1:B:122:ARG:O	1:B:124:ASN:ND2	2.48	0.47
1:B:207:ILE:HB	2:D:567:ILE:HD13	1.96	0.47
2:C:423:VAL:O	2:C:424:ASN:HB2	2.15	0.46
1:B:11:ILE:HB	1:B:178:LEU:O	2.16	0.46
2:C:324:PRO:HB2	2:C:571:PHE:HE2	1.81	0.46
2:D:513:ASP:OD2	2:D:516:LEU:HB2	2.16	0.46
2:C:309:PRO:HA	2:C:312:PHE:CD2	2.50	0.46
1:B:102:VAL:HG23	1:B:102:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:ILE:O	2:C:307:ILE:HG22	2.16	0.46
1:B:75:TYR:CE1	1:B:79:LYS:HD2	2.50	0.46
1:B:73:LEU:HD13	1:B:77:ARG:NH2	2.31	0.46
2:D:342:GLN:NE2	2:D:352:SER:OG	2.48	0.46
1:B:10:ASP:OD2	1:B:73:LEU:HD22	2.16	0.46
1:B:21:GLU:C	1:B:23:LYS:N	2.69	0.45
1:B:108:ASN:HB2	4:B:610:NDP:O2A	2.16	0.45
1:A:144:ASN:H	1:A:144:ASN:ND2	2.14	0.45
1:B:102:VAL:HG23	1:B:124:ASN:HA	1.97	0.45
2:D:350:VAL:HG12	2:D:553:TYR:CD1	2.50	0.45
2:C:499:PHE:CE1	2:D:340:ASN:HB3	2.52	0.45
1:B:41:GLY:N	1:B:195:VAL:HG23	2.30	0.45
1:B:165:GLY:HA3	1:B:169:VAL:HB	1.97	0.45
2:C:487:LEU:HD23	2:C:487:LEU:N	2.31	0.45
1:B:28:LYS:CG	1:B:29:ASN:H	2.30	0.45
1:B:95:SER:O	1:B:97:LYS:N	2.49	0.45
1:B:77:ARG:O	1:B:80:TYR:HB3	2.16	0.45
1:B:147:GLU:N	1:B:147:GLU:OE1	2.49	0.45
2:C:312:PHE:HB2	2:C:316:ASN:ND2	2.32	0.45
2:C:289:ASP:HA	2:C:292:TYR:CD2	2.52	0.45
1:B:5:VAL:HG13	1:B:9:PHE:CD2	2.52	0.44
1:A:65:VAL:HA	1:A:159:TYR:CD2	2.52	0.44
1:B:16:ALA:HA	1:B:185:THR:HB	1.99	0.44
2:C:307:ILE:CG2	2:C:561:LYS:HE2	2.47	0.44
2:C:303:ASN:O	2:C:304:LYS:CB	2.65	0.44
2:C:340:ASN:HB3	2:D:499:PHE:CE1	2.52	0.44
1:A:206:GLN:HE21	1:A:229:THR:HG21	1.83	0.44
1:B:41:GLY:H	1:B:195:VAL:HG23	1.83	0.44
2:D:309:PRO:HA	2:D:312:PHE:HD2	1.80	0.44
2:C:509:GLN:HB3	2:C:512:CYS:SG	2.58	0.44
1:B:25:GLU:C	1:B:27:LYS:N	2.70	0.44
1:B:180:LYS:HE2	2:C:285:GLU:OE1	2.17	0.44
1:B:121:ASN:ND2	1:B:121:ASN:N	2.64	0.44
1:B:41:GLY:HA2	1:B:47:PRO:HD3	2.00	0.44
2:D:312:PHE:HE1	2:D:561:LYS:HG2	1.80	0.43
1:B:127:LEU:HA	1:B:143:ILE:HG13	2.00	0.43
1:A:172:GLU:OE2	4:A:610:NDP:N7A	2.51	0.43
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.18	0.43
1:B:121:ASN:HD22	1:B:121:ASN:N	2.15	0.43
1:A:42:ASN:HB2	1:A:192:GLU:O	2.18	0.43
1:A:127:LEU:O	4:A:610:NDP:H1B	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:493:LEU:CD2	2:D:492:ILE:HG21	2.48	0.43
2:D:567:ILE:HA	2:D:568:PRO:HD3	1.88	0.43
1:B:23:LYS:O	1:B:24:ASN:ND2	2.51	0.43
