



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:51 PM GMT

PDB ID : 4DPH  
Title : Quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with P65 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.; Taweethai, S.; Vanichtanakul, J.; Arwon, U.; Fantauzzi, P.; Yuvaniyama, J.; Charman, W.N.; Matthews, D.  
Deposited on : 2012-02-13  
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

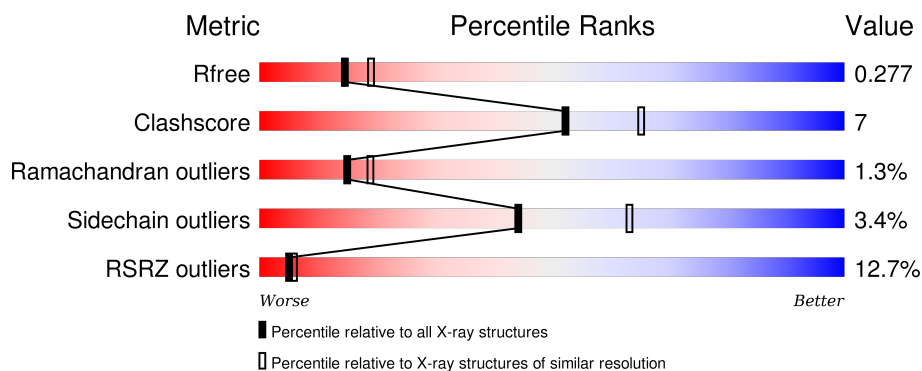
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	608	<div> <div>9%</div> <div>74%</div> <div>13%</div> <div>12%</div> </div>
1	B	608	<div> <div>13%</div> <div>71%</div> <div>14%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BME	A	705	-	-	-	X

## 2 Entry composition [i](#)

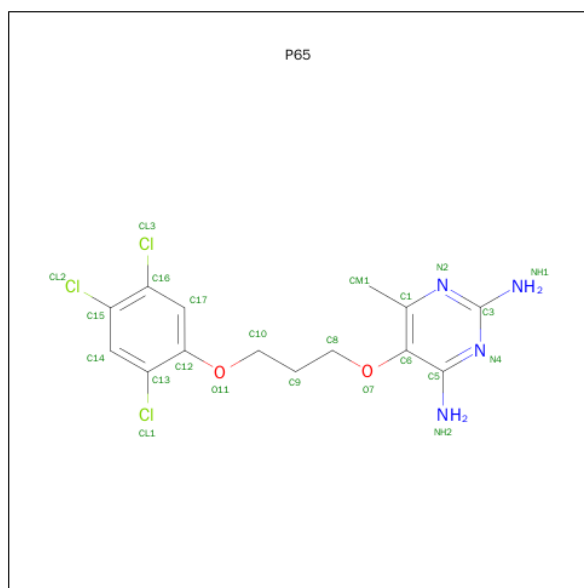
There are 6 unique types of molecules in this entry. The entry contains 9473 atoms, of which 0 are hydrogens and 0 are deuteriums.

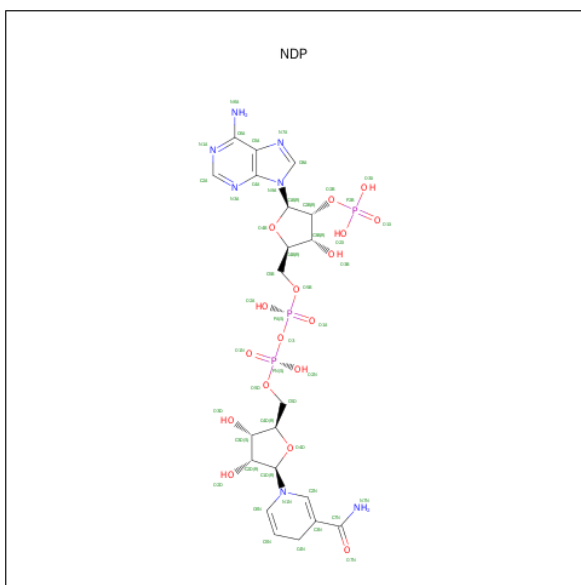
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4472	2890	740	817	25			
1	B	529	Total	C	N	O	S	0	0	0
			4395	2845	725	800	25			

