



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:23 PM GMT

PDB ID : 4DP3  
Title : Quadruple mutant (N51I+C59R+S108N+I164L)plasmodium falciparum dihydrofolate reductase-thymidylatesynthase (PfDHFR-TS) complexed with P218 and NADPH  
Authors : Yuthavong, Y.; Vilaivan, T.; Kamchonwongpaisan, S.; Charman, S.A.; McLennan, D.N.; White, K.L.; Vivas, L.; Bongard, E.; Chitnumsub, P.; Tarnchompoo, B.; Thongphanchang, C.; Taweechai, S.; Vanichtanakul, J.; Arwon, U.; Fantauzzi, P.; Yuvaniyama, J.; Charman, W.N.; Matthews, D.  
Deposited on : 2012-02-13  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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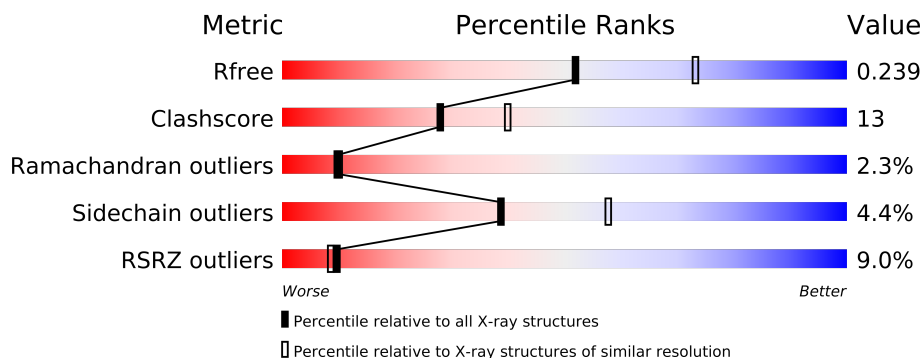
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	608	
1	B	608	

## 2 Entry composition i

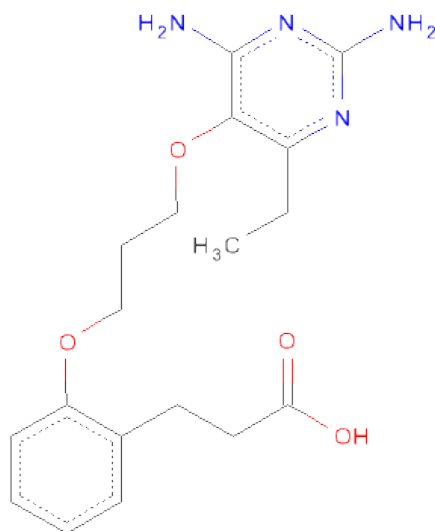
There are 5 unique types of molecules in this entry. The entry contains 9667 atoms, of which 0 are hydrogen and 0 are deuterium.

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-thymidylatesynthase.

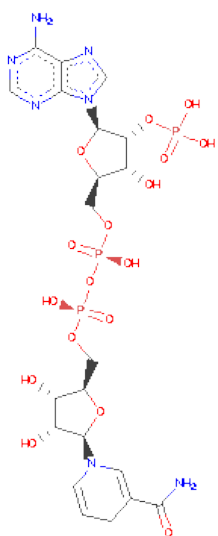
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4539	2931	751	830	27			
1	B	544	Total	C	N	O	S	0	0	0
			4529	2924	751	828	26			

- Molecule 2 is 3-(2-{3-[(2,4-DIAMINO-6-ETHYLPYRIMIDIN-5-YL)OXY]PROPOXY}PHE NYL)PROPANOICACID (three-letter code: MMV) (formula: C<sub>18</sub>H<sub>24</sub>N<sub>4</sub>O<sub>4</sub>).



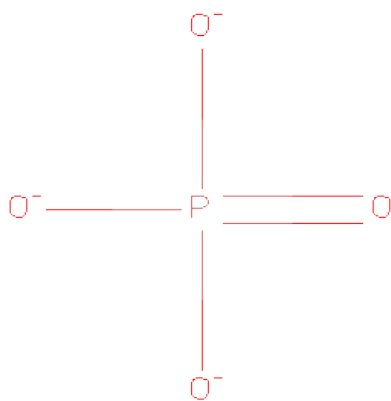
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	18	4	4		
2	B	1	Total	C	N	O	0	0
			26	18	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

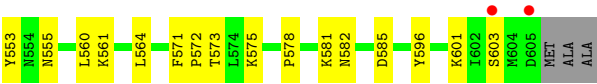


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total 233	O 233	0	0
5	B	208	Total 208	O 208	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.50Å 156.20Å 164.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.90-2.40) 96.6 (19.90-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.239 0.205 , 0.239	Depositor DCC
$R_{free}$ test set	2903 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.6	EDS
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 57640 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: NDP, PO4, MMV

