



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2019 – 02:42 AM EDT

PDB ID : 2C4G  
Title : STRUCTURE OF CDK2-CYCLIN A WITH PHA-533514  
Authors : Cameron, A.; Fogliatto, G.; Pevarello, P.; Fancelli, D.; Vulpetti, A.; Amici, R.; Villa, M.; Pittala, V.; Ciomei, M.; Mercurio, C.; Bischoff, J.R.; Roletto, F.; Varasi, M.; Brasca, M.G.  
Deposited on : 2005-10-19  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

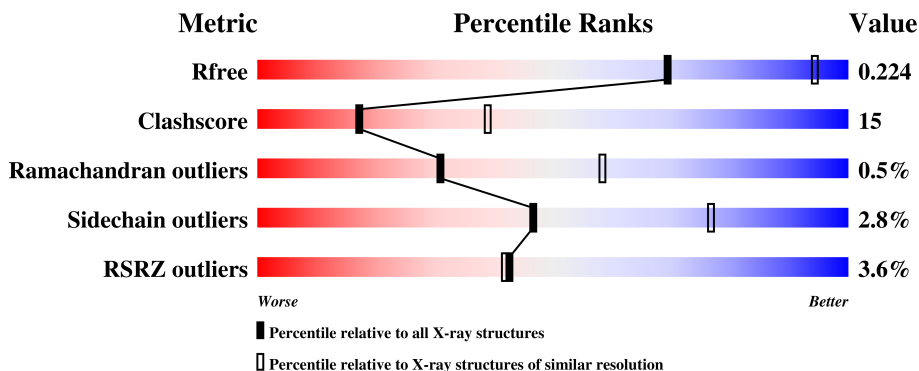
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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	309	 4% 64% 30% . .
1	C	309	 5% 67% 28% . .
2	B	265	 3% 73% 23% . .
2	D	265	 2% 71% 24% . .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9187 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.

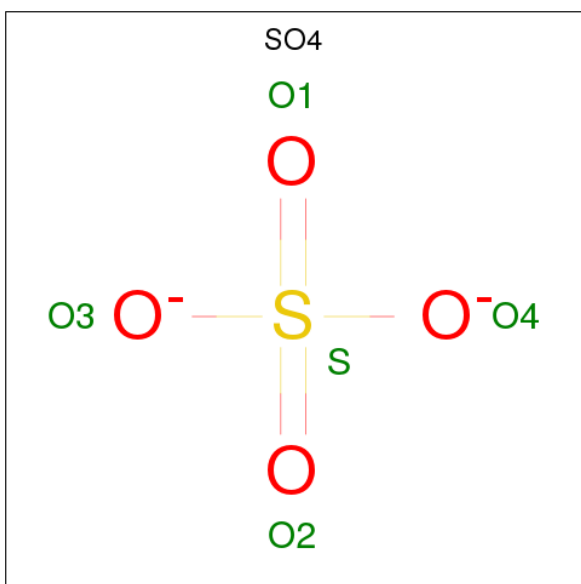
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	Total 2419	C 1573	N 411	O 427	S 8	0	0	0
1	C	300	Total 2412	C 1568	N 410	O 426	S 8	0	0	0

- Molecule 2 is a protein called CYCLIN A2.

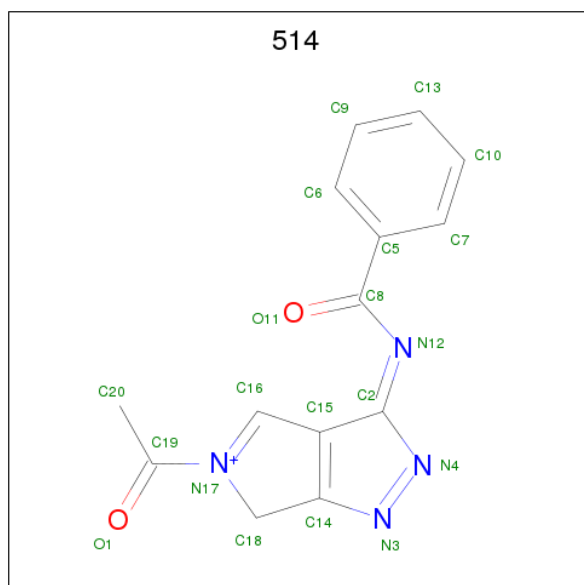
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	258	Total 2084	C 1350	N 339	O 384	S 11	0	0	0
2	D	258	Total 2084	C 1350	N 339	O 384	S 11	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is (3Z)-5-ACETYL-3-(BENZOYLIMINO)-3,6-DIHYDROPYRROLO[3,4-C]PYRAZOL-5-IUM (three-letter code: 514) (formula: C<sub>14</sub>H<sub>11</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 14 4 2	0	0
4	C	1	Total C N O 20 14 4 2	0	0