2:D:421:ARG:NH1	2:D:421:ARG:HG2	2.31	0.43
1:B:210:VAL:O	1:B:210:VAL:HG23	2.19	0.43
2:D:353:LYS:HG3	2:D:356:TYR:OH	2.18	0.43
2:D:600:GLU:HG3	6:D:1084:HOH:O	2.17	0.43
1:A:102:VAL:HB	1:A:164:LEU:CD1	2.49	0.43
2:C:411:GLU:H	2:C:411:GLU:CD	2.21	0.43
2:D:508:TYR:CD1	2:D:508:TYR:C	2.92	0.42
1:A:166:GLY:HA3	4:A:610:NDP:O1A	2.19	0.42
1:B:164:LEU:CD1	3:B:609:RJ6:H8A	2.50	0.42
1:A:133:LYS:HG3	1:A:134:GLU:N	2.33	0.42
2:C:556:HIS:HA	2:C:604:MET:O	2.20	0.42
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.55	0.42
2:C:492:ILE:HG21	2:D:493:LEU:CD2	2.49	0.42
1:A:231:ASN:HA	1:A:231:ASN:HD22	1.53	0.42
2:D:346:THR:OG1	2:D:348:VAL:HG23	2.19	0.42
1:B:115:LYS:HG2	1:B:115:LYS:H	1.62	0.42
1:B:181:LYS:HE3	1:B:227:LYS:NZ	2.35	0.42
1:B:23:LYS:HA	1:B:23:LYS:HD2	1.90	0.42
1:B:141:TYR:CE2	1:B:156:LEU:HD11	2.54	0.42
2:D:310:ASN:O	2:D:313:GLN:NE2	2.46	0.42
1:A:40:LEU:O	4:A:610:NDP:H2N	2.19	0.42
2:C:327:GLN:NE2	2:C:359:LYS:O	2.47	0.42
1:B:127:LEU:HD22	4:B:610:NDP:C2A	2.49	0.42
1:B:27:LYS:O	1:B:28:LYS:HB2	2.20	0.42
1:A:112:ILE:HA	1:A:113:PRO:HD3	1.94	0.42
1:A:18:CYS:HA	1:A:187:ILE:HB	2.02	0.42
1:A:208:ILE:HD13	1:A:227:LYS:HB2	2.01	0.42
1:B:50:CYS:SG	1:B:55:MET:CE	3.08	0.41
1:A:166:GLY:HA3	4:A:610:NDP:O2A	2.20	0.41
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.56	0.41
1:B:20:VAL:CG2	1:B:38:ARG:NH2	2.83	0.41
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.85	0.41
1:B:221:LEU:N	1:B:221:LEU:HD23	2.34	0.41
2:D:336:MET:HE3	2:D:560:LEU:HB2	2.02	0.41
2:C:308:HIS:N	2:C:309:PRO:CD	2.84	0.41
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.85	0.41
1:B:94:ASN:O	1:B:95:SER:OG	2.29	0.41
2:C:472:ILE:C	2:C:473:LEU:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG13	1:A:9:PHE:HD2	1.86	0.41
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.56	0.41
1:B:171:GLN:HE21	1:B:175:GLU:CG	2.35	0.40
2:C:309:PRO:HG3	2:C:337:MET:HE2	2.02	0.40
1:B:170:TYR:OH	4:B:610:NDP:H41N	2.20	0.40
1:A:221:LEU:HD23	1:A:221:LEU:N	2.36	0.40
2:D:336:MET:CE	2:D:557:ILE:HG23	2.47	0.40
1:B:50:CYS:SG	1:B:55:MET:HE1	2.61	0.40
2:C:588:ILE:HG23	2:C:589:SER:N	2.36	0.40
1:B:106:ARG:HD3	1:B:128:SER:OG	2.21	0.40
2:D:456:LEU:O	2:D:459:ILE:HG13	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	217/280 (78%)	200 (92%)	16 (7%)	1 (0%)	34	58