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	1/4644 (0.0%)	0.71	2/6267 (0.0%)
1	B	0.38	0/4634	0.72	6/6254 (0.1%)
All	All	0.39	1/9278 (0.0%)	0.72	8/12521 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	CYS	CB-SG	-5.06	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLY	N-CA-C	-10.23	87.53	113.10
1	B	165	GLY	N-CA-C	7.31	131.38	113.10
1	B	300	GLU	N-CA-C	-6.50	93.45	111.00
1	B	166	GLY	N-CA-C	-6.45	96.99	113.10
1	A	165	GLY	N-CA-C	5.93	127.92	113.10
1	B	299	LYS	N-CA-C	5.32	125.36	111.00
1	B	26	GLY	N-CA-C	-5.21	100.07	113.10
1	B	305	ASN	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4539	0	4501	94	0
1	B	4529	0	4490	144	0
2	A	26	0	23	1	0
2	B	26	0	23	0	0
3	A	48	0	26	3	0
3	B	48	0	26	5	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	233	0	0	6	0
5	B	208	0	0	12	0
All	All	9667	0	9089	232	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (232) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:301:GLU:C	1:B:303:ASN:H	1.48	1.06
1:B:490:CYS:SG	5:B:989:HOH:O	2.21	0.96
1:B:299:LYS:C	1:B:301:GLU:H	1.64	0.91
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.53	0.89
1:B:137:ASP:HB3	5:B:895:HOH:O	1.78	0.83
1:A:59:ARG:O	1:A:63:THR:HG23	1.79	0.82
1:B:299:LYS:HG3	1:B:301:GLU:HA	1.61	0.81
1:B:301:GLU:C	1:B:303:ASN:N	2.26	0.80
1:A:329:LEU:HD22	1:A:564:LEU:HD12	1.64	0.78
1:A:298:GLU:HG3	1:A:299:LYS:O	1.84	0.77
1:B:299:LYS:HE2	1:B:301:GLU:HB3	1.66	0.76
1:A:302:LYS:HG2	1:A:302:LYS:O	1.86	0.74
1:B:415:ASN:HB2	5:B:894:HOH:O	1.86	0.74
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.28	0.74
1:B:59:ARG:O	1:B:63:THR:HG23	1.91	0.71
1:B:573:THR:HG23	5:B:879:HOH:O	1.88	0.71
1:A:454:ASP:OD2	1:A:457:LYS:HG3	1.91	0.70
1:B:4:GLN:HB3	1:B:7:ASP:OD2	1.92	0.69
1:B:494:CYS:SG	1:B:525:TYR:HE2	2.15	0.69
1:A:376:LEU:HD22	1:A:379:ILE:HD11	1.75	0.69
1:B:582:ASN:HB3	5:B:901:HOH:O	1.93	0.68
1:B:299:LYS:C	1:B:301:GLU:N	2.37	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ASN:HB2	1:B:148:ASP:OD2	1.93	0.67
1:B:65:VAL:HG22	1:B:159:TYR:CB	2.24	0.67
1:B:108:ASN:ND2	1:B:165:GLY:O	2.28	0.67
1:A:490:CYS:SG	5:A:1016:HOH:O	2.53	0.66
1:B:81:LEU:CD2	1:B:83:LYS:HE2	2.26	0.66
1:B:42:ASN:HB2	1:B:193:CYS:HA	1.78	0.66
1:B:345:ARG:HD3	5:B:876:HOH:O	1.97	0.65
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.79	0.65
1:A:21:GLU:HB2	5:A:994:HOH:O	1.96	0.65
1:B:131:LEU:HD22	1:B:136:PHE:HE2	1.60	0.65
1:B:304:LYS:HD3	1:B:337:MET:O	1.96	0.65
1:B:415:ASN:C	1:B:415:ASN:HD22	2.00	0.64
1:B:166:GLY:HA3	3:B:702:NDP:PA	2.38	0.64
1:A:171:GLN:O	1:A:175:GLU:HG3	1.97	0.64
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.79	0.64
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.81	0.63
1:A:2:MET:SD	1:A:2:MET:O	2.56	0.63
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.32	0.63
1:A:100:ASN:OD1	1:A:159:TYR:HB3	1.98	0.63
1:B:306:SER:C	1:B:307:ILE:HG12	2.19	0.62
1:A:494:CYS:SG	1:A:525:TYR:HE2	2.22	0.62