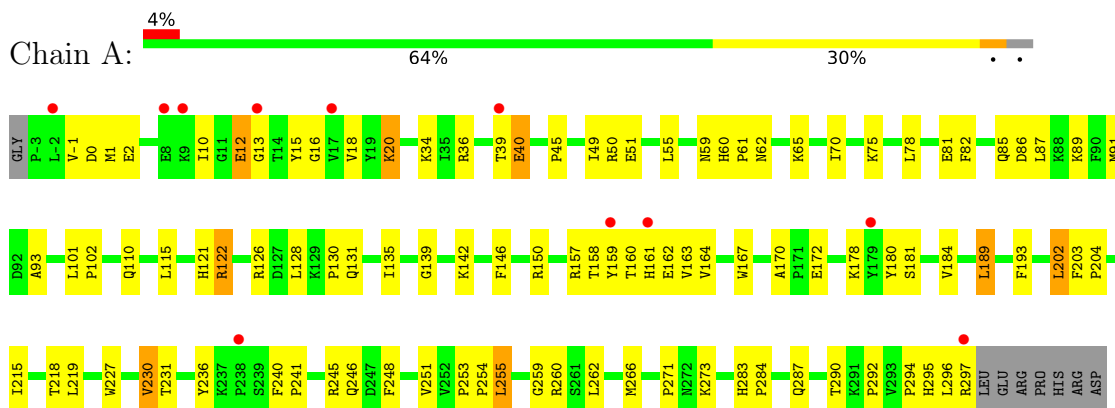
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	40	Total O 40 40	0	0
5	B	26	Total O 26 26	0	0
5	C	34	Total O 34 34	0	0
5	D	38	Total O 38 38	0	0

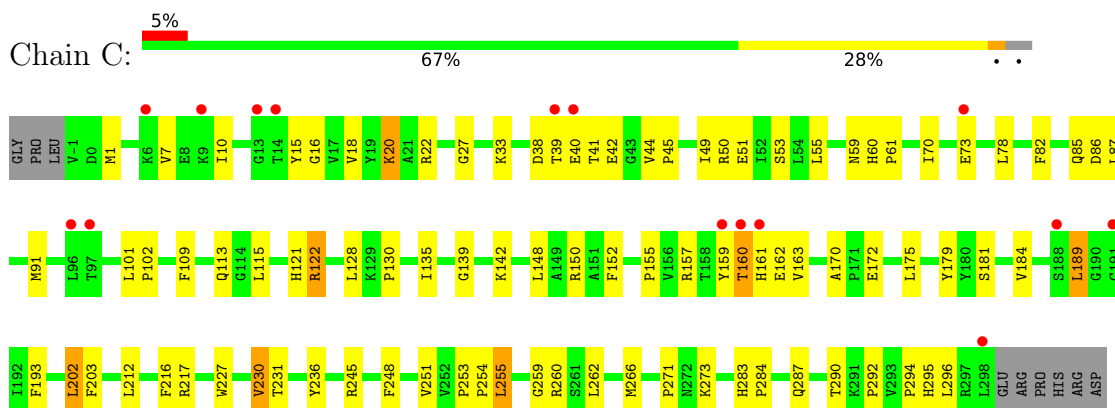
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

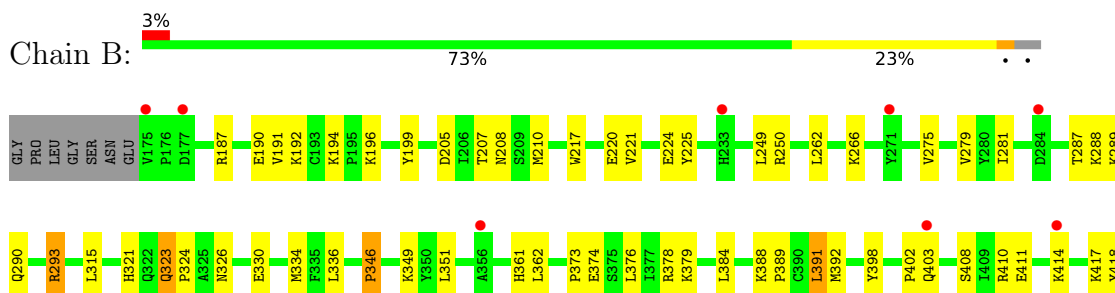
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