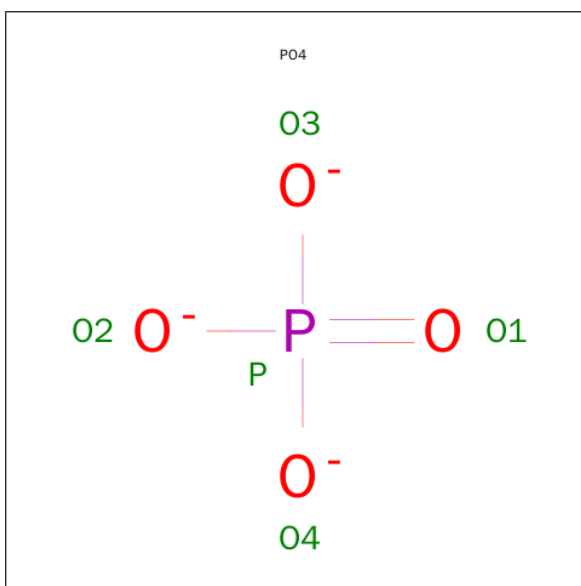
- Molecule 2 is 2,4-DIAMINO-6-METHYL-5-[3-(2,4,5-TRICHLOROPHENOXY)PROPYLOXY]PYRIMIDINE (three-letter code: P65) (formula: C<sub>14</sub>H<sub>15</sub>Cl<sub>3</sub>N<sub>4</sub>O<sub>2</sub>).





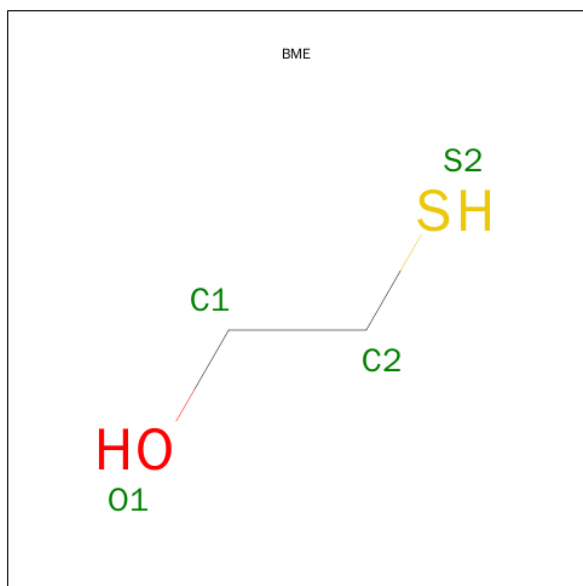
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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



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

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



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

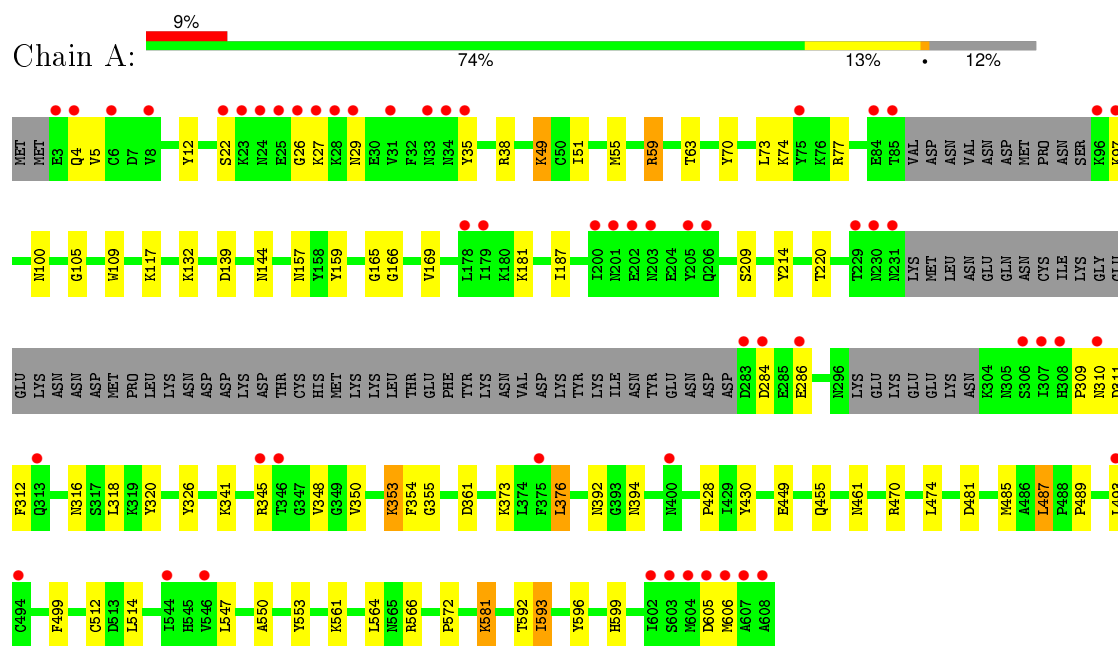
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		
6	B	209	Total	O	0	0
			209	209		