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.81	0.61
1:B:299:LYS:HE3	1:B:301:GLU:HB2	1.82	0.61
1:B:299:LYS:CE	1:B:301:GLU:HB3	2.30	0.61
1:B:299:LYS:HG2	1:B:299:LYS:O	2.00	0.61
1:B:114:LYS:HB2	5:B:931:HOH:O	2.01	0.59
1:A:124:ASN:N	1:A:124:ASN:HD22	1.99	0.59
1:B:23:LYS:O	1:B:25:GLU:N	2.32	0.59
1:A:72:LYS:HB3	1:A:72:LYS:NZ	2.17	0.59
1:B:81:LEU:HG	1:B:83:LYS:HE2	1.85	0.59
1:A:582:ASN:HB2	5:A:949:HOH:O	2.01	0.58
1:B:23:LYS:C	1:B:25:GLU:H	2.07	0.58
1:B:575:LYS:HG3	5:B:1003:HOH:O	2.03	0.58
1:A:454:ASP:CG	1:A:457:LYS:HG3	2.25	0.57
1:B:301:GLU:O	1:B:303:ASN:N	2.34	0.57
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.39	0.57
1:B:299:LYS:CE	1:B:301:GLU:CB	2.82	0.57
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.39	0.57
1:B:169:VAL:O	1:B:173:PHE:HD2	1.88	0.56
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.39	0.56
1:B:494:CYS:SG	1:B:525:TYR:CE2	2.98	0.56
1:B:115:LYS:HE3	1:B:116:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:51:ILE:CD1	1:A:187:ILE:HD12	2.32	0.56
1:B:470:ARG:HD3	5:B:888:HOH:O	2.05	0.55
1:B:1:MET:HA	1:B:1:MET:HE2	1.88	0.55
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.41	0.55
1:B:357:ILE:CD1	1:B:546:VAL:HG22	2.37	0.55
1:A:494:CYS:SG	1:A:525:TYR:CE2	3.00	0.55
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.89	0.55
1:A:493:LEU:HD12	1:A:493:LEU:C	2.26	0.55
1:B:171:GLN:O	1:B:175:GLU:HG2	2.06	0.55
1:A:307:ILE:HG21	1:A:312:PHE:HE2	1.72	0.54
1:B:300:GLU:OE1	1:B:302:LYS:HE3	2.07	0.54
1:A:373:LYS:HE2	1:A:375:PHE:CZ	2.42	0.54
1:A:22:SER:C	1:A:23:LYS:HG2	2.28	0.54
1:A:284:ASP:HB2	1:A:287:GLU:OE1	2.08	0.54
1:A:312:PHE:CE1	1:A:564:LEU:HD23	2.43	0.54
1:B:493:LEU:HD12	1:B:493:LEU:C	2.29	0.54
1:A:16:ALA:HA	1:A:185:THR:HB	1.90	0.53
1:B:299:LYS:HG3	1:B:301:GLU:CA	2.34	0.53
1:B:575:LYS:CG	5:B:1003:HOH:O	2.56	0.53
1:B:298:GLU:HG2	1:B:299:LYS:N	2.23	0.53
1:A:146:VAL:HG21	1:A:176:LYS:HE3	1.90	0.52
1:A:357:ILE:HD13	1:A:357:ILE:C	2.30	0.52
1:B:547:LEU:N	1:B:547:LEU:HD23	2.25	0.52
1:B:58:PHE:CE1	1:B:164:LEU:HD22	2.45	0.52
1:B:308:HIS:ND1	1:B:308:HIS:N	2.56	0.52
1:B:95:SER:OG	1:B:96:LYS:N	2.43	0.52
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.45	0.52
1:A:63:THR:HG22	1:A:122:ARG:HD3	1.91	0.51
1:B:108:ASN:HB2	1:B:165:GLY:O	2.10	0.51
1:A:376:LEU:HD13	1:A:527:ILE:HD11	1.92	0.51
1:B:555:ASN:HB3	5:B:963:HOH:O	2.11	0.51
1:B:299:LYS:HE2	1:B:301:GLU:CB	2.37	0.51
1:A:112:ILE:HD11	2:A:701:MMV:H15	1.91	0.51
1:A:63:THR:HG22	1:A:122:ARG:CD	2.39	0.51
1:A:192:GLU:HA	5:A:994:HOH:O	2.10	0.51
1:B:95:SER:O	1:B:96:LYS:HG2	2.10	0.50
1:B:144:ASN:O	3:B:702:NDP:H2A	2.12	0.50
1:B:134:GLU:C	1:B:136:PHE:H	2.14	0.50
1:B:169:VAL:HG23	3:B:702:NDP:O1A	2.10	0.50
1:B:312:PHE:HB2	1:B:316:ASN:ND2	2.26	0.50
1:A:485:MET:SD	1:A:489:PRO:HD3	2.52	0.50
1:B:305:ASN:N	5:B:1008:HOH:O	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:ARG:HB2	3:B:702:NDP:O3X	2.13	0.49