- Molecule 1: CELL DIVISION PROTEIN KINASE 2

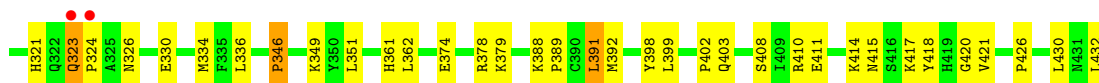


- Molecule 2: CYCLIN A2





• Molecule 2: CYCLIN A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.99Å 191.99Å 205.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.93-2.70) 99.5 (29.92-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.68Å)	Xtrriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.233 , 0.250 0.227 , 0.224	Depositor DCC
$R_{free}$ test set	1238 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 514

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	0.35	0/2482	0.63	1/3370 (0.0%)
1	C	0.34	0/2474	0.63	1/3359 (0.0%)
2	B	0.33	0/2134	0.59	0/2897
2	D	0.43	0/2134	0.63	1/2897 (0.0%)
All	All	0.36	0/9224	0.62	3/12523 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	178	TYR	N-CA-C	-7.34	91.18	111.00
1	A	20	LYS	N-CA-C	-5.30	96.69	111.00
1	C	20	LYS	N-CA-C	-5.05	97.36	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	2419	0	2470	86	0
1	C	2412	0	2463	79	0
2	B	2084	0	2107	53	0
2	D	2084	0	2107	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	20	0	11	1	0
4	C	20	0	11	1	0
5	A	40	0	0	3	0
5	B	26	0	0	0	0
5	C	34	0	0	2	0
5	D	38	0	0	1	0
All	All	9187	0	9169	271	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 15.