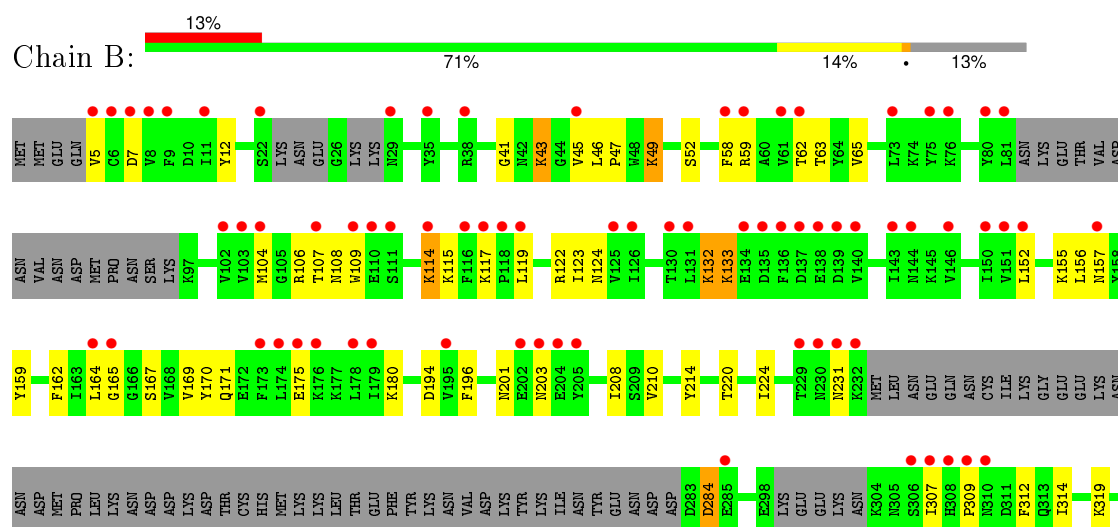
### 3 Residue-property plots

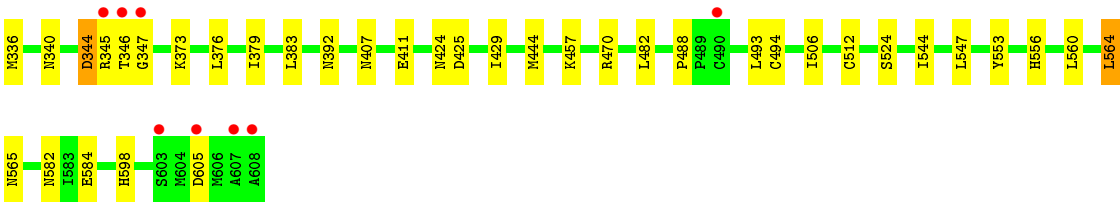
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.95Å 156.45Å 164.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.66 – 2.38 51.79 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (54.66-2.38) 99.1 (51.79-2.38)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.219 , 0.286 0.213 , 0.277	Depositor DCC
$R_{free}$ test set	3072 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 60475 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9473	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 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, PO4, P65, BME

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	0.71	0/4576	0.74	4/6178 (0.1%)
1	B	0.67	1/4497 (0.0%)	0.71	1/6071 (0.0%)
All	All	0.69	1/9073 (0.0%)	0.73	5/12249 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	CYS	CB-SG	-5.35	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	487	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	361	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	383	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	59	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4472	0	4426	49	0
1	B	4395	0	4346	73	0
2	A	23	0	15	1	0
2	B	23	0	15	0	0
3	A	48	0	26	2	0
3	B	48	0	26	5	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	12	0	18	0	0
5	B	4	0	6	0	0
6	A	229	0	0	6	0
6	B	209	0	0	12	0
All	All	9473	0	8878	120	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 7.