1:B:81:LEU:CG	1:B:83:LYS:HE2	2.42	0.48
1:A:206:GLN:HG2	1:A:229:THR:HG22	1.94	0.48
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.95	0.48
1:B:168:VAL:O	1:B:172:GLU:HG2	2.13	0.48
1:A:423:VAL:O	1:A:424:ASN:HB2	2.14	0.48
1:B:29:ASN:O	1:B:30:GLU:C	2.52	0.48
1:B:28:LYS:HG3	1:B:29:ASN:N	2.29	0.48
1:B:43:LYS:H	1:B:194:ASP:CG	2.17	0.48
1:B:303:ASN:C	1:B:304:LYS:HG3	2.33	0.48
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.78	0.48
1:B:21:GLU:C	1:B:23:LYS:H	2.17	0.48
1:B:141:TYR:N	1:B:141:TYR:CD2	2.82	0.47
1:A:214:TYR:O	1:A:220:THR:HA	2.14	0.47
1:B:115:LYS:HE3	1:B:116:PHE:CE2	2.49	0.47
1:A:307:ILE:CG2	1:A:312:PHE:HE2	2.26	0.47
1:B:102:VAL:HG11	1:B:122:ARG:HD2	1.96	0.47
1:A:315:TYR:HB2	1:A:564:LEU:O	2.14	0.47
1:B:572:PRO:HB3	1:B:596:TYR:HA	1.96	0.47
1:B:345:ARG:NH2	4:B:703:PO4:O1	2.47	0.47
1:B:145:LYS:HA	3:B:702:NDP:N1A	2.29	0.47
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.96	0.47
1:B:308:HIS:O	1:B:311:ASP:HB2	2.15	0.46
1:B:78:CYS:O	1:B:82:ASN:N	2.47	0.46
1:B:1:MET:HA	1:B:1:MET:CE	2.45	0.46
1:B:300:GLU:CD	1:B:302:LYS:HE3	2.36	0.46
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.51	0.46
1:A:373:LYS:HE2	1:A:375:PHE:CE2	2.51	0.46
1:A:289:ASP:HA	1:A:292:TYR:CD2	2.50	0.46
1:A:297:LYS:O	1:A:298:GLU:O	2.34	0.46
1:B:301:GLU:HG3	1:B:301:GLU:O	2.16	0.46
1:A:382:GLU:O	1:A:385:TRP:HB3	2.14	0.46
1:A:165:GLY:HA2	1:A:169:VAL:HB	1.97	0.46
1:B:299:LYS:HE3	1:B:301:GLU:CB	2.43	0.46
1:B:102:VAL:HB	1:B:164:LEU:HD11	1.97	0.46
1:B:553:TYR:HB3	1:B:555:ASN:OD1	2.15	0.46
1:B:65:VAL:HG22	1:B:159:TYR:HB2	1.97	0.46
1:B:382:GLU:O	1:B:385:TRP:HB3	2.16	0.46
1:A:193:CYS:N	5:A:994:HOH:O	2.48	0.45
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.81	0.45
1:B:459:ILE:HG13	1:B:460:ILE:N	2.31	0.45
1:B:136:PHE:CE2	1:B:142:ILE:HD11	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:580:ILE:O	1:A:581:LYS:HD3	2.16	0.45
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.51	0.45
1:B:141:TYR:H	1:B:141:TYR:HD2	1.63	0.45
1:A:357:ILE:HD13	1:A:358:MET:N	2.31	0.45
1:B:63:THR:HG22	1:B:122:ARG:CD	2.46	0.45
1:B:578:PRO:O	1:B:581:LYS:HE3	2.16	0.45
1:A:319:LYS:HG3	1:A:320:TYR:CD2	2.51	0.45
1:A:2:MET:O	1:A:3:GLU:C	2.54	0.44
1:A:485:MET:O	1:A:486:ALA:C	2.54	0.44
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.99	0.44
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.99	0.44
1:A:166:GLY:HA3	3:A:702:NDP:O1A	2.17	0.44
1:A:506:ILE:HG12	1:A:544:ILE:HB	2.00	0.44
1:B:65:VAL:HG22	1:B:159:TYR:HB3	1.97	0.44
1:A:210:VAL:HG21	1:A:326:TYR:HE2	1.82	0.44
1:B:35:TYR:CZ	1:B:38:ARG:HD3	2.53	0.44
1:B:12:TYR:CE1	1:B:180:LYS:HB3	2.53	0.44
1:B:43:LYS:N	1:B:194:ASP:OD2	2.44	0.44
1:B:216:SER:O	1:B:219:THR:HG22	2.18	0.44
1:B:312:PHE:CE1	1:B:561:LYS:HG2	2.53	0.44
1:B:118:PRO:HB2	1:B:124:ASN:ND2	2.32	0.44
1:B:299:LYS:CG	1:B:301:GLU:CA	2.96	0.44
1:B:1:MET:C	1:B:3:GLU:H	2.19	0.44
1:A:421:ARG:HH11	1:A:421:ARG:HG2	1.83	0.44
