Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 PM GMT

PDB ID	:	4MX3
Title	:	Crystal Structure of PKA RIalpha Homodimer
Authors	:	Bruystens, J.G.H.; Wu, J.; Fortezzo, A.; Kornev, A.P.; Blumenthal, D.A.; Taylor, S.S.
Deposited on	:	2013-09-25
Resolution	:	3.88 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 ①) were used in the production of this report:

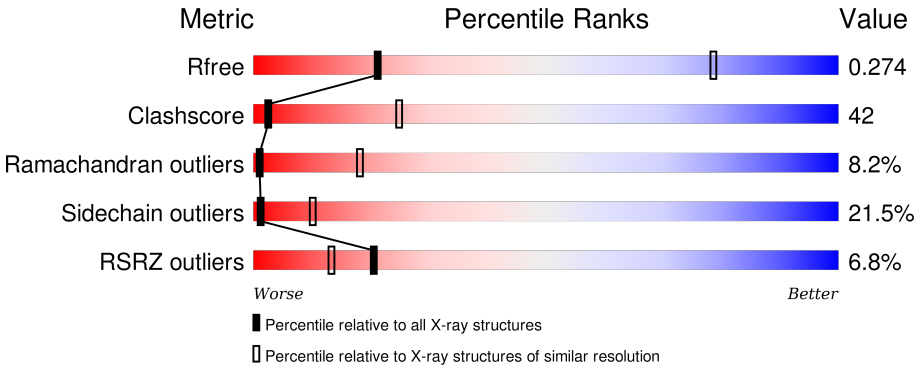
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.88 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	1005 (4.24-3.52)
Clashscore	102246	1026 (4.20-3.56)
Ramachandran outliers	100387	1003 (4.22-3.54)
Sidechain outliers	100360	1043 (4.24-3.52)
RSRZ outliers	91569	1009 (4.24-3.52)

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 <=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	379	6% 30% 30% 10% • 28%
1	B	379	4% 26% 30% 14% • 29%

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
2	CMP	A	402	-	-	-	X
2	CMP	B	402	-	-	-	X

2 Entry composition

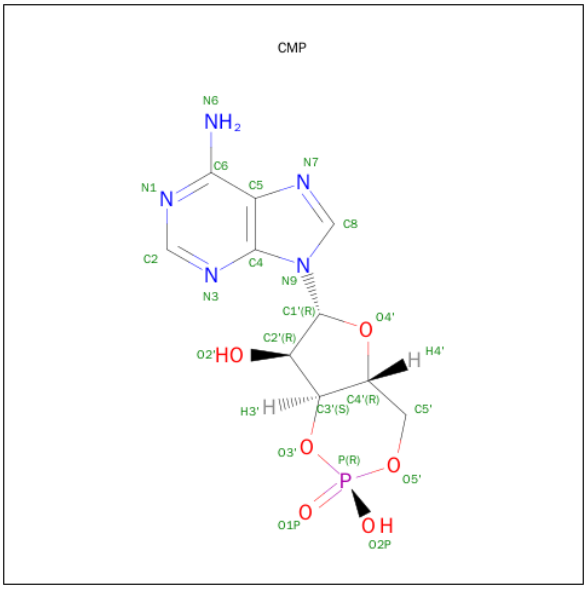
There are 2 unique types of molecules in this entry. The entry contains 4217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cAMP-dependent protein kinase type I-alpha regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2073	1322	348	395	8			
1	B	269	Total	C	N	O	S	0	0	0
			2056	1310	345	393	8			

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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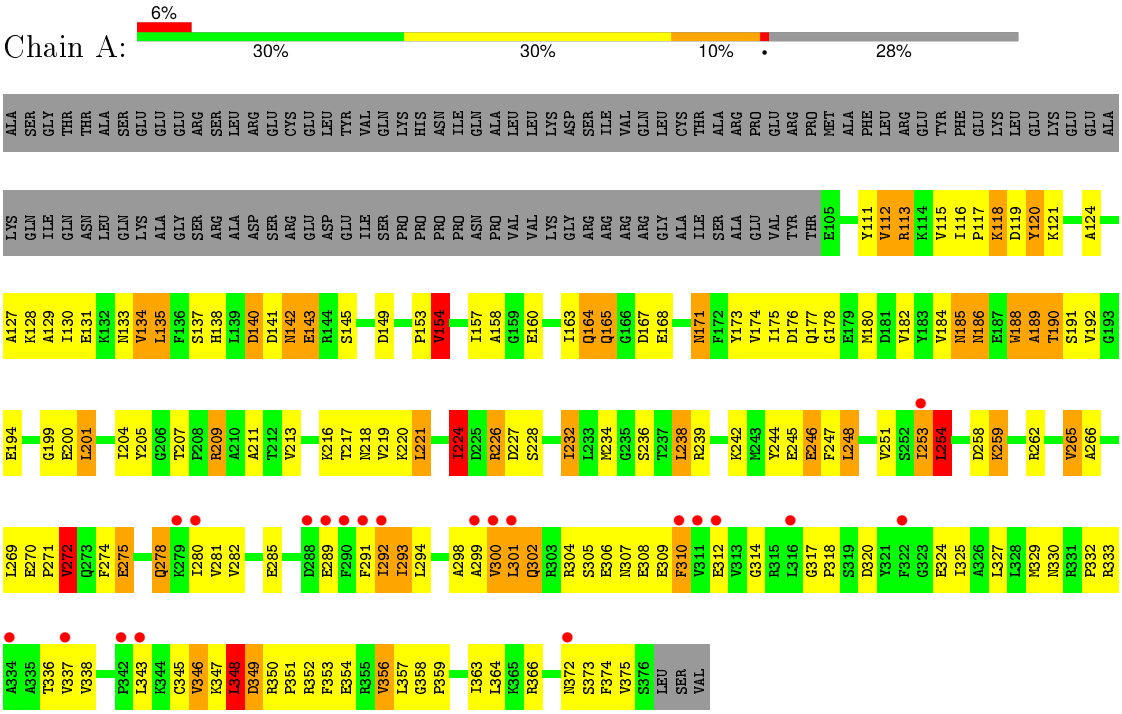
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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 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.