All (271) 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)
2:D:323:GLN:HB2	2:D:324:PRO:HD3	1.38	1.05
2:D:289:LYS:O	2:D:293:ARG:HG3	1.73	0.86
2:B:323:GLN:HB2	2:B:324:PRO:HD3	1.68	0.76
2:B:205:ASP:OD2	2:B:250:ARG:HG3	1.86	0.75
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.68	0.75
1:A:128:LEU:HD13	1:A:189:LEU:HD13	1.69	0.75
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.69	0.74
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.69	0.73
1:A:51:GLU:O	1:A:55:LEU:HB2	1.88	0.73
1:C:51:GLU:O	1:C:55:LEU:HB2	1.88	0.73
2:D:279:VAL:HG21	2:D:288:LYS:HG2	1.72	0.70
2:B:323:GLN:CB	2:B:324:PRO:HD3	2.22	0.70
1:C:227:TRP:O	1:C:230:VAL:HG22	1.92	0.70
2:D:289:LYS:HE2	2:D:293:ARG:NH1	2.08	0.69
2:D:346:PRO:O	2:D:349:LYS:HG2	1.93	0.68
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.74	0.68
2:B:346:PRO:O	2:B:349:LYS:HG2	1.93	0.68
1:C:231:THR:HA	1:C:236:TYR:CD1	2.29	0.68
1:A:231:THR:HA	1:A:236:TYR:CD1	2.29	0.68
2:D:289:LYS:HE2	2:D:293:ARG:HH11	1.57	0.67
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.59	0.67
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.77	0.66
2:D:323:GLN:HB2	2:D:324:PRO:CD	2.21	0.66
1:A:227:TRP:O	1:A:230:VAL:HG22	1.96	0.66
1:C:10:ILE:HD11	1:C:82:PHE:HE2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:PRO:HA	2:B:410:ARG:NH1	2.12	0.65
2:B:374:GLU:HG3	2:B:378:ARG:NH1	2.12	0.65
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.80	0.64
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.78	0.64
1:A:93:ALA:HB1	1:A:297:ARG:HD2	1.79	0.63
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.79	0.63
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.63	0.63
2:D:374:GLU:HG3	2:D:378:ARG:NH1	2.13	0.63
1:A:10:ILE:HB	1:A:18:VAL:O	1.98	0.63
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.64	0.62
2:B:275:VAL:O	2:B:279:VAL:HG23	1.99	0.62
2:D:402:PRO:HA	2:D:410:ARG:NH1	2.14	0.62
2:D:388:LYS:O	2:D:392:MET:HG2	2.00	0.61
2:B:191:VAL:HG12	2:B:191:VAL:O	1.99	0.61
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.82	0.61
2:B:207:THR:HG23	2:B:210:MET:H	1.65	0.61
1:C:61:PRO:O	1:C:142:LYS:HE2	2.01	0.60
1:A:157:ARG:HH12	1:A:178:LYS:HE2	1.66	0.60
2:D:191:VAL:HG12	2:D:191:VAL:O	2.01	0.60
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.82	0.60
1:A:227:TRP:O	1:A:230:VAL:CG2	2.50	0.59
1:A:284:PRO:O	1:A:287:GLN:HB2	2.02	0.59
1:A:61:PRO:O	1:A:142:LYS:HE2	2.01	0.59
1:A:-1:VAL:HG11	2:D:296:HIS:CE1	2.37	0.59
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.85	0.59
2:D:192:LYS:C	2:D:194:LYS:H	2.06	0.59
2:D:175:VAL:N	2:D:176:PRO:HD3	2.18	0.59
2:B:192:LYS:C	2:B:194:LYS:H	2.06	0.58
2:B:323:GLN:HG3	2:B:324:PRO:HD3	1.84	0.58
2:D:415:ASN:ND2	5:D:2036:HOH:O	2.37	0.58
2:D:330:GLU:O	2:D:334:MET:HG2	2.04	0.58
1:C:227:TRP:O	1:C:230:VAL:CG2	2.50	0.58
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.86	0.58
1:A:163:VAL:HG12	1:A:180:TYR:OH	2.04	0.58
2:B:402:PRO:HA	2:B:410:ARG:HH11	1.69	0.57
1:A:0:ASP:OD2	2:D:300:LYS:HE3	2.04	0.57
2:B:336:LEU:HD13	2:B:362:LEU:HD23	1.87	0.57
2:B:330:GLU:O	2:B:334:MET:HG2	2.04	0.56
1:C:284:PRO:O	1:C:287:GLN:HB2	2.04	0.56
1:C:60:HIS:ND1	1:C:61:PRO:HD2	2.20	0.56
2:B:388:LYS:O	2:B:392:MET:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG22	1:C:39:THR:O	2.05	0.56
2:D:323:GLN:H	2:D:323:GLN:NE2	2.02	0.56