1:A:172:GLU:O	1:A:176:LYS:HG3	2.17	0.43
1:B:172:GLU:O	1:B:176:LYS:HG3	2.17	0.43
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.54	0.43
1:B:307:ILE:CG2	1:B:312:PHE:CE2	3.01	0.43
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.83	0.43
1:A:516:LEU:HD21	1:A:604:MET:CG	2.48	0.43
1:B:459:ILE:O	1:B:463:ILE:HG13	2.19	0.43
1:A:553:TYR:HB3	1:A:555:ASN:OD1	2.18	0.43
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.54	0.43
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.53	0.43
1:B:131:LEU:HD22	1:B:136:PHE:CE2	2.48	0.43
1:A:318:LEU:HD23	1:A:318:LEU:N	2.34	0.43
1:B:9:PHE:CE2	1:B:150:ILE:HG23	2.54	0.43
1:A:22:SER:O	1:A:25:GLU:OE1	2.37	0.42
1:A:40:LEU:O	1:A:47:PRO:HD3	2.18	0.42
1:A:603:SER:HA	5:A:1015:HOH:O	2.19	0.42
1:B:513:ASP:OD2	1:B:516:LEU:HB2	2.19	0.42
1:B:97:LYS:O	1:B:99:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:514:LEU:HD21	1:B:550:ALA:HB1	2.00	0.42
1:A:166:GLY:HA3	3:A:702:NDP:O2A	2.18	0.42
1:A:376:LEU:O	1:A:380:ILE:HG13	2.17	0.42
1:B:134:GLU:HG2	1:B:134:GLU:H	1.57	0.42
1:A:560:LEU:HG	1:A:604:MET:CE	2.50	0.42
1:A:72:LYS:HB3	1:A:72:LYS:HZ3	1.81	0.42
1:A:510:ARG:HG3	1:A:511:SER:N	2.34	0.42
1:A:557:ILE:O	1:A:561:LYS:HG3	2.19	0.42
1:B:41:GLY:O	1:B:193:CYS:HB3	2.20	0.42
1:A:22:SER:HB2	1:A:25:GLU:CD	2.40	0.42
1:B:344:ASP:O	1:B:346:THR:N	2.52	0.42
1:B:128:SER:HB3	1:B:131:LEU:HB2	2.02	0.42
1:B:299:LYS:CE	1:B:301:GLU:HB2	2.46	0.42
1:B:307:ILE:HG23	1:B:561:LYS:HE2	2.00	0.42
1:B:303:ASN:O	1:B:304:LYS:HG3	2.20	0.42
1:B:582:ASN:HB2	1:B:585:ASP:OD2	2.20	0.42
1:B:221:LEU:HD23	1:B:221:LEU:N	2.35	0.42
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.02	0.42
1:A:514:LEU:HD21	1:A:550:ALA:HB1	2.02	0.42
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.85	0.41
1:B:125:VAL:CG1	1:B:143:ILE:HD11	2.49	0.41
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.88	0.41
1:A:20:VAL:HG11	1:A:38:ARG:HG3	2.02	0.41
1:B:415:ASN:ND2	1:B:415:ASN:O	2.42	0.41
1:A:459:ILE:O	1:A:463:ILE:HG13	2.20	0.41
1:A:303:ASN:ND2	1:A:338:ASN:OD1	2.54	0.41
1:A:63:THR:HG22	1:A:122:ARG:NE	2.36	0.41
1:A:516:LEU:CD2	1:A:604:MET:HG3	2.50	0.41
1:B:357:ILE:HD13	1:B:546:VAL:HG22	2.03	0.41
1:A:560:LEU:HG	1:A:604:MET:HE1	2.02	0.41
1:B:306:SER:O	1:B:307:ILE:HG12	2.21	0.41
1:B:324:PRO:HG2	1:B:365:TYR:CZ	2.56	0.41
1:A:344:ASP:O	1:A:346:THR:N	2.54	0.41
1:A:604:MET:HB3	1:A:604:MET:HE3	1.97	0.41
1:A:499:PHE:CZ	1:B:340:ASN:HB3	2.56	0.41
1:B:63:THR:HG22	1:B:122:ARG:NE	2.37	0.40
1:B:309:PRO:C	1:B:311:ASP:H	2.25	0.40
1:A:210:VAL:HG23	1:A:210:VAL:O	2.20	0.40
1:B:284:ASP:OD1	1:B:284:ASP:N	2.53	0.40
1:A:189:SER:HG	1:A:191:TYR:HE2	1.69	0.40
1:A:283:ASP:OD1	1:A:284:ASP:N	2.54	0.40
1:A:493:LEU:O	1:A:493:LEU:HD12	2.21	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	539/608 (89%)	507 (94%)	21 (4%)	11 (2%)	11	13
1	B	538/608 (88%)	484 (90%)	40 (7%)	14 (3%)	8	8
All	All	1077/1216 (89%)	991 (92%)	61 (6%)	25 (2%)	10	10