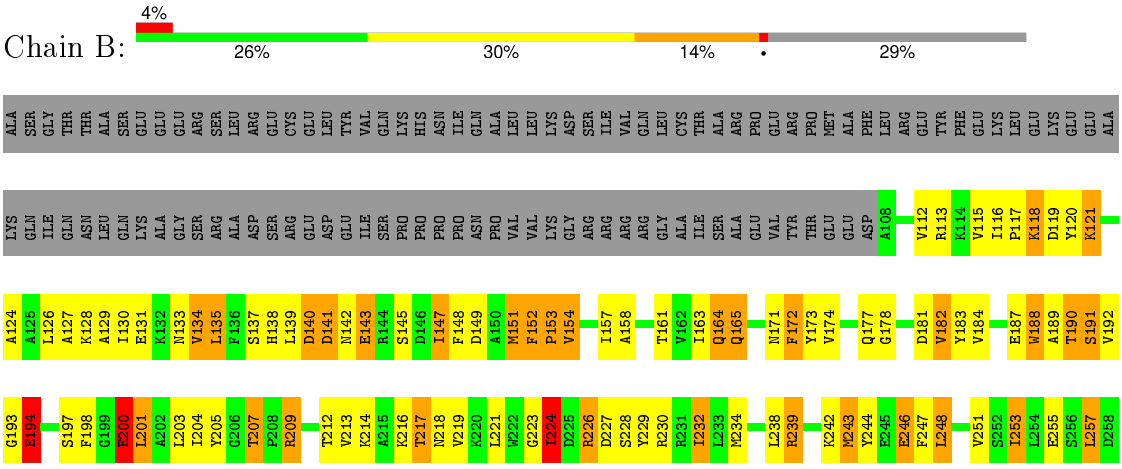
- Molecule 1: cAMP-dependent protein kinase type I-alpha regulatory subunit

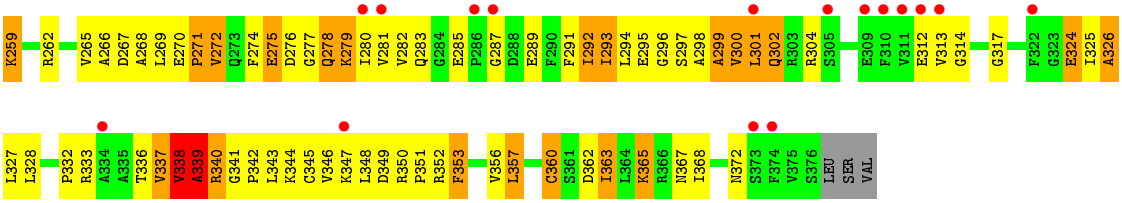
Chain A:



- Molecule 1: cAMP-dependent protein kinase type I-alpha regulatory subunit

Chain B:




K259
R262
V265
A266
D267
A268
L269
E270
P271
V272
Q273
F274
E275
D276
G277
Q278
K279
I280
V281
V282
Q283
G284
E285
P286
G287
D288
E289
F290
F291
I292
I293
L294
E295
G296
S297
A298
A299
V300
L301
Q302
R303
R304
S305
E309
F310
V311
E312
V313
G314
G317
F322
G323
E324
I325
A326
L327
L328
P332
R333
A334
A335
T336
V337
V338
A339
R340
G341
P342
L343
K344
C345
V346
K347
L348
D349
R350
P351
R352
F353
V356
L357
C360
S361
D362
I363
L364
K365
R366
N367
I368
N372
S373
F374
V375
S376
LEU
SER
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.67Å 104.67Å 218.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.88 47.19 – 3.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-3.88) 97.8 (47.19-3.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.78 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.260 , 0.287 0.250 , 0.274	Depositor DCC
R_{free} test set	549 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	125.4	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 141.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 11554 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4217	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.82	2/2112 (0.1%)	0.92	9/2862 (0.3%)
1	B	0.82	6/2095 (0.3%)	0.95	9/2838 (0.3%)
All	All	0.82	8/4207 (0.2%)	0.93	18/5700 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLU	CD-OE1	-7.40	1.17	1.25
1	A	246	GLU	CD-OE2	-6.66	1.18	1.25
1	B	134	VAL	CB-CG1	-5.74	1.40	1.52
1	B	134	VAL	CB-CG2	-5.68	1.41	1.52
1	A	143	GLU	CD-OE1	-5.56	1.19	1.25
1	B	200	GLU	CB-CG	-5.49	1.41	1.52
1	B	246	GLU	CD-OE2	-5.05	1.20	1.25
1	B	246	GLU	CD-OE1	-5.02	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	ALA	CB-CA-C	-10.82	93.87	110.10
1	A	254	LEU	CA-CB-CG	8.04	133.79	115.30
1	B	338	VAL	CB-CA-C	6.96	124.62	111.40
1	B	246	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	B	339	ALA	N-CA-C	5.81	126.69	111.00
1	B	239	ARG	CB-CG-CD	-5.81	96.50	111.60
1	A	154	VAL	CB-CA-C	-5.80	100.38	111.40
1	B	299	ALA	CB-CA-C	5.79	118.79	110.10