All (120) 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:425:ASP:HA	1:B:444:MET:CE	1.76	1.13
1:B:425:ASP:HA	1:B:444:MET:HE3	1.21	1.11
1:B:392:ASN:HA	1:B:444:MET:HE2	1.40	1.03
1:B:376:LEU:HD22	1:B:379:ILE:HD11	1.43	0.98
1:B:547:LEU:HG	6:B:957:HOH:O	1.61	0.97
1:B:584:GLU:HG3	6:B:803:HOH:O	1.66	0.94
1:A:461:ASN:HB3	6:A:973:HOH:O	1.70	0.90
1:B:425:ASP:CA	1:B:444:MET:HE3	2.03	0.89
1:B:392:ASN:HA	1:B:444:MET:CE	2.07	0.85
1:B:307:ILE:HG12	6:B:996:HOH:O	1.77	0.83
1:B:524:SER:HB2	6:B:915:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HG23	3:B:702:NDP:O1A	1.81	0.79
1:B:425:ASP:HA	1:B:444:MET:HE1	1.67	0.74
1:B:171:GLN:HE21	1:B:175:GLU:HG3	1.53	0.73
1:B:210:VAL:HB	6:B:948:HOH:O	1.90	0.72
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.54	0.71
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.31	0.70
1:B:512:CYS:SG	1:B:547:LEU:HD22	2.33	0.69
1:A:4:GLN:HB2	6:A:847:HOH:O	1.94	0.68
1:A:59:ARG:O	1:A:63:THR:HG23	1.94	0.67
1:B:7:ASP:HA	1:B:180:LYS:HE3	1.76	0.66
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.32	0.64
1:A:493:LEU:HD12	1:A:493:LEU:C	2.18	0.64
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.34	0.63
1:A:312:PHE:CE1	1:A:564:LEU:HD23	2.34	0.63
1:B:210:VAL:O	1:B:210:VAL:HG23	1.97	0.62
1:B:425:ASP:CA	1:B:444:MET:CE	2.65	0.62
1:B:424:ASN:O	1:B:444:MET:HE1	2.00	0.61
1:A:74:LYS:C	6:A:959:HOH:O	2.39	0.60
1:B:43:LYS:N	1:B:194:ASP:OD2	2.29	0.60
1:B:167:SER:HB3	3:B:702:NDP:O2N	2.02	0.59
1:B:392:ASN:CA	1:B:444:MET:HE2	2.26	0.58
1:B:132:LYS:HD2	1:B:133:LYS:HD2	1.85	0.57
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.03	0.57
1:A:166:GLY:HA3	3:A:702:NDP:O1A	2.05	0.57
1:B:45:VAL:HG12	1:B:46:LEU:H	1.71	0.56
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.87	0.56
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.39	0.56
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.87	0.56
1:B:373:LYS:HG3	1:B:598:HIS:CE1	2.41	0.55
1:B:493:LEU:HD12	1:B:493:LEU:C	2.26	0.55
1:B:407:ASN:ND2	6:B:991:HOH:O	2.39	0.55
1:B:425:ASP:CB	1:B:444:MET:HE3	2.38	0.54
1:B:171:GLN:NE2	1:B:175:GLU:HG3	2.22	0.53
1:A:312:PHE:HE1	1:A:564:LEU:HD23	1.74	0.53
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.45	0.51
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.44	0.51
1:B:482:LEU:HD22	1:B:488:PRO:HB3	1.93	0.51
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.46	0.51
1:B:307:ILE:HG23	6:B:958:HOH:O	2.11	0.51
1:B:307:ILE:CG2	1:B:312:PHE:HE2	2.23	0.51
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:OH	1:A:157:ASN:OD1	2.28	0.50
1:A:428:PRO:HG2	1:A:481:ASP:HB3	1.93	0.50
1:B:65:VAL:HG22	1:B:159:TYR:CB	2.41	0.50
1:A:214:TYR:O	1:A:220:THR:HA	2.11	0.50
1:B:122:ARG:O	1:B:124:ASN:ND2	2.42	0.49
1:B:201:ASN:HD21	1:B:203:ASN:HB2	1.77	0.49
1:B:5:VAL:N	6:B:967:HOH:O	2.46	0.49
1:A:27:LYS:HG2	1:A:27:LYS:O	2.13	0.49
1:A:514:LEU:HD21	1:A:550:ALA:HB1	1.95	0.49
1:B:376:LEU:HD22	1:B:379:ILE:CD1	2.31	0.49
1:A:581:LYS:HA	1:A:581:LYS:HE3	1.94	0.49