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.42	0.55
1:C:53:SER:HB3	2:D:304:PHE:O	2.05	0.55
1:A:16:GLY:HA3	1:A:34:LYS:O	2.06	0.55
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.88	0.55
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.42	0.55
1:A:91:MET:HE2	1:A:130:PRO:HB3	1.89	0.55
2:B:321:HIS:CE1	2:B:379:LYS:HD2	2.40	0.55
1:C:148:LEU:HD13	1:C:163:VAL:HG13	1.86	0.55
1:C:38:ASP:HB3	1:C:42:GLU:HB2	1.89	0.55
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.89	0.55
2:D:205:ASP:OD2	2:D:250:ARG:HG3	2.07	0.55
1:A:262:LEU:HG	1:A:266:MET:HE2	1.89	0.54
1:C:122:ARG:O	1:C:122:ARG:HD2	2.08	0.54
1:C:10:ILE:HD11	1:C:82:PHE:CE2	2.41	0.54
2:D:175:VAL:N	2:D:176:PRO:CD	2.70	0.54
2:D:205:ASP:OD1	2:D:250:ARG:NH1	2.41	0.54
1:A:159:TYR:CZ	1:A:161:HIS:HB2	2.42	0.53
2:B:414:LYS:HA	2:B:420:GLY:HA2	1.90	0.53
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.89	0.53
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.43	0.53
2:B:287:THR:HG22	2:B:289:LYS:H	1.73	0.53
1:A:128:LEU:HD13	1:A:189:LEU:CD1	2.39	0.53
2:D:175:VAL:O	2:D:175:VAL:HG12	2.09	0.53
1:C:87:LEU:O	1:C:91:MET:HG3	2.09	0.52
2:D:287:THR:HG22	2:D:288:LYS:N	2.24	0.52
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.91	0.52
1:A:-1:VAL:HG22	1:C:73:GLU:HG3	1.91	0.52
2:D:402:PRO:HA	2:D:410:ARG:HH11	1.74	0.52
1:C:262:LEU:HG	1:C:266:MET:HE2	1.91	0.52
2:D:175:VAL:O	2:D:176:PRO:C	2.48	0.52
2:B:323:GLN:CG	2:B:324:PRO:HD3	2.39	0.52
2:B:411:GLU:O	2:B:414:LYS:HG2	2.10	0.52
1:A:122:ARG:HD2	1:A:122:ARG:O	2.10	0.52
1:A:193:PHE:CD2	1:A:266:MET:HE1	2.45	0.52
1:A:1:MET:HE2	1:A:70:ILE:HG12	1.91	0.51
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.44	0.51
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.46	0.51
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.91	0.51
2:B:323:GLN:HB2	2:B:324:PRO:CD	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:THR:HG22	2:D:289:LYS:H	1.74	0.51
1:C:175:LEU:HD21	1:C:212:LEU:HD21	1.92	0.51
1:C:40:GLU:HG3	1:C:41:THR:HG23	1.93	0.51
1:A:262:LEU:HG	1:A:266:MET:CE	2.40	0.51
2:B:205:ASP:OD1	2:B:250:ARG:NH2	2.44	0.51
2:B:287:THR:HG22	2:B:288:LYS:N	2.25	0.51
1:C:212:LEU:HG	1:C:216:PHE:CZ	2.46	0.51
1:C:85:GLN:HG2	1:C:86:ASP:N	2.26	0.51
1:A:159:TYR:CD1	1:A:160:THR:N	2.79	0.51
1:C:121:HIS:O	1:C:122:ARG:HG3	2.10	0.51
1:A:85:GLN:HG2	1:A:86:ASP:N	2.26	0.50
1:C:159:TYR:O	1:C:161:HIS:N	2.43	0.50
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.45	0.50
1:C:135:ILE:HD12	1:C:296:LEU:HD21	1.93	0.50
1:C:248:PHE:HB3	1:C:260:ARG:HD2	1.92	0.50
1:A:121:HIS:O	1:A:122:ARG:HG3	2.11	0.50
1:A:-1:VAL:HG13	1:C:73:GLU:HG2	1.92	0.50
2:D:398:TYR:CD2	2:D:426:PRO:HB3	2.47	0.50
1:A:115:LEU:HD22	1:A:189:LEU:HD22	1.93	0.50
1:A:135:ILE:HD12	1:A:296:LEU:HD21	1.93	0.50
1:A:170:ALA:HB1	1:A:172:GLU:OE2	2.11	0.50
2:B:417:LYS:HE3	2:B:418:TYR:CE2	2.47	0.49
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.47	0.49
1:C:20:LYS:HG3	1:C:82:PHE:CE2	2.47	0.49
1:A:12:GLU:HG3	1:A:13:GLY:N	2.27	0.49
1:A:160:THR:HG21	5:A:2021:HOH:O	2.12	0.49
1:A:245:ARG:HH11	1:A:245:ARG:HG3	1.76	0.49
1:C:248:PHE:HB2	5:C:2013:HOH:O	2.11	0.49
1:A:135:ILE:HB	5:A:2017:HOH:O	2.12	0.49
2:D:287:THR:HB	2:D:290:GLN:H	1.78	0.48
2:D:411:GLU:O	2:D:414:LYS:HG2	2.13	0.48
1:A:126:ARG:O	1:A:164:VAL:HG22	2.13	0.48