1	A	142	ASN	N-CA-CB	-5.68	100.38	110.60
1	A	254	LEU	CB-CG-CD2	-5.56	101.54	111.00
1	A	112	VAL	CB-CA-C	-5.36	101.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ARG	CB-CG-CD	-5.35	97.68	111.60
1	A	189	ALA	N-CA-CB	5.34	117.57	110.10
1	A	134	VAL	CB-CA-C	-5.24	101.45	111.40
1	B	337	VAL	N-CA-C	5.21	125.06	111.00
1	B	338	VAL	N-CA-C	5.13	124.86	111.00
1	A	113	ARG	N-CA-CB	-5.13	101.36	110.60
1	B	337	VAL	CB-CA-C	-5.13	101.65	111.40

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	2073	0	1989	145	0
1	B	2056	0	1977	204	0
2	A	44	0	22	8	0
2	B	44	0	22	5	0
All	All	4217	0	4010	343	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 42.

All (343) 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:A:402:CMP:C2	2:A:402:CMP:H2	0.97	1.48
2:A:401:CMP:C2	2:A:401:CMP:H2	0.97	1.48
2:B:401:CMP:H2	2:B:401:CMP:C2	0.97	1.48
2:B:402:CMP:H2	2:B:402:CMP:C2	0.97	1.48
1:B:153:PRO:O	1:B:154:VAL:HG22	1.41	1.21
1:A:253:ILE:H	1:A:253:ILE:HD13	1.10	1.13
1:B:182:VAL:HG23	1:B:213:VAL:HG22	1.32	1.12
1:B:253:ILE:HD12	1:B:253:ILE:H	1.01	1.10
1:B:278:GLN:O	1:B:338:VAL:HG13	1.49	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:O	1:A:265:VAL:HG23	1.52	1.08
1:B:163:ILE:HG23	1:B:209:ARG:HD2	1.31	1.06
1:B:301:LEU:O	1:B:302:GLN:HB2	1.60	1.01
1:A:301:LEU:O	1:A:302:GLN:HB2	1.59	1.01
1:B:294:LEU:HD11	1:B:346:VAL:HG13	1.38	1.00
1:A:163:ILE:CG2	1:A:209:ARG:HD2	1.90	1.00
1:A:253:ILE:H	1:A:253:ILE:CD1	1.76	0.99
1:B:253:ILE:CD1	1:B:253:ILE:H	1.79	0.93
1:A:163:ILE:HG23	1:A:209:ARG:HD2	1.46	0.93
1:B:281:VAL:CG1	1:B:333:ARG:HD3	1.99	0.93
1:A:373:SER:HB2	2:A:402:CMP:HN62	1.33	0.92
1:B:300:VAL:HG23	1:B:314:GLY:O	1.69	0.92
1:A:300:VAL:O	1:A:301:LEU:HG	1.71	0.91
1:B:173:TYR:HB3	1:B:221:LEU:HD12	1.50	0.90
1:B:253:ILE:N	1:B:253:ILE:HD12	1.86	0.89
1:A:188:TRP:CD1	1:A:189:ALA:N	2.39	0.89
1:B:281:VAL:HG13	1:B:333:ARG:HD3	1.50	0.89
1:A:178:GLY:HA3	1:A:219:VAL:HG12	1.56	0.88
1:B:163:ILE:HG23	1:B:209:ARG:CD	2.04	0.86
1:A:133:ASN:OD1	1:A:135:LEU:HB2	1.76	0.86
1:B:126:LEU:HD11	1:B:151:MET:CE	2.06	0.85
1:B:289:GLU:OE2	1:B:347:LYS:HD3	1.75	0.85
1:A:244:TYR:O	1:A:248:LEU:HD12	1.77	0.85
1:B:352:ARG:O	1:B:356:VAL:HG22	1.76	0.84
1:B:265:VAL:HG12	1:B:356:VAL:HB	1.57	0.84
1:B:158:ALA:H	1:B:218:ASN:HD22	1.22	0.83
1:B:300:VAL:O	1:B:301:LEU:HG	1.79	0.83