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.94	0.48
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.94	0.48
1:A:376:LEU:HD12	1:A:593:ILE:HD11	1.95	0.48
1:B:12:TYR:HE1	1:B:180:LYS:HD2	1.78	0.48
1:B:59:ARG:O	1:B:63:THR:HG23	2.12	0.48
1:A:55:MET:HE1	2:A:701:P65:CL1	2.51	0.48
1:A:311:ASP:OD2	1:A:561:LYS:NZ	2.42	0.48
1:B:152:LEU:O	1:B:156:LEU:HD12	2.13	0.48
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.54	0.47
1:B:336:MET:CE	1:B:560:LEU:HB2	2.43	0.47
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.95	0.47
1:B:108:ASN:ND2	3:B:702:NDP:H5N	2.30	0.46
1:B:344:ASP:O	1:B:346:THR:N	2.48	0.46
1:B:553:TYR:O	1:B:556:HIS:HB2	2.15	0.46
1:A:512:CYS:SG	1:A:547:LEU:CD2	3.04	0.46
1:B:411:GLU:HB2	6:B:869:HOH:O	2.15	0.45
1:A:105:GLY:CA	1:A:169:VAL:HG21	2.46	0.45
1:B:582:ASN:HB3	6:B:803:HOH:O	2.15	0.45
1:B:171:GLN:HG3	1:B:175:GLU:OE2	2.16	0.45
1:B:43:LYS:HE3	1:B:43:LYS:HB2	1.58	0.45
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.51	0.45
1:A:355:GLY:HA2	1:A:547:LEU:O	2.16	0.45
1:B:214:TYR:O	1:B:220:THR:HA	2.17	0.45
1:B:114:LYS:HD2	1:B:115:LYS:N	2.33	0.44
1:A:318:LEU:HD11	1:A:326:TYR:OH	2.16	0.44
1:A:35:TYR:CZ	1:A:38:ARG:HD2	2.53	0.44
1:B:106:ARG:HE	3:B:702:NDP:P2B	2.40	0.44
1:B:312:PHE:CE1	1:B:564:LEU:HD23	2.52	0.44
1:B:109:TRP:CE2	1:B:117:LYS:HD2	2.53	0.44
1:B:165:GLY:HA3	1:B:170:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLY:N	1:A:169:VAL:HG21	2.33	0.43
1:A:29:ASN:OD1	1:A:373:LYS:NZ	2.51	0.43
1:A:312:PHE:HB2	1:A:316:ASN:ND2	2.34	0.43
1:B:344:ASP:O	1:B:347:GLY:N	2.52	0.43
1:B:210:VAL:O	1:B:210:VAL:CG2	2.67	0.43
1:A:392:ASN:OD1	1:A:394:ASN:HB2	2.19	0.43
1:A:312:PHE:HB2	1:A:316:ASN:HD22	1.84	0.43
1:B:470:ARG:NE	6:B:974:HOH:O	2.52	0.42
1:A:109:TRP:CH2	1:A:117:LYS:HD2	2.54	0.42
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.84	0.42
1:B:314:ILE:HB	1:B:565:ASN:HB3	2.02	0.42
1:A:77:ARG:N	6:A:959:HOH:O	2.53	0.41
1:A:70:TYR:HA	1:A:73:LEU:HD12	2.01	0.41
1:A:353:LYS:HE2	1:A:353:LYS:HB3	1.65	0.41
1:B:62:THR:HA	1:B:162:PHE:CE2	2.56	0.41
1:A:485:MET:SD	1:A:489:PRO:HD3	2.61	0.41
1:A:209:SER:OG	1:A:320:TYR:HD2	2.04	0.41
1:A:77:ARG:HG3	6:A:995:HOH:O	2.21	0.41
1:A:455:GLN:HB3	1:A:474:LEU:HD12	2.02	0.41
1:A:566:ARG:HD3	1:A:599:HIS:CG	2.56	0.41
1:A:493:LEU:CD1	1:A:493:LEU:C	2.89	0.40
1:B:157:ASN:HB3	6:B:904:HOH:O	2.21	0.40
1:B:133:LYS:HD2	1:B:133:LYS:H	1.87	0.40
1:A:286:GLU:HG2	1:B:319:LYS:HD3	2.02	0.40
1:B:108:ASN:HD21	3:B:702:NDP:H5N	1.87	0.40
4:A:703:PO4:O1	6:A:999:HOH:O	2.22	0.40
1:B:284:ASP:OD1	1:B:284:ASP:N	2.47	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	530/608 (87%)	491 (93%)	31 (6%)	8 (2%)	13	15
1	B	518/608 (85%)	474 (92%)	38 (7%)	6 (1%)	16	21
All	All	1048/1216 (86%)	965 (92%)	69 (7%)	14 (1%)	15	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	LYS
1	B	345	ARG
1	A	139	ASP
1	A	49	LYS
1	A	284	ASP
1	A	430	TYR
1	A	22	SER
1	A	26	GLY
1	A	310	ASN
1	B	119	LEU
1	A	309	PRO
1	B	309	PRO
1	B	123	ILE
1	B	429	ILE