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	23	LYS
1	A	298	GLU
1	A	304	LYS
1	B	28	LYS
1	B	299	LYS
1	A	3	GLU
1	A	310	ASN
1	A	345	ARG
1	A	430	TYR
1	B	22	SER
1	B	27	LYS
1	B	29	ASN
1	B	115	LYS
1	B	345	ARG
1	B	430	TYR
1	A	309	PRO
1	B	114	LYS
1	B	133	LYS
1	B	302	LYS
1	A	26	GLY
1	A	284	ASP
1	B	24	ASN
1	B	298	GLU

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Mol	Chain	Res	Type
1	B	309	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/570 (90%)	487 (96%)	23 (4%)	38	57
1	B	509/570 (89%)	487 (96%)	22 (4%)	40	59
All	All	1019/1140 (89%)	974 (96%)	45 (4%)	39	58

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	21	GLU
1	A	25	GLU
1	A	27	LYS
1	A	28	LYS
1	A	59	ARG
1	A	63	THR
1	A	84	GLU
1	A	85	THR
1	A	104	MET
1	A	124	ASN
1	A	144	ASN
1	A	286	GLU
1	A	318	LEU
1	A	357	ILE
1	A	402	ARG
1	A	449	GLU
1	A	459	ILE
1	A	491	HIS
1	A	524	SER
1	A	564	LEU
1	A	605	ASP
1	A	606	MET
1	B	4	GLN