1:A:253:ILE:N	1:A:253:ILE:HD13	1.93	0.83
1:A:299:ALA:HB1	1:A:312:GLU:HG3	1.61	0.83
1:A:294:LEU:HD11	1:A:346:VAL:HG13	1.61	0.82
1:B:201:LEU:HD23	1:B:201:LEU:H	1.42	0.81
1:A:173:TYR:HB3	1:A:221:LEU:HD12	1.59	0.81
1:B:172:PHE:CD1	1:B:229:TYR:CE1	2.68	0.81
1:A:115:VAL:HG22	1:A:149:ASP:HB3	1.63	0.81
1:A:271:PRO:O	1:A:272:VAL:HB	1.82	0.80
1:B:282:VAL:HA	1:B:336:THR:HG23	1.64	0.80
1:B:244:TYR:HB3	1:B:248:LEU:HD12	1.64	0.79
1:A:281:VAL:CG1	1:A:333:ARG:HE	1.96	0.79
1:B:172:PHE:HD2	1:B:173:TYR:N	1.81	0.79
1:B:133:ASN:OD1	1:B:135:LEU:HB2	1.84	0.78
1:B:153:PRO:O	1:B:154:VAL:CG2	2.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HG21	1:A:209:ARG:HD2	1.67	0.75
1:B:244:TYR:HB3	1:B:248:LEU:CD1	2.16	0.75
1:A:281:VAL:O	1:A:336:THR:HG23	1.87	0.75
1:B:126:LEU:HD11	1:B:151:MET:HE2	1.67	0.75
1:A:291:PHE:HD2	1:A:345:CYS:HG	1.35	0.75
1:B:172:PHE:HD1	1:B:229:TYR:CE1	2.04	0.74
1:A:293:ILE:HG22	1:A:318:PRO:HA	1.70	0.74
1:B:204:ILE:HG21	1:B:238:LEU:HD21	1.70	0.74
1:B:278:GLN:O	1:B:338:VAL:CG1	2.35	0.73
1:B:262:ARG:O	1:B:265:VAL:CG2	2.37	0.73
1:B:298:ALA:HB1	1:B:338:VAL:O	1.87	0.72
1:B:182:VAL:CG2	1:B:213:VAL:HG22	2.16	0.72
1:B:280:ILE:N	1:B:338:VAL:HG22	2.04	0.72
1:B:299:ALA:O	1:B:337:VAL:HG12	1.89	0.72
1:B:221:LEU:HD23	1:B:221:LEU:N	2.04	0.72
1:B:281:VAL:HG13	1:B:333:ARG:CD	2.20	0.72
1:A:201:LEU:H	1:A:201:LEU:HD23	1.52	0.72
1:A:165:GLN:HE22	1:A:211:ALA:HA	1.53	0.71
1:A:165:GLN:NE2	1:A:211:ALA:HA	2.05	0.71
1:B:201:LEU:H	1:B:201:LEU:CD2	2.03	0.70
1:B:280:ILE:H	1:B:338:VAL:HG22	1.54	0.70
1:B:296:GLY:HA2	1:B:342:PRO:HB2	1.73	0.70
1:B:324:GLU:O	1:B:328:LEU:HB2	1.91	0.70
1:A:352:ARG:O	1:A:356:VAL:HG22	1.92	0.70
1:B:126:LEU:HD11	1:B:151:MET:HE3	1.71	0.70
1:B:158:ALA:H	1:B:218:ASN:ND2	1.89	0.70
1:A:221:LEU:HD23	1:A:221:LEU:N	2.07	0.70
1:A:244:TYR:HB3	1:A:248:LEU:HD12	1.73	0.69
1:B:203:LEU:HD22	1:B:226:ARG:HB2	1.73	0.69
1:A:281:VAL:HG13	1:A:333:ARG:HE	1.57	0.69
1:A:120:TYR:HD2	1:B:145:SER:HA	1.57	0.69
1:A:348:LEU:HD23	1:A:353:PHE:HA	1.75	0.69
1:B:172:PHE:CD2	1:B:173:TYR:N	2.60	0.69
1:B:130:ILE:HD11	1:B:151:MET:CE	2.23	0.68
1:B:265:VAL:CG1	1:B:356:VAL:HB	2.23	0.68
1:B:190:THR:HG23	1:B:191:SER:N	2.09	0.67
1:B:262:ARG:O	1:B:265:VAL:HG23	1.93	0.67
1:A:190:THR:CG2	1:A:191:SER:N	2.56	0.67
1:B:274:PHE:HB2	1:B:343:LEU:CD2	2.23	0.67
1:B:279:LYS:HA	1:B:338:VAL:HG11	1.75	0.67