### 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	501/570 (88%)	484 (97%)	17 (3%)	44	63
1	B	492/570 (86%)	475 (96%)	17 (4%)	43	62
All	All	993/1140 (87%)	959 (97%)	34 (3%)	44	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	49	LYS

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	132	LYS
1	A	144	ASN
1	A	341	LYS
1	A	345	ARG
1	A	348	VAL
1	A	353	LYS
1	A	376	LEU
1	A	449	GLU
1	A	487	LEU
1	A	581	LYS
1	A	592	THR
1	A	593	ILE
1	A	605	ASP
1	A	606	MET
1	B	43	LYS
1	B	49	LYS
1	B	52	SER
1	B	104	MET
1	B	107	THR
1	B	114	LYS
1	B	132	LYS
1	B	133	LYS
1	B	155	LYS
1	B	196	PHE
1	B	208	ILE
1	B	231	ASN
1	B	284	ASP
1	B	344	ASP
1	B	457	LYS
1	B	564	LEU
1	B	605	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	144	ASN
1	A	294	ASN
1	A	316	ASN
1	A	394	ASN
1	A	424	ASN

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Mol	Chain	Res	Type
1	A	554	ASN
1	B	99	GLN
1	B	171	GLN
1	B	201	ASN
1	B	203	ASN
1	B	305	ASN
1	B	316	ASN
1	B	394	ASN
1	B	424	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](#)