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Mol	Chain	Res	Type
1	B	23	LYS
1	B	27	LYS
1	B	31	VAL
1	B	50	CYS
1	B	55	MET
1	B	71	GLU
1	B	107	THR
1	B	127	LEU
1	B	134	GLU
1	B	135	ASP
1	B	139	ASP
1	B	143	ILE
1	B	145	LYS
1	B	195	VAL
1	B	306	SER
1	B	308	HIS
1	B	344	ASP
1	B	415	ASN
1	B	547	LEU
1	B	601	LYS
1	B	603	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	144	ASN
1	A	231	ASN
1	A	294	ASN
1	A	394	ASN
1	A	407	ASN
1	A	415	ASN
1	A	424	ASN
1	A	554	ASN
1	B	94	ASN
1	B	231	ASN
1	B	316	ASN
1	B	394	ASN
1	B	415	ASN
1	B	424	ASN
1	B	551	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
2	MMV	A	701	-	27,27,27	1.13	2 (7%)	35,35,35	1.86	6 (17%)
3	NDP	A	702	-	52,52,52	1.73	9 (17%)	80,80,80	1.84	17 (21%)
4	PO4	A	703	-	4,4,4	3.30	3 (75%)	6,6,6	0.30	0
2	MMV	B	701	-	27,27,27	1.47	6 (22%)	35,35,35	1.89	8 (22%)
3	NDP	B	702	-	52,52,52	1.77	8 (15%)	80,80,80	1.81	19 (23%)
4	PO4	B	703	-	4,4,4	3.36	3 (75%)	6,6,6	0.32	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	MMV	A	701	-	-	0/15/15/15	0/2/2/2
3	NDP	A	702	-	-	0/35/77/77	0/3/5/5
4	PO4	A	703	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMV	B	701	-	-	0/15/15/15	0/2/2/2
3	NDP	B	702	-	-	0/35/77/77	0/3/5/5
4	PO4	B	703	-	-	0/0/0/0	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NDP	C2N-C3N	5.54	1.45	1.34
3	A	702	NDP	C2N-C3N	5.38	1.45	1.34
3	B	702	NDP	C4N-C5N	-4.89	1.38	1.49
3	A	702	NDP	C4N-C5N	-4.71	1.38	1.49
3	A	702	NDP	C4N-C3N	-4.64	1.41	1.50
3	B	702	NDP	C4N-C3N	-4.44	1.41	1.50
4	B	703	PO4	P-O2	4.07	1.69	1.52
4	A	703	PO4	P-O2	4.05	1.69	1.52
3	B	702	NDP	C8A-N9A	3.94	1.42	1.36
4	A	703	PO4	P-O4	3.73	1.67	1.52
4	B	703	PO4	P-O3	3.66	1.67	1.52
4	B	703	PO4	P-O4	3.65	1.67	1.52
3	A	702	NDP	C8A-N9A	3.63	1.42	1.36
2	B	701	MMV	O26-C24	3.53	1.34	1.22
2	B	701	MMV	C6-C1	-3.16	1.39	1.41
4	A	703	PO4	P-O1	3.07	1.68	1.52
3	A	702	NDP	C2N-N1N	2.71	1.41	1.36
3	B	702	NDP	C6N-C5N	2.70	1.39	1.33
2	A	701	MMV	C6-C1	-2.66	1.39	1.41
3	B	702	NDP	C2N-N1N	2.57	1.41	1.36
2	B	701	MMV	O25-C24	-2.52	1.21	1.30
3	A	702	NDP	C6N-C5N	2.49	1.38	1.33
3	B	702	NDP	C3B-C2B	-2.45	1.47	1.53
2	B	701	MMV	C16-C17	2.32	1.44	1.40
3	B	702	NDP	C4A-N3A	2.25	1.39	1.35
3	A	702	NDP	PA-O3	-2.21	1.55	1.59
2	B	701	MMV	C3-N2	-2.17	1.31	1.35
3	A	702	NDP	C4A-N3A	2.10	1.38	1.35
2	A	701	MMV	C3-N4	-2.05	1.31	1.35
2	B	701	MMV	C3-N4	-2.03	1.31	1.35
3	A	702	NDP	C3B-C4B	-2.01	1.47	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	MMV	C3-N4-C5	6.95	121.02	115.99
3	A	702	NDP	O4B-C1B-N9A	6.90	114.86	108.44
2	B	701	MMV	C3-N4-C5	6.08	120.39	115.99
3	B	702	NDP	O4B-C1B-N9A	5.71	113.75	108.44
3	A	702	NDP	C4B-O4B-C1B	-4.83	104.51	109.75
3	B	702	NDP	C3N-C2N-N1N	-4.42	116.78	123.05
3	A	702	NDP	C3N-C2N-N1N	-4.27	116.98	123.05
3	B	702	NDP	C1D-N1N-C2N	-4.15	113.95	121.02
3	A	702	NDP	N3A-C2A-N1A	-4.10	125.28	128.71
3	A	702	NDP	C1D-N1N-C2N	-4.09	114.06	121.02
3	B	702	NDP	C5N-C4N-C3N	4.07	123.61	112.60
3	A	702	NDP	C5N-C4N-C3N	4.05	123.57	112.60
3	B	702	NDP	N3A-C2A-N1A	-3.94	125.42	128.71
3	B	702	NDP	C4B-O4B-C1B	-3.85	105.57	109.75
3	A	702	NDP	C3B-C2B-C1B	-3.79	95.35	102.73
2	B	701	MMV	C3-N2-C1	3.70	121.16	116.96
2	B	701	MMV	O26-C24-C23	-3.62	110.57	123.03
2	B	701	MMV	O25-C24-C23	3.49	126.55	114.22
2	A	701	MMV	C23-C22-C17	3.41	120.27	112.24
3	B	702	NDP	O4B-C1B-C2B	3.39	110.11	106.95
2	A	701	MMV	C3-N2-C1	3.31	120.72	116.96
3	B	702	NDP	O3B-C3B-C4B	3.25	120.65	111.08
3	B	702	NDP	C8A-N9A-C4A	-3.07	104.56	106.90
3	A	702	NDP	C8A-N9A-C4A	-3.02	104.59	106.90
3	B	702	NDP	PN-O3-PA	2.97	140.41	131.68