1:B:188:TRP:CD1	1:B:188:TRP:C	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASP:H	1:B:143:GLU:HG3	1.59	0.66
1:B:275:GLU:N	1:B:278:GLN:HE22	1.93	0.66
1:B:293:ILE:HG21	1:B:317:GLY:O	1.96	0.66
1:A:262:ARG:O	1:A:265:VAL:CG2	2.37	0.66
1:B:274:PHE:HB2	1:B:343:LEU:HD23	1.77	0.65
1:B:291:PHE:O	1:B:292:ILE:HG12	1.97	0.65
1:B:188:TRP:CD1	1:B:189:ALA:N	2.65	0.65
1:A:145:SER:HB2	1:B:121:LYS:HD3	1.78	0.65
1:B:275:GLU:H	1:B:278:GLN:HE22	1.45	0.64
1:B:244:TYR:O	1:B:248:LEU:HD12	1.97	0.64
1:B:128:LYS:HG3	1:B:129:ALA:N	2.13	0.64
1:B:300:VAL:HA	1:B:337:VAL:HA	1.79	0.64
1:B:301:LEU:O	1:B:302:GLN:CB	2.40	0.64
1:B:157:ILE:HA	1:B:218:ASN:ND2	2.13	0.63
1:B:130:ILE:HD11	1:B:151:MET:HE1	1.80	0.63
1:A:301:LEU:O	1:A:302:GLN:CB	2.41	0.63
1:B:163:ILE:CG2	1:B:209:ARG:CD	2.77	0.63
1:B:313:VAL:HG11	2:B:402:CMP:N6	2.14	0.62
1:B:280:ILE:HD11	1:B:343:LEU:HD21	1.79	0.62
1:A:244:TYR:HB3	1:A:248:LEU:CD1	2.28	0.62
1:A:348:LEU:O	1:A:349:ASP:O	2.18	0.62
1:A:204:ILE:HG21	1:A:238:LEU:HD21	1.81	0.62
1:B:221:LEU:HD23	1:B:221:LEU:H	1.63	0.62
1:A:350:ARG:O	1:A:354:GLU:HG3	1.99	0.61
1:A:275:GLU:N	1:A:278:GLN:HE22	1.98	0.61
1:A:163:ILE:HG23	1:A:209:ARG:CD	2.26	0.61
1:A:201:LEU:N	1:A:201:LEU:HD23	2.15	0.61
1:A:293:ILE:HG21	1:A:317:GLY:O	2.00	0.61
1:B:279:LYS:HA	1:B:338:VAL:HG21	1.82	0.60
1:B:116:ILE:O	1:B:118:LYS:HD2	2.00	0.60
1:B:300:VAL:HG12	1:B:301:LEU:H	1.67	0.60
1:A:293:ILE:HG21	1:A:317:GLY:C	2.22	0.60
1:B:253:ILE:O	1:B:360:CYS:SG	2.60	0.59
1:B:299:ALA:O	1:B:337:VAL:CG1	2.49	0.59
1:B:152:PHE:H	1:B:152:PHE:HD2	1.51	0.59
1:A:190:THR:HG23	1:A:191:SER:H	1.67	0.59
1:A:145:SER:HA	1:B:120:TYR:HD2	1.67	0.59
1:B:209:ARG:NH1	2:B:401:CMP:O1P	2.36	0.59
1:B:262:ARG:O	1:B:265:VAL:HG22	2.02	0.59
1:A:300:VAL:HG21	2:A:402:CMP:N7	2.18	0.58
1:A:275:GLU:H	1:A:278:GLN:HE22	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:OD1	1:B:119:ASP:HB2	2.03	0.58
1:A:349:ASP:OD1	1:A:351:PRO:HG2	2.04	0.58
1:B:353:PHE:CD2	1:B:357:LEU:HD23	2.38	0.58
1:B:140:ASP:OD1	1:B:143:GLU:HG3	2.03	0.58
1:B:301:LEU:HA	1:B:312:GLU:HA	1.86	0.58
1:B:152:PHE:CD2	1:B:152:PHE:N	2.72	0.57
1:A:188:TRP:CD1	1:A:188:TRP:C	2.76	0.57
1:A:188:TRP:CG	1:A:189:ALA:N	2.72	0.57
1:B:133:ASN:HD21	1:B:135:LEU:HD12	1.69	0.57
1:B:251:VAL:HG12	1:B:253:ILE:HD13	1.87	0.57