10 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	P65	A	701	-	23,24,24	3.14	4 (17%)	29,33,33	2.14	10 (34%)
3	NDP	A	702	-	42,52,52	1.57	5 (11%)	55,80,80	1.75	10 (18%)
4	PO4	A	703	-	4,4,4	0.47	0	6,6,6	0.31	0
5	BME	A	704	-	3,3,3	0.37	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BME	A	705	-	3,3,3	0.48	0	2,2,2	0.29	0
5	BME	A	706	-	3,3,3	0.33	0	2,2,2	0.57	0
2	P65	B	701	-	23,24,24	3.41	3 (13%)	29,33,33	1.53	4 (13%)
3	NDP	B	702	-	42,52,52	1.53	5 (11%)	55,80,80	1.76	3 (5%)
4	PO4	B	703	-	4,4,4	0.37	0	6,6,6	0.29	0
5	BME	B	704	-	3,3,3	0.43	0	2,2,2	0.61	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	P65	A	701	-	-	0/8/8/8	0/2/2/2
3	NDP	A	702	-	-	0/30/77/77	0/5/5/5
4	PO4	A	703	-	-	0/0/0/0	0/0/0/0
5	BME	A	704	-	-	0/1/1/1	0/0/0/0
5	BME	A	705	-	-	0/1/1/1	0/0/0/0
5	BME	A	706	-	-	0/1/1/1	0/0/0/0
2	P65	B	701	-	-	0/8/8/8	0/2/2/2
3	NDP	B	702	-	-	0/30/77/77	0/5/5/5
4	PO4	B	703	-	-	0/0/0/0	0/0/0/0
5	BME	B	704	-	-	0/1/1/1	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	P65	C15-CL2	-9.74	1.49	1.73
2	B	701	P65	C13-CL1	-9.58	1.50	1.73
2	A	701	P65	C15-CL2	-8.95	1.51	1.73
2	B	701	P65	C16-CL3	-8.69	1.52	1.73
2	A	701	P65	C16-CL3	-8.17	1.53	1.73
2	A	701	P65	C13-CL1	-7.82	1.54	1.73
3	B	702	NDP	C2N-C3N	2.13	1.39	1.34
2	A	701	P65	C1-N2	2.21	1.37	1.34
3	A	702	NDP	C2N-C3N	2.50	1.40	1.34
3	A	702	NDP	C2A-N1A	2.53	1.38	1.33
3	B	702	NDP	C2A-N1A	2.66	1.39	1.33
3	B	702	NDP	C6N-C5N	3.24	1.39	1.33
3	A	702	NDP	C2A-N3A	3.47	1.38	1.32
3	B	702	NDP	C2A-N3A	3.53	1.38	1.32
3	A	702	NDP	C6N-C5N	3.68	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NDP	O7N-C7N	6.65	1.41	1.24
3	A	702	NDP	O7N-C7N	6.73	1.41	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NDP	N3A-C2A-N1A	-11.46	120.12	128.89
3	A	702	NDP	N3A-C2A-N1A	-9.75	121.43	128.89
2	A	701	P65	N4-C3-N2	-3.44	119.90	125.53
3	A	702	NDP	C4A-C5A-N7A	-3.24	106.50	109.48
2	B	701	P65	N4-C3-N2	-2.82	120.92	125.53
2	A	701	P65	C16-C15-CL2	-2.61	114.34	120.87
3	B	702	NDP	PN-O3-PA	-2.57	125.51	132.73
3	A	702	NDP	O2B-C2B-C1B	-2.50	100.28	110.02
3	A	702	NDP	N6A-C6A-N1A	-2.33	114.20	119.20
3	A	702	NDP	C1D-N1N-C2N	-2.30	116.91	120.91
2	A	701	P65	C14-C13-C12	-2.29	117.64	120.99
3	A	702	NDP	C1B-N9A-C4A	-2.17	123.67	126.94
3	A	702	NDP	PN-O3-PA	-2.16	126.67	132.73
3	A	702	NDP	O2N-PN-O1N	2.07	123.74	112.53
3	A	702	NDP	O4D-C1D-N1N	2.15	112.62	108.07
3	A	702	NDP	O4B-C1B-N9A	2.26	112.82	108.10
2	A	701	P65	C14-C13-CL1	2.27	122.00	118.50
3	B	702	NDP	O2A-PA-O3	2.36	115.81	105.09
2	B	701	P65	C10-O11-C12	2.39	123.50	117.64
2	A	701	P65	CM1-C1-N2	2.92	120.97	116.34
2	A	701	P65	NH1-C3-N2	3.09	122.32	117.20
2	B	701	P65	C3-N4-C5	3.30	120.80	117.04
2	A	701	P65	C14-C15-CL2	3.40	123.74	118.50
2	A	701	P65	C17-C16-CL3	4.00	124.67	118.50
2	A	701	P65	C3-N4-C5	4.09	121.69	117.04
2	B	701	P65	C3-N2-C1	4.10	120.48	117.01
2	A	701	P65	C3-N2-C1	4.24	120.60	117.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	P65	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NDP	2	0
4	A	703	PO4	1	0
3	B	702	NDP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	538/608 (88%)	0.67	55 (10%) 9 10	26, 39, 81, 98	0