1	B	217/280 (78%)	184 (85%)	27 (12%)	6 (3%)	6	9
2	C	324/328 (99%)	301 (93%)	18 (6%)	5 (2%)	13	25
2	D	324/328 (99%)	301 (93%)	18 (6%)	5 (2%)	13	25
All	All	1082/1216 (89%)	986 (91%)	79 (7%)	17 (2%)	12	23

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	B	24	ASN
1	B	27	LYS
2	C	304	LYS

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Mol	Chain	Res	Type
2	C	307	ILE
2	C	308	HIS
2	C	309	PRO
2	D	308	HIS
2	D	309	PRO
2	D	345	ARG
1	B	23	LYS
1	B	115	LYS
1	B	165	GLY
2	D	606	MET
2	C	430	TYR
2	D	430	TYR
1	B	140	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	210/268 (78%)	206 (98%)	4 (2%)	65	85
1	B	210/268 (78%)	206 (98%)	4 (2%)	65	85
2	C	300/302 (99%)	296 (99%)	4 (1%)	76	91
2	D	300/302 (99%)	295 (98%)	5 (2%)	68	87
All	All	1020/1140 (90%)	1003 (98%)	17 (2%)	68	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	49	LYS
1	A	144	ASN
1	A	231	ASN
1	B	2	MET
1	B	124	ASN
1	B	127	LEU
1	B	164	LEU

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Mol	Chain	Res	Type
2	C	288	ASP
2	C	303	ASN
2	C	487	LEU
2	C	605	ASP
2	D	287	GLU
2	D	440	GLU
2	D	555	ASN
2	D	564	LEU
2	D	606	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	99	GLN
1	A	144	ASN
1	A	206	GLN
1	A	231	ASN
1	B	24	ASN
1	B	99	GLN
1	B	121	ASN
1	B	171	GLN
2	C	303	ASN
2	C	316	ASN
2	C	394	ASN
2	C	415	ASN
2	C	424	ASN
2	C	554	ASN
2	C	555	ASN
2	D	316	ASN
2	D	342	GLN
2	D	394	ASN
2	D	407	ASN
2	D	415	ASN
2	D	424	ASN

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 ⓘ

6 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$
3	RJ6	A	609	-	11,17,17	1.04	1 (9%)	14,22,22	2.83	5 (35%)
4	NDP	A	610	-	42,52,52	1.71	7 (16%)	55,80,80	1.85	12 (21%)
3	RJ6	B	609	-	11,17,17	0.77	0	14,22,22	3.23	5 (35%)
4	NDP	B	610	-	42,52,52	1.67	6 (14%)	55,80,80	1.93	17 (30%)
5	UMP	C	611	-	16,21,21	2.17	5 (31%)	23,31,31	3.27	8 (34%)
5	UMP	D	611	-	16,21,21	2.12	5 (31%)	23,31,31	3.26	7 (30%)

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
3	RJ6	A	609	-	-	0/7/12/12	0/1/1/1
4	NDP	A	610	-	-	0/30/77/77	0/5/5/5
3	RJ6	B	609	-	-	0/7/12/12	0/1/1/1
4	NDP	B	610	-	-	0/30/77/77	0/5/5/5
5	UMP	C	611	-	-	0/6/22/22	0/2/2/2
5	UMP	D	611	-	-	0/6/22/22	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	NDP	C4N-C5N	-5.23	1.37	1.49