1:B:277:GLY:HA2	1:B:339:ALA:HB2	1.86	0.57
1:B:296:GLY:HA3	1:B:342:PRO:O	2.05	0.57
1:A:165:GLN:NE2	1:A:211:ALA:CA	2.67	0.57
1:A:121:LYS:NZ	1:B:145:SER:HB2	2.20	0.57
1:B:352:ARG:O	1:B:356:VAL:CG2	2.51	0.56
1:A:291:PHE:O	1:A:292:ILE:HG12	2.04	0.56
1:A:317:GLY:O	1:A:320:ASP:HB2	2.04	0.56
1:B:158:ALA:N	1:B:218:ASN:HD22	1.97	0.56
1:A:140:ASP:OD1	1:A:143:GLU:HG3	2.05	0.56
1:A:281:VAL:HG11	1:A:333:ARG:HE	1.69	0.56
1:B:204:ILE:CG2	1:B:238:LEU:HD21	2.34	0.56
1:B:124:ALA:O	1:B:127:ALA:HB3	2.06	0.56
1:A:145:SER:HA	1:B:120:TYR:CD2	2.40	0.56
1:B:271:PRO:O	1:B:272:VAL:HB	2.06	0.56
1:B:172:PHE:HD2	1:B:172:PHE:C	2.09	0.56
1:B:140:ASP:OD1	1:B:143:GLU:CG	2.53	0.56
1:B:201:LEU:N	1:B:201:LEU:CD2	2.69	0.55
1:A:184:VAL:C	1:A:186:ASN:H	2.08	0.55
1:B:172:PHE:CE2	1:B:173:TYR:O	2.59	0.55
1:B:296:GLY:CA	1:B:342:PRO:HB2	2.35	0.55
1:B:279:LYS:HA	1:B:338:VAL:CG1	2.35	0.55
1:A:145:SER:HB2	1:B:121:LYS:CD	2.36	0.55
1:A:119:ASP:OD2	1:A:121:LYS:HG2	2.06	0.55
1:B:253:ILE:HG22	1:B:363:ILE:HG23	1.90	0.54
1:B:173:TYR:CB	1:B:221:LEU:HD12	2.31	0.54
1:B:182:VAL:HG12	1:B:190:THR:H	1.72	0.54
1:A:294:LEU:HD12	1:A:345:CYS:HA	1.90	0.54
1:A:190:THR:HG23	1:A:191:SER:N	2.21	0.54
1:A:298:ALA:HB1	1:A:338:VAL:O	2.06	0.54
1:B:165:GLN:H	1:B:212:THR:CB	2.21	0.54
1:A:209:ARG:NH1	2:A:401:CMP:O1P	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HD12	1:B:360:CYS:HB3	1.90	0.54
1:A:200:GLU:OE2	1:A:201:LEU:CD2	2.56	0.54
1:B:172:PHE:CD2	1:B:172:PHE:C	2.81	0.54
1:A:120:TYR:CD2	1:B:145:SER:HA	2.41	0.53
1:B:353:PHE:CE2	1:B:357:LEU:HD23	2.42	0.53
1:B:228:SER:O	1:B:232:ILE:HG13	2.09	0.53
1:B:270:GLU:O	1:B:271:PRO:O	2.25	0.53
1:B:276:ASP:OD1	1:B:341:GLY:N	2.42	0.53
1:B:287:GLY:HA3	1:B:326:ALA:HB1	1.90	0.53
1:B:130:ILE:CD1	1:B:151:MET:HE1	2.38	0.53
1:A:291:PHE:HD2	1:A:345:CYS:SG	2.32	0.53
1:B:190:THR:CG2	1:B:191:SER:N	2.72	0.53
1:B:200:GLU:OE2	1:B:201:LEU:CD2	2.57	0.53
1:B:161:THR:HG23	1:B:214:LYS:HG3	1.90	0.53
1:B:178:GLY:HA3	1:B:219:VAL:HG12	1.90	0.52
1:A:294:LEU:HD12	1:A:345:CYS:CA	2.40	0.52
1:A:358:GLY:N	1:A:359:PRO:CD	2.72	0.52
1:A:350:ARG:N	1:A:351:PRO:HD2	2.24	0.52
1:B:177:GLN:HA	1:B:194:GLU:OE1	2.10	0.52
1:A:302:GLN:H	1:A:310:PHE:HB3	1.75	0.52
1:B:283:GLN:HB2	1:B:336:THR:OG1	2.09	0.52
1:A:228:SER:O	1:A:232:ILE:HG13	2.09	0.52
1:B:365:LYS:O	1:B:368:ILE:HG22	2.09	0.52