3	A	702	NDP	C4N-C3N-C2N	-2.91	118.14	121.68
2	A	701	MMV	C10-C9-C5	-2.81	108.00	115.23
3	B	702	NDP	O3B-C3B-C2B	2.75	119.29	111.20
3	A	702	NDP	O7N-C7N-N7N	-2.75	115.99	122.93
3	B	702	NDP	C3B-C2B-C1B	-2.74	97.40	102.73
3	A	702	NDP	PN-O3-PA	2.73	139.69	131.68
2	A	701	MMV	C14-O15-C16	2.71	124.31	117.65
3	B	702	NDP	O7N-C7N-N7N	-2.71	116.08	122.93
2	B	701	MMV	O15-C16-C17	2.71	119.53	115.56
2	A	701	MMV	N2-C3-N4	-2.66	121.01	125.55
2	B	701	MMV	N2-C3-N4	-2.63	121.07	125.55
3	A	702	NDP	C3D-C2D-C1D	-2.61	96.15	101.35
3	B	702	NDP	C2B-C3B-C4B	2.56	108.03	101.94
3	A	702	NDP	O3B-C3B-C2B	2.56	118.74	111.20
3	B	702	NDP	C4N-C3N-C2N	-2.56	118.56	121.68
2	B	701	MMV	C23-C22-C17	2.53	118.21	112.24
2	B	701	MMV	O15-C14-C13	2.36	117.69	108.42
3	B	702	NDP	C3D-C2D-C1D	-2.32	96.73	101.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NDP	C6N-N1N-C2N	2.30	122.45	119.44
3	B	702	NDP	C4N-C5N-C6N	-2.20	118.56	122.61
3	B	702	NDP	C2D-C3D-C4D	2.20	107.04	102.65
3	A	702	NDP	O3B-C3B-C4B	2.14	117.39	111.08
3	B	702	NDP	C6N-N1N-C2N	2.12	122.21	119.44
3	A	702	NDP	C2D-C3D-C4D	2.06	106.76	102.65
3	A	702	NDP	C4N-C5N-C6N	-2.03	118.87	122.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	545/608 (89%)	0.04	35 (6%) 19 17	22, 37, 92, 120	0
1	B	544/608 (89%)	0.34	64 (11%) 5 5	22, 43, 104, 121	0
All	All	1089/1216 (89%)	0.19	99 (9%) 10 8	22, 40, 99, 121	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	8.5
1	A	24	ASN	8.2
1	B	301	GLU	8.1
1	B	1	MET	7.8
1	B	303	ASN	7.7
1	B	26	GLY	7.7
1	A	2	MET	7.5
1	B	231	ASN	6.8
1	A	606	MET	6.7
1	B	94	ASN	6.6
1	A	85	THR	6.2
1	B	75	TYR	6.1
1	A	23	LYS	6.1
1	A	283	ASP	6.1
1	B	345	ARG	6.0
1	A	301	GLU	6.0
1	B	27	LYS	5.9
1	A	1	MET	5.8
1	B	300	GLU	5.6
1	B	25	GLU	5.6
1	B	299	LYS	5.6
1	A	230	ASN	5.4
1	B	2	MET	5.3
1	A	231	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLU	5.3
1	A	303	ASN	5.1
1	A	26	GLY	5.1
1	B	346	THR	5.0
1	A	345	ARG	4.9
1	B	230	ASN	4.8
1	B	95	SER	4.7
1	B	81	LEU	4.7
1	B	24	ASN	4.6
1	A	299	LYS	4.5
1	B	302	LYS	4.5
1	A	28	LYS	4.4
1	B	298	GLU	4.3
1	A	25	GLU	4.1
1	A	302	LYS	4.1
1	B	136	PHE	4.1
1	A	96	LYS	4.0
1	A	29	ASN	4.0
1	A	346	THR	3.9
1	B	130	THR	3.8
1	B	23	LYS	3.7
1	B	28	LYS	3.7
1	B	83	LYS	3.6
1	B	29	ASN	3.5
1	B	82	ASN	3.5
1	B	96	LYS	3.5
1	B	135	ASP	3.4
1	B	4	GLN	3.3
1	B	203	ASN	3.2
1	B	605	ASP	3.1
1	B	126	ILE	3.0
1	B	97	LYS	3.0
1	B	118	PRO	3.0
1	A	307	ILE	3.0
1	A	75	TYR	2.9
1	A	49	LYS	2.9
1	A	347	GLY	2.9
1	B	283	ASP	2.9
1	A	284	ASP	2.8
1	B	3	GLU	2.8
1	A	22	SER	2.8
1	B	306	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	605	ASP	2.8
1	B	134	GLU	2.6
1	A	306	SER	2.6
1	A	97	LYS	2.6
1	B	22	SER	2.6
1	B	305	ASN	2.5
1	B	43	LYS	2.5
1	B	144	ASN	2.4
1	B	310	ASN	2.4
1	A	84	GLU	2.4
1	B	284	ASP	2.3
1	B	139	ASP	2.3
1	B	309	PRO	2.3
1	B	343	SER	2.3
1	B	307	ILE	2.3
1	A	298	GLU	2.3
1	B	35	TYR	2.3
1	B	347	GLY	2.3
1	A	72	LYS	2.2
1	B	110	GLU	2.2
1	B	603	SER	2.2
1	B	164	LEU	2.2
1	B	114	LYS	2.2
1	B	105	GLY	2.2
1	A	286	GLU	2.2
1	B	125	VAL	2.1
1	B	165	GLY	2.1
1	B	103	VAL	2.0
1	A	348	VAL	2.0
1	B	157	ASN	2.0
1	B	104	MET	2.0
1	B	115	LYS	2.0
1	B	132	LYS	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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MMV	A	701	26/26	0.13	0.37	30,32,36,39	0
2	MMV	B	701	26/26	0.18	-0.02	56,60,62,64	0
3	NDP	B	702	48/48	0.22	-0.05	75,86,105,105	0
4	PO4	A	703	5/5	0.15	-0.18	53,56,58,59	0
4	PO4	B	703	5/5	0.14	-0.22	45,49,52,53	0
3	NDP	A	702	48/48	0.10	-0.76	38,44,51,52	0

## 6.5 Other polymers

There are no such residues in this entry.