4	B	610	NDP	C4N-C5N	-5.13	1.38	1.49
5	D	611	UMP	P-OP3	-2.52	1.45	1.54
4	B	610	NDP	C3B-C2B	-2.47	1.47	1.53
5	C	611	UMP	P-OP3	-2.47	1.45	1.54
4	A	610	NDP	C3B-C2B	-2.34	1.47	1.53
5	D	611	UMP	P-OP2	-2.16	1.46	1.54
4	B	610	NDP	C3B-C4B	-2.13	1.47	1.53
5	C	611	UMP	P-OP2	-2.13	1.47	1.54
3	A	609	RJ6	C2-C3	-2.05	1.35	1.38
4	A	610	NDP	O4B-C1B	2.06	1.43	1.41
4	A	610	NDP	C2D-C1D	2.08	1.60	1.53
4	A	610	NDP	C4A-N3A	2.12	1.38	1.35
5	D	611	UMP	O4'-C4'	2.17	1.50	1.45
5	C	611	UMP	O4'-C4'	2.44	1.50	1.45
4	B	610	NDP	C4A-N3A	2.74	1.39	1.35
4	A	610	NDP	C6N-C5N	2.82	1.38	1.33
4	B	610	NDP	C6N-C5N	2.98	1.39	1.33
5	D	611	UMP	O4'-C1'	4.09	1.51	1.42
5	C	611	UMP	O4'-C1'	4.30	1.52	1.42
4	B	610	NDP	C2N-C3N	4.60	1.46	1.34
4	A	610	NDP	C2N-C3N	5.12	1.47	1.34
5	D	611	UMP	C4-N3	5.44	1.43	1.33
5	C	611	UMP	C4-N3	5.45	1.43	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	NDP	N3A-C2A-N1A	-4.91	125.13	128.89
4	A	610	NDP	N3A-C2A-N1A	-4.62	125.36	128.89
4	A	610	NDP	C4B-O4B-C1B	-4.49	104.79	109.72
4	A	610	NDP	C3N-C2N-N1N	-4.43	116.79	123.14
4	B	610	NDP	C3N-C2N-N1N	-4.22	117.09	123.14
4	B	610	NDP	C4B-O4B-C1B	-3.93	105.39	109.72
5	D	611	UMP	O4'-C1'-C2'	-3.59	99.11	106.27
4	B	610	NDP	C1D-N1N-C2N	-3.49	114.83	120.91
4	A	610	NDP	C3B-C2B-C1B	-3.44	96.07	102.73
5	C	611	UMP	O4'-C1'-C2'	-3.40	99.50	106.27
5	C	611	UMP	C5-C4-N3	-3.01	115.41	123.12
5	D	611	UMP	C5-C4-N3	-2.87	115.76	123.12
4	A	610	NDP	C1D-N1N-C2N	-2.87	115.92	120.91
4	B	610	NDP	O7N-C7N-N7N	-2.75	115.93	122.76
4	A	610	NDP	O7N-C7N-N7N	-2.62	116.24	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	RJ6	C2-C1-C6	-2.58	116.54	120.99
5	D	611	UMP	O4'-C4'-C3'	-2.57	99.20	105.67
3	A	609	RJ6	C4-C3-C2	-2.46	116.74	120.99
4	B	610	NDP	C3B-C2B-C1B	-2.46	97.97	102.73
5	C	611	UMP	O4'-C4'-C3'	-2.44	99.54	105.67
3	B	609	RJ6	C4-C3-C2	-2.41	116.83	120.99
4	B	610	NDP	C4N-C5N-C6N	-2.36	118.69	122.58
3	A	609	RJ6	C2-C1-C6	-2.26	117.09	120.99
4	A	610	NDP	C4N-C5N-C6N	-2.12	119.09	122.58
4	B	610	NDP	C3D-C2D-C1D	-2.01	97.36	101.40
4	B	610	NDP	C2D-C3D-C4D	2.06	106.84	102.61
5	C	611	UMP	C2'-C3'-C4'	2.07	107.07	102.77
4	B	610	NDP	O2B-C2B-C3B	2.14	119.82	111.51
4	B	610	NDP	O4B-C1B-C2B	2.17	110.53	106.60
3	A	609	RJ6	C10-O9-C3	2.17	122.60	117.51
5	D	611	UMP	C4'-O4'-C1'	2.28	115.24	109.47