2:D:191:VAL:O	2:D:191:VAL:CG1	2.61	0.48
1:A:131:GLN:HG2	5:A:2016:HOH:O	2.12	0.48
2:B:191:VAL:O	2:B:191:VAL:CG1	2.60	0.48
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.78	0.48
2:B:418:TYR:O	2:B:421:VAL:HG13	2.14	0.48
1:C:15:TYR:CD1	1:C:16:GLY:N	2.81	0.48
1:C:172:GLU:HG2	1:C:271:PRO:HG3	1.95	0.48
2:D:418:TYR:O	2:D:421:VAL:HG13	2.14	0.48
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:417:LYS:HE3	2:D:418:TYR:CE2	2.48	0.48
1:A:248:PHE:HB3	1:A:260:ARG:HD2	1.95	0.48
1:A:20:LYS:HG3	1:A:82:PHE:CE2	2.49	0.47
1:A:89:LYS:HD2	4:A:306:514:H10	1.97	0.47
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.44	0.47
1:A:2:GLU:HG3	2:D:293:ARG:NH2	2.30	0.47
2:B:287:THR:HB	2:B:290:GLN:H	1.79	0.47
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.49	0.47
2:B:217:TRP:O	2:B:221:VAL:HG23	2.15	0.47
2:B:374:GLU:HG3	2:B:378:ARG:HH12	1.80	0.47
1:C:60:HIS:CE1	1:C:61:PRO:HD2	2.49	0.47
2:D:287:THR:HG22	2:D:288:LYS:H	1.79	0.47
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.50	0.46
1:A:87:LEU:O	1:A:91:MET:HG3	2.16	0.46
1:A:251:VAL:C	1:A:253:PRO:HD3	2.36	0.46
1:A:2:GLU:CG	2:D:293:ARG:HH22	2.28	0.46
1:A:253:PRO:CB	1:A:254:PRO:HD3	2.46	0.46
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.80	0.46
1:C:251:VAL:C	1:C:253:PRO:HD3	2.36	0.46
1:C:15:TYR:HE1	1:C:18:VAL:HG23	1.80	0.46
1:C:193:PHE:CD2	1:C:266:MET:HE1	2.51	0.46
1:A:181:SER:O	1:A:184:VAL:HG22	2.15	0.46
1:A:39:THR:O	1:A:40:GLU:HB3	2.16	0.46
1:C:91:MET:CE	1:C:130:PRO:HB3	2.45	0.46
1:C:262:LEU:HG	1:C:266:MET:CE	2.45	0.46
2:B:220:GLU:HG3	2:B:408:SER:OG	2.16	0.45
1:C:159:TYR:C	1:C:161:HIS:N	2.69	0.45
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.16	0.45
2:D:217:TRP:O	2:D:221:VAL:HG23	2.15	0.45
1:A:121:HIS:C	1:A:122:ARG:HG3	2.36	0.45
1:A:158:THR:HA	1:A:180:TYR:CE1	2.50	0.45
1:A:215:ILE:HG23	1:A:219:LEU:HD12	1.98	0.45
1:C:290:THR:C	1:C:292:PRO:HD3	2.37	0.45
2:D:175:VAL:HG12	2:D:177:ASP:CG	2.37	0.45
1:A:159:TYR:HD1	1:A:160:THR:N	2.15	0.45
1:A:159:TYR:CE2	1:A:162:GLU:HG3	2.51	0.45
2:B:196:LYS:HB2	2:B:199:TYR:HB3	1.99	0.45
1:C:217:ARG:HD2	5:C:2028:HOH:O	2.16	0.45
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.52	0.45
2:D:210:MET:HE1	2:D:250:ARG:HG2	1.99	0.45
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:HG2	1:C:179:TYR:CE1	2.52	0.45
1:C:181:SER:O	1:C:184:VAL:HG22	2.16	0.45
1:C:115:LEU:HD22	1:C:189:LEU:HD22	1.97	0.44
2:D:175:VAL:HG12	2:D:177:ASP:OD2	2.16	0.44
2:D:277:GLU:HA	2:D:280:TYR:CD1	2.52	0.44
1:A:91:MET:CE	1:A:130:PRO:HB3	2.47	0.44
2:B:249:LEU:HD12	1:C:27:GLY:HA3	1.99	0.44
1:C:227:TRP:HB3	1:C:230:VAL:HG22	2.00	0.44
2:B:287:THR:HG22	2:B:288:LYS:H	1.81	0.44
2:D:323:GLN:CB	2:D:324:PRO:HD3	2.26	0.44
1:A:51:GLU:HG3	1:A:146:PHE:HB2	1.98	0.44
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.99	0.44
1:C:1:MET:HE3	1:C:70:ILE:HG12	2.00	0.44
1:A:15:TYR:HD1	1:A:15:TYR:H	1.66	0.44
1:A:-1:VAL:HG22	1:C:73:GLU:CG	2.48	0.44
2:B:224:GLU:HG3	2:B:225:TYR:CD1	2.53	0.43
2:D:315:LEU:HA	2:D:315:LEU:HD23	1.84	0.43
2:D:398:TYR:CE2	2:D:426:PRO:HB3	2.52	0.43
2:B:323:GLN:CB	2:B:324:PRO:CD	2.95	0.43
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.80	0.43
1:A:93:ALA:CB	1:A:297:ARG:HD2	2.48	0.43
1:A:36:ARG:NH1	1:A:75:LYS:HE2	2.34	0.43
2:B:262:LEU:HD11	2:B:266:LYS:HE3	2.00	0.43
1:C:18:VAL:HG22	1:C:33:LYS:HD3	2.01	0.43