1:A:253:ILE:N	1:A:253:ILE:CD1	2.56	0.52
1:A:158:ALA:H	1:A:218:ASN:HD22	1.58	0.52
1:B:152:PHE:HD2	1:B:152:PHE:N	2.05	0.51
1:A:258:ASP:O	1:A:259:LYS:C	2.47	0.51
1:B:182:VAL:CG1	1:B:182:VAL:O	2.58	0.51
1:A:324:GLU:HG2	1:A:325:ILE:HG13	1.92	0.51
1:A:300:VAL:HG23	1:A:314:GLY:O	2.11	0.51
1:B:205:TYR:HB2	1:B:207:THR:CG2	2.41	0.51
1:B:205:TYR:HB2	1:B:207:THR:HG23	1.93	0.51
1:A:175:ILE:HA	1:A:221:LEU:HB3	1.93	0.51
1:A:251:VAL:HB	1:A:254:LEU:HD12	1.93	0.51
1:B:118:LYS:NZ	1:B:151:MET:O	2.44	0.51
1:A:153:PRO:O	1:A:154:VAL:HG22	2.10	0.51
1:B:277:GLY:HA2	1:B:339:ALA:CB	2.40	0.50
1:B:244:TYR:CE2	1:B:269:LEU:HD11	2.46	0.50
1:A:251:VAL:HB	1:A:254:LEU:CD1	2.41	0.50
1:B:183:TYR:HA	1:B:188:TRP:HA	1.93	0.50
1:A:204:ILE:HG12	1:A:234:MET:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG13	1:A:356:VAL:HB	1.94	0.49
1:A:336:THR:HG22	1:A:337:VAL:N	2.27	0.49
1:B:230:ARG:HA	1:B:234:MET:HB2	1.95	0.49
1:A:270:GLU:C	1:A:271:PRO:O	2.50	0.49
1:A:301:LEU:HB3	1:A:310:PHE:HB3	1.95	0.48
1:A:253:ILE:HG21	1:A:364:LEU:CD2	2.43	0.48
1:A:185:ASN:O	1:A:186:ASN:HB2	2.13	0.48
1:B:172:PHE:HE2	1:B:173:TYR:O	1.95	0.48
1:B:243:MET:HG3	1:B:243:MET:O	2.13	0.48
1:B:216:LYS:C	1:B:217:THR:HG22	2.34	0.48
1:A:157:ILE:HG12	1:A:160:GLU:OE2	2.14	0.48
1:A:177:GLN:O	1:A:219:VAL:HA	2.13	0.48
1:B:140:ASP:O	1:B:142:ASN:N	2.47	0.48
1:B:139:LEU:HD21	1:B:147:ILE:HD13	1.96	0.48
1:A:304:ARG:C	1:A:306:GLU:H	2.17	0.48
1:A:271:PRO:O	1:A:272:VAL:CB	2.55	0.48
1:A:310:PHE:N	1:A:310:PHE:CD2	2.82	0.48
1:B:181:ASP:OD2	1:B:216:LYS:HG3	2.14	0.48
1:B:279:LYS:HA	1:B:338:VAL:CG2	2.42	0.48
1:B:285:GLU:O	1:B:333:ARG:HG3	2.14	0.48
1:B:115:VAL:HG22	1:B:149:ASP:HB3	1.95	0.47
1:B:257:LEU:HD21	1:B:360:CYS:HB2	1.96	0.47
1:B:147:ILE:HG22	1:B:148:PHE:N	2.30	0.47
1:A:180:MET:HA	1:A:216:LYS:H	1.79	0.47
1:B:193:GLY:O	1:B:194:GLU:C	2.53	0.47
1:B:295:GLU:HB3	1:B:344:LYS:HD2	1.96	0.47
1:B:172:PHE:CE1	1:B:229:TYR:CE1	3.02	0.47
1:A:124:ALA:O	1:A:127:ALA:HB3	2.14	0.47
1:B:327:LEU:HD22	1:B:350:ARG:CB	2.45	0.47
1:B:183:TYR:HE2	1:B:188:TRP:HE3	1.62	0.47
1:B:277:GLY:CA	1:B:339:ALA:HB2	2.44	0.47
1:A:184:VAL:C	1:A:186:ASN:N	2.67	0.47
1:A:310:PHE:N	1:A:310:PHE:HD2	2.13	0.47
1:A:158:ALA:H	1:A:218:ASN:ND2	2.13	0.47
1:A:226:ARG:CG	1:A:227:ASP:N	2.78	0.46
1:A:128:LYS:CG	1:A:129:ALA:N	2.78	0.46
1:B:182:VAL:CG1	1:B:189:ALA:HB3	2.45	0.46