4	B	610	NDP	PN-O3-PA	2.33	139.27	132.73
5	C	611	UMP	C4'-O4'-C1'	2.33	115.36	109.47
4	A	610	NDP	O3B-C3B-C4B	2.45	118.40	111.05
4	A	610	NDP	O3B-C3B-C2B	2.49	118.34	111.16
4	B	610	NDP	C2B-C3B-C4B	2.57	107.94	101.85
4	A	610	NDP	PN-O3-PA	2.79	140.56	132.73
4	B	610	NDP	O3B-C3B-C2B	2.82	119.31	111.16
4	A	610	NDP	O4B-C1B-N9A	2.98	114.33	108.10
5	C	611	UMP	C2'-C1'-N1	3.14	121.78	114.16
4	B	610	NDP	O3B-C3B-C4B	3.25	120.81	111.05
4	B	610	NDP	O4B-C1B-N9A	3.78	116.01	108.10
5	D	611	UMP	C2'-C1'-N1	3.84	123.50	114.16
4	A	610	NDP	C5N-C4N-C3N	4.01	123.56	112.52
4	B	610	NDP	C5N-C4N-C3N	4.03	123.61	112.52
3	B	609	RJ6	C3-C2-C1	4.22	125.15	118.53
3	A	609	RJ6	C3-C2-C1	4.50	125.59	118.53
5	D	611	UMP	O4'-C1'-N1	5.68	117.56	107.72
5	C	611	UMP	O4'-C1'-N1	5.71	117.61	107.72
3	B	609	RJ6	C10-O9-C3	7.24	134.46	117.51
3	B	609	RJ6	C8-O7-C1	7.42	134.88	117.51
3	A	609	RJ6	C8-O7-C1	8.15	136.60	117.51
5	D	611	UMP	C4-N3-C2	12.28	126.31	114.14
5	C	611	UMP	C4-N3-C2	12.45	126.47	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	609	RJ6	6	0
4	A	610	NDP	7	0
3	B	609	RJ6	3	0
4	B	610	NDP	6	0
5	D	611	UMP	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	221/280 (78%)	0.64	28 (12%) 5 3	22, 41, 86, 90	0
1	B	221/280 (78%)	2.08	83 (37%) 0 0	30, 81, 90, 90	0
2	C	326/328 (99%)	0.36	20 (6%) 25 20	22, 31, 74, 90	0
2	D	326/328 (99%)	0.19	21 (6%) 23 18	19, 28, 73, 90	0
All	All	1094/1216 (89%)	0.71	152 (13%) 4 2	19, 36, 90, 90	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	MET	12.8
1	A	1	MET	12.6
1	B	1	MET	11.9
1	A	2	MET	10.7
1	B	95	SER	9.7
1	B	231	ASN	9.5
1	B	3	GLU	8.9
1	B	27	LYS	8.9
1	B	93	PRO	8.6
1	B	94	ASN	8.2
1	B	29	ASN	7.8
1	B	136	PHE	7.4
1	B	26	GLY	6.8
1	B	232	LYS	6.8
2	D	345	ARG	6.5
1	B	9	PHE	6.4
1	B	23	LYS	6.3
1	A	85	THR	6.3
1	B	96	LYS	6.3
1	B	165	GLY	6.0
1	A	31	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	75	TYR	5.8
1	B	25	GLU	5.7
1	B	70	TYR	5.6
1	B	81	LEU	5.6
1	A	231	ASN	5.6
1	B	24	ASN	5.6
1	B	97	LYS	5.6
2	C	299	LYS	5.6
2	C	301	GLU	5.6
1	B	76	LYS	5.2
2	D	283	ASP	5.1
2	C	303	ASN	5.1
1	B	138	GLU	5.1
1	B	157	ASN	5.1
1	B	5	VAL	5.0
1	A	29	ASN	4.9
1	A	23	LYS	4.9
1	B	116	PHE	4.8
1	A	25	GLU	4.7
2	C	307	ILE	4.6
1	A	26	GLY	4.6
1	B	28	LYS	4.6
1	A	230	ASN	4.5
1	B	159	TYR	4.5
1	B	139	ASP	4.5
2	C	300	GLU	4.4