2:D:220:GLU:HG3	2:D:408:SER:OG	2.18	0.43
2:B:326:ASN:O	2:B:330:GLU:HG3	2.19	0.43
2:D:210:MET:CE	2:D:250:ARG:HG2	2.49	0.43
1:C:121:HIS:C	1:C:122:ARG:HG3	2.39	0.43
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.54	0.43
1:C:60:HIS:HA	1:C:61:PRO:HD3	1.89	0.42
2:B:373:PRO:HG2	2:B:376:LEU:HB2	2.01	0.42
1:C:159:TYR:O	1:C:160:THR:C	2.57	0.42
1:A:39:THR:HG22	1:A:39:THR:O	2.18	0.42
2:B:373:PRO:CG	2:B:376:LEU:HD12	2.48	0.42
1:A:193:PHE:HD2	1:A:266:MET:HE1	1.85	0.42
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.82	0.42
1:C:128:LEU:HD13	1:C:189:LEU:CD1	2.43	0.42
1:A:245:ARG:HG3	1:A:245:ARG:NH1	2.35	0.42
1:A:240:PHE:HA	1:A:241:PRO:HD3	1.86	0.42
1:A:45:PRO:O	1:A:49:ILE:HG12	2.19	0.42
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ARG:HG2	2:B:293:ARG:NH1	2.35	0.42
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.42
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.55	0.42
1:C:50:ARG:NH1	1:C:150:ARG:NE	2.68	0.42
1:C:155:PRO:HD3	2:D:316:THR:HG21	2.02	0.42
1:C:231:THR:HA	1:C:236:TYR:CE1	2.54	0.42
2:D:208:ASN:HA	2:D:208:ASN:HD22	1.64	0.42
2:D:430:LEU:HB3	2:D:432:LEU:HG	2.02	0.42
2:B:192:LYS:C	2:B:194:LYS:N	2.73	0.41
1:C:7:VAL:HB	1:C:20:LYS:O	2.19	0.41
1:C:50:ARG:NH1	1:C:150:ARG:HE	2.18	0.41
2:D:326:ASN:O	2:D:330:GLU:HG3	2.19	0.41
1:C:49:ILE:CG2	2:D:306:LEU:HD12	2.46	0.41
2:D:399:LEU:HD23	2:D:426:PRO:HG2	2.03	0.41
1:A:1:MET:CE	1:A:70:ILE:HG12	2.50	0.41
2:B:208:ASN:HA	2:B:208:ASN:HD22	1.72	0.41
2:B:430:LEU:HB3	2:B:432:LEU:HG	2.02	0.41
1:A:157:ARG:NH1	1:A:157:ARG:HG3	2.33	0.41
1:C:121:HIS:O	1:C:122:ARG:NH1	2.52	0.41
2:D:262:LEU:HD11	2:D:266:LYS:HE3	2.02	0.41
1:A:218:THR:HA	1:A:246:GLN:CG	2.50	0.41
1:C:109:PHE:O	1:C:113:GLN:HG3	2.21	0.41
1:A:290:THR:C	1:A:292:PRO:HD3	2.40	0.41
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.35	0.41
2:B:187:ARG:HD2	2:B:190:GLU:OE2	2.20	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.94	0.41
1:C:85:GLN:HA	4:C:306:514:C10	2.50	0.41
2:B:190:GLU:HG3	2:B:351:LEU:HD22	2.02	0.41
2:D:281:ILE:HG13	2:D:281:ILE:H	1.68	0.41
2:D:192:LYS:C	2:D:194:LYS:N	2.73	0.41
1:A:65:LYS:H	1:A:81:GLU:HG2	1.86	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.55	0.41
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.56	0.41
1:C:70:ILE:N	1:C:70:ILE:HD12	2.35	0.40
1:A:40:GLU:OE2	1:A:45:PRO:HG3	2.22	0.40
1:A:101:LEU:N	1:A:102:PRO:CD	2.84	0.40
1:A:50:ARG:NH1	1:A:150:ARG:NE	2.69	0.40
2:D:175:VAL:O	2:D:177:ASP:N	2.54	0.40
1:A:60:HIS:HA	1:A:61:PRO:HD3	1.89	0.40
1:C:1:MET:HE3	1:C:70:ILE:CG1	2.51	0.40
1:A:2:GLU:HG3	2:D:293:ARG:HH22	1.87	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	299/309 (97%)	273 (91%)	24 (8%)	2 (1%)	24	50
1	C	298/309 (96%)	271 (91%)	25 (8%)	2 (1%)	24	50
2	B	256/265 (97%)	245 (96%)	11 (4%)	0	100	100
2	D	256/265 (97%)	244 (95%)	10 (4%)	2 (1%)	21	47
All	All	1109/1148 (97%)	1033 (93%)	70 (6%)	6 (0%)	31	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	C	162	GLU
2	D	178	TYR
1	C	160	THR
2	D	177	ASP
1	A	12	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/273 (97%)	257 (97%)	9 (3%)	40	71
1	C	265/273 (97%)	256 (97%)	9 (3%)	40	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	232/237 (98%)	227 (98%)	5 (2%)	55	83
2	D	232/237 (98%)	227 (98%)	5 (2%)	55	83
All	All	995/1020 (98%)	967 (97%)	28 (3%)	47	77