1	B	529/608 (87%)	0.90	81 (15%) 3 3	24, 43, 96, 116	0
All	All	1067/1216 (87%)	0.78	136 (12%) 5 6	24, 41, 91, 116	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	THR	11.3
1	B	138	GLU	8.7
1	A	26	GLY	8.1
1	B	151	VAL	7.6
1	B	136	PHE	7.6
1	B	232	LYS	7.5
1	A	24	ASN	7.3
1	A	25	GLU	7.2
1	A	31	VAL	7.1
1	B	231	ASN	7.0
1	B	306	SER	6.4
1	B	346	THR	6.2
1	B	130	THR	6.1
1	B	607	ALA	5.8
1	A	29	ASN	5.6
1	B	345	ARG	5.6
1	B	118	PRO	5.6
1	A	231	ASN	5.4
1	A	608	ALA	5.4
1	B	75	TYR	5.2
1	A	230	ASN	5.1
1	B	9	PHE	5.1
1	A	607	ALA	4.9
1	B	178	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	80	TYR	4.6
1	B	307	ILE	4.5
1	B	310	ASN	4.5
1	B	62	THR	4.4
1	A	283	ASP	4.4
1	B	135	ASP	4.4
1	A	606	MET	4.3
1	A	28	LYS	4.3
1	B	608	ALA	4.3
1	B	7	ASP	4.2
1	A	27	LYS	4.2
1	A	200	ILE	4.2
1	B	8	VAL	4.2
1	B	116	PHE	4.1
1	B	309	PRO	4.1
1	A	310	ASN	4.0
1	B	230	ASN	4.0
1	A	345	ARG	3.9
1	B	204	GLU	3.9
1	B	131	LEU	3.9
1	B	109	TRP	3.8
1	B	126	ILE	3.7
1	B	29	ASN	3.7
1	A	306	SER	3.6
1	B	152	LEU	3.6
1	A	35	TYR	3.6
1	B	134	GLU	3.6
1	A	23	LYS	3.5
1	B	229	THR	3.5
1	B	140	VAL	3.4
1	A	22	SER	3.4
1	B	347	GLY	3.4
1	B	111	SER	3.4
1	B	110	GLU	3.4
1	B	102	VAL	3.3
1	B	103	VAL	3.2
1	B	11	ILE	3.2
1	B	285	GLU	3.2
1	A	346	THR	3.1
1	A	203	ASN	3.1
1	A	3	GLU	3.1
1	A	33	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLU	3.1
1	B	22	SER	3.1
1	A	313	GLN	3.1
1	B	104	MET	3.0
1	A	604	MET	3.0
1	A	8	VAL	2.9
1	B	146	VAL	2.9
1	B	58	PHE	2.9
1	B	45	VAL	2.9
1	B	157	ASN	2.9
1	A	201	ASN	2.8
1	A	97	LYS	2.8
1	A	34	ASN	2.7
1	A	546	VAL	2.7
1	B	195	VAL	2.7
1	B	173	PHE	2.7
1	B	107	THR	2.7
1	B	61	VAL	2.7
1	B	38	ARG	2.7
1	B	164	LEU	2.6
1	B	35	TYR	2.6
1	A	375	PHE	2.6
1	A	4	GLN	2.6
1	A	206	GLN	2.5
1	B	59	ARG	2.5
1	B	308	HIS	2.5
1	B	203	ASN	2.5
1	B	137	ASP	2.5
1	A	307	ILE	2.5
1	B	139	ASP	2.5
1	A	286	GLU	2.5
1	A	6	CYS	2.5
1	B	202	GLU	2.5
1	B	81	LEU	2.5
1	B	119	LEU	2.5
1	B	165	GLY	2.5
1	B	205	TYR	2.4
1	A	494	CYS	2.4
1	B	179	ILE	2.4
1	A	605	ASP	2.4
1	A	75	TYR	2.4
1	B	150	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	144	ASN	2.3
1	B	5	VAL	2.3
1	B	605	ASP	2.3
1	B	175	GLU	2.3
1	B	603	SER	2.3
1	B	6	CYS	2.3
1	B	117	LYS	2.3
1	B	143	ILE	2.3
1	A	84	GLU	2.3
1	B	125	VAL	2.3
1	A	205	TYR	2.3
1	A	603	SER	2.3
1	A	178	LEU	2.3
1	B	490	CYS	2.2
1	A	308	HIS	2.2
1	A	96	LYS	2.2
1	A	284	ASP	2.2
1	A	400	ASN	2.2
1	B	76	LYS	2.2
1	B	176	LYS	2.2
1	A	229	THR	2.2
1	A	602	ILE	2.1
1	A	179	ILE	2.1
1	B	174	LEU	2.1
1	B	114	LYS	2.1
1	A	544	ILE	2.0
1	B	73	LEU	2.0
1	A	493	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	BME	A	705	4/4	0.66	0.30	12.64	89,90,90,91	0
5	BME	B	704	4/4	0.86	0.16	1.33	65,67,68,71	0
2	P65	A	701	23/23	0.92	0.14	-0.08	26,31,53,58	0
3	NDP	B	702	48/48	0.88	0.22	-0.09	83,88,102,104	0
3	NDP	A	702	48/48	0.96	0.14	-0.19	43,50,53,54	0
4	PO4	B	703	5/5	0.97	0.14	-0.55	48,48,50,51	0
2	P65	B	701	23/23	0.88	0.17	-0.59	59,66,77,79	0
4	PO4	A	703	5/5	0.96	0.15	-0.65	61,62,62,62	0
5	BME	A	704	4/4	0.78	0.17	-	90,92,93,94	0
5	BME	A	706	4/4	0.94	0.32	-	77,77,77,78	0

## 6.5 Other polymers

There are no such residues in this entry.