2	D	305	ASN	4.3
1	B	134	GLU	4.1
1	A	96	LYS	4.1
1	A	24	ASN	4.0
1	B	73	LEU	4.0
1	A	28	LYS	4.0
2	D	607	ALA	3.9
1	B	131	LEU	3.9
2	D	608	ALA	3.9
1	B	141	TYR	3.8
2	D	348	VAL	3.8
1	B	137	ASP	3.8
1	A	30	GLU	3.7
1	A	27	LYS	3.7
2	D	309	PRO	3.7
1	B	22	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	C	283	ASP	3.5
1	B	66	ASN	3.5
1	B	35	TYR	3.5
1	B	118	PRO	3.3
2	D	284	ASP	3.3
1	B	230	ASN	3.3
1	A	3	GLU	3.2
2	C	608	ALA	3.2
2	C	302	LYS	3.2
1	B	156	LEU	3.2
1	B	67	GLU	3.1
2	D	299	LYS	3.1
2	D	606	MET	3.1
1	B	4	GLN	3.1
1	A	22	SER	3.1
1	B	45	VAL	3.1
1	B	135	ASP	3.1
1	B	140	VAL	2.9
2	D	346	THR	2.9
1	B	151	VAL	2.8
1	A	229	THR	2.8
1	A	4	GLN	2.8
1	B	80	TYR	2.8
1	B	7	ASP	2.8
1	B	58	PHE	2.7
2	D	308	HIS	2.7
1	A	84	GLU	2.7
2	D	310	ASN	2.6
1	B	105	GLY	2.6
2	C	310	ASN	2.6
1	B	115	LYS	2.6
1	B	155	LYS	2.6
1	B	228	LYS	2.6
1	B	65	VAL	2.6
2	D	304	LYS	2.6
2	C	284	ASP	2.6
1	B	146	VAL	2.5
1	B	40	LEU	2.5
1	B	104	MET	2.5
2	D	306	SER	2.5
1	B	74	LYS	2.5
2	C	298	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	46	LEU	2.5
1	B	168	VAL	2.4
1	B	113	PRO	2.4
1	B	123	ILE	2.4
2	D	347	GLY	2.4
2	C	308	HIS	2.4
2	C	375	PHE	2.4
1	B	98	LEU	2.4
1	A	33	ASN	2.3
1	B	229	THR	2.3
2	C	546	VAL	2.3
2	C	286	GLU	2.3
1	A	35	TYR	2.3
1	A	206	GLN	2.2
1	B	78	CYS	2.2
1	B	106	ARG	2.2
1	A	72	LYS	2.2
2	D	313	GLN	2.2
1	B	172	GLU	2.2
1	B	201	ASN	2.2
1	B	203	ASN	2.2
2	C	291	VAL	2.2
1	A	178	LEU	2.2
2	C	287	GLU	2.2
2	C	346	THR	2.2
2	C	345	ARG	2.2
1	B	13	ALA	2.2
1	B	206	GLN	2.2
1	B	195	VAL	2.1
2	D	285	GLU	2.1
1	A	49	LYS	2.1
1	B	43	LYS	2.1
1	B	6	CYS	2.1
1	B	44	GLY	2.1
2	D	344	ASP	2.1
1	B	153	LEU	2.1
1	B	103	VAL	2.1
2	D	605	ASP	2.1
1	B	208	ILE	2.1
2	D	307	ILE	2.1
1	A	75	TYR	2.1
1	B	164	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	119	LEU	2.0
1	B	152	LEU	2.0
1	B	173	PHE	2.0
2	C	559	SER	2.0
1	A	177	LYS	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, 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
5	UMP	D	611	20/20	0.84	0.42	12.94	75,86,90,90	0
3	RJ6	A	609	17/17	0.88	0.29	5.21	37,51,60,62	0
3	RJ6	B	609	17/17	0.67	0.46	3.57	85,89,90,90	0
5	UMP	C	611	20/20	0.87	0.31	2.73	76,87,90,90	0
4	NDP	A	610	48/48	0.96	0.19	1.20	40,44,59,60	0
4	NDP	B	610	48/48	0.83	0.28	0.22	87,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.