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	78	LEU
1	A	122	ARG
1	A	189	LEU
1	A	202	LEU
1	A	230	VAL
1	A	255	LEU
1	A	273	LYS
1	A	295	HIS
2	B	293	ARG
2	B	323	GLN
2	B	346	PRO
2	B	391	LEU
2	B	403	GLN
1	C	59	ASN
1	C	78	LEU
1	C	122	ARG
1	C	189	LEU
1	C	202	LEU
1	C	230	VAL
1	C	255	LEU
1	C	273	LYS
1	C	295	HIS
2	D	209	SER
2	D	323	GLN
2	D	346	PRO
2	D	391	LEU
2	D	403	GLN

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	59	ASN

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Mol	Chain	Res	Type
1	A	113	GLN
2	B	208	ASN
2	B	296	HIS
2	B	317	GLN
2	B	396	GLN
2	B	419	HIS
2	B	425	ASN
1	C	59	ASN
2	D	208	ASN
2	D	296	HIS
2	D	323	GLN
2	D	396	GLN
2	D	415	ASN
2	D	419	HIS
2	D	425	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](#)

4 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	SO4	A	305	-	4,4,4	0.36	0	6,6,6	0.09	0
4	514	A	306	-	15,22,22	3.31	8 (53%)	15,31,31	2.15	4 (26%)
4	514	C	306	-	15,22,22	3.47	10 (66%)	15,31,31	2.27	4 (26%)
3	SO4	D	433	-	4,4,4	0.34	0	6,6,6	0.05	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
3	SO4	A	305	-	-	0/0/0/0	0/0/0/0
4	514	A	306	-	-	1/8/33/33	0/3/3/3
4	514	C	306	-	-	1/8/33/33	0/3/3/3
3	SO4	D	433	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	306	514	C5-C8	-5.30	1.41	1.49
4	C	306	514	C5-C8	-4.63	1.42	1.49
4	A	306	514	C13-C10	2.09	1.43	1.38
4	C	306	514	C13-C9	2.20	1.43	1.38
4	A	306	514	C14-N3	2.27	1.39	1.36
4	C	306	514	C13-C10	2.28	1.44	1.38
4	C	306	514	C9-C6	2.30	1.43	1.38
4	C	306	514	C10-C7	2.36	1.44	1.38
4	A	306	514	C7-C5	3.09	1.44	1.39
4	A	306	514	C6-C5	3.18	1.44	1.39
4	C	306	514	C7-C5	3.60	1.45	1.39
4	C	306	514	C6-C5	3.81	1.45	1.39
4	C	306	514	C2-N4	4.02	1.39	1.34
4	A	306	514	C2-N4	4.05	1.39	1.34
4	A	306	514	C16-C15	4.53	1.47	1.40
4	C	306	514	C16-C15	4.89	1.47	1.40
4	A	306	514	C2-N12	7.59	1.47	1.33
4	C	306	514	C2-N12	8.01	1.48	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	306	514	C15-C2-N4	-4.48	102.99	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	306	514	C15-C2-N4	-4.18	103.45	109.67
4	C	306	514	N12-C2-N4	-2.52	124.44	128.14
4	A	306	514	N12-C2-N4	-2.46	124.52	128.14
4	A	306	514	C5-C8-N12	2.86	119.35	114.92
4	C	306	514	C5-C8-N12	3.04	119.63	114.92
4	A	306	514	C15-C2-N12	5.61	132.03	122.78
4	C	306	514	C15-C2-N12	5.93	132.57	122.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	306	514	C15-C2-N12-C8
4	A	306	514	C15-C2-N12-C8

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	514	1	0
4	C	306	514	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, 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	301/309 (97%)	0.06	11 (3%) 41 40	39, 61, 125, 163	0
1	C	300/309 (97%)	0.25	15 (5%) 29 27	39, 73, 130, 168	0
2	B	258/265 (97%)	0.04	9 (3%) 44 43	40, 65, 106, 174	0
2	D	258/265 (97%)	-0.12	5 (1%) 66 68	34, 55, 105, 194	0
All	All	1117/1148 (97%)	0.07	40 (3%) 42 42	34, 63, 120, 194	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	323	GLN	7.7
2	D	177	ASP	5.8
1	A	297	ARG	5.5
1	A	39	THR	5.2
1	C	96	LEU	5.0
1	C	161	HIS	4.9
2	D	175	VAL	4.8
1	C	298	LEU	4.4
2	B	175	VAL	4.2
1	C	159	TYR	3.8
2	D	324	PRO	3.6
1	A	238	PRO	3.4
1	C	97	THR	3.3
1	C	9	LYS	3.3
1	A	159	TYR	3.2
1	C	160	THR	3.1
1	A	161	HIS	2.9
1	C	14	THR	2.9
1	C	40	GLU	2.7
1	C	73	GLU	2.6
2	B	432	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	39	THR	2.6
1	C	13	GLY	2.5
1	C	188	SER	2.5
2	B	177	ASP	2.5
2	B	403	GLN	2.4
1	C	6	LYS	2.4
1	A	8	GLU	2.3
2	B	233	HIS	2.3
1	A	17	VAL	2.3
1	A	-2	LEU	2.2
2	B	271	TYR	2.2
1	A	9	LYS	2.2
1	C	191	CYS	2.1
2	D	193	CYS	2.1
2	B	356	ALA	2.1
1	A	179	TYR	2.1
2	B	414	LYS	2.0
2	B	284	ASP	2.0
1	A	13	GLY	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	305	5/5	0.81	0.29	160,160,161,161	0
3	SO4	D	433	5/5	0.88	0.39	139,139,140,140	0
4	514	C	306	20/20	0.90	0.24	82,82,82,82	0
4	514	A	306	20/20	0.94	0.18	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.