1:B:172:PHE:CE2	1:B:174:VAL:HG23	2.51	0.46
1:B:294:LEU:HD12	1:B:345:CYS:CA	2.45	0.46
1:B:338:VAL:CG1	1:B:339:ALA:N	2.79	0.46
1:B:294:LEU:HD12	1:B:345:CYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:HD12	1:B:232:ILE:HG21	1.98	0.46
1:A:246:GLU:O	1:A:247:PHE:C	2.53	0.46
1:B:163:ILE:CG2	1:B:209:ARG:HD3	2.46	0.45
1:B:297:SER:O	1:B:340:ARG:CB	2.64	0.45
1:A:163:ILE:CG2	1:A:164:GLN:N	2.78	0.45
1:A:205:TYR:HB2	1:A:207:THR:HG23	1.98	0.45
1:A:119:ASP:HB2	1:B:149:ASP:OD1	2.16	0.45
1:B:246:GLU:O	1:B:247:PHE:C	2.54	0.45
1:B:181:ASP:OD1	1:B:191:SER:HB2	2.16	0.45
1:B:251:VAL:HG12	1:B:253:ILE:CD1	2.46	0.45
1:A:329:MET:O	1:A:330:ASN:HB2	2.16	0.45
1:A:373:SER:HB2	2:A:402:CMP:N6	2.16	0.45
1:B:157:ILE:O	1:B:158:ALA:C	2.54	0.45
1:A:226:ARG:HG3	1:A:227:ASP:N	2.32	0.45
2:A:401:CMP:N3	2:A:401:CMP:H3'	2.32	0.45
1:B:126:LEU:CD1	1:B:151:MET:HE3	2.43	0.45
1:A:174:VAL:HG12	1:A:174:VAL:O	2.15	0.45
1:A:121:LYS:HZ3	1:B:145:SER:HB2	1.81	0.45
1:A:358:GLY:N	1:A:359:PRO:HD3	2.32	0.45
1:A:201:LEU:N	1:A:201:LEU:CD2	2.79	0.44
1:B:112:VAL:CG1	1:B:113:ARG:N	2.79	0.44
1:B:356:VAL:HG23	1:B:357:LEU:HD22	2.00	0.44
1:B:272:VAL:HG11	1:B:347:LYS:HE3	1.99	0.44
1:A:157:ILE:O	1:A:158:ALA:C	2.55	0.44
1:B:349:ASP:HB3	1:B:352:ARG:HB2	1.99	0.44
1:A:348:LEU:O	1:A:349:ASP:C	2.56	0.44
1:A:185:ASN:O	1:A:186:ASN:CB	2.65	0.44
1:A:289:GLU:OE2	1:A:347:LYS:HD2	2.18	0.44
1:A:300:VAL:O	1:A:301:LEU:CG	2.56	0.44
1:B:274:PHE:HB2	1:B:343:LEU:HD21	1.99	0.44
1:A:115:VAL:HG12	1:A:117:PRO:HD3	2.00	0.44
1:A:285:GLU:O	1:A:333:ARG:HG2	2.17	0.44
1:A:306:GLU:O	1:A:308:GLU:N	2.46	0.44
1:A:176:ASP:HB3	1:A:220:LYS:O	2.18	0.44
1:A:199:GLY:HA2	2:A:401:CMP:H4'	1.99	0.43
1:B:253:ILE:HG22	1:B:363:ILE:CG2	2.48	0.43
1:A:327:LEU:HD23	1:A:353:PHE:CD2	2.53	0.43
1:B:349:ASP:OD1	1:B:351:PRO:HD2	2.18	0.43
1:A:274:PHE:CD2	1:A:280:ILE:HG12	2.53	0.43
1:B:266:ALA:C	1:B:268:ALA:H	2.21	0.43
1:B:352:ARG:HG3	1:B:352:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG22	1:A:213:VAL:HG22	2.00	0.43
1:A:282:VAL:HA	1:A:336:THR:HG23	2.01	0.43
1:B:115:VAL:HG12	1:B:117:PRO:HD3	2.00	0.43
1:A:182:VAL:HG12	1:A:182:VAL:O	2.18	0.43
1:A:113:ARG:O	1:A:115:VAL:HG23	2.18	0.42
1:A:120:TYR:O	1:A:121:LYS:C	2.58	0.42
1:A:293:ILE:HD11	1:A:343:LEU:HD11	2.01	0.42
1:A:258:ASP:C	1:A:258:ASP:OD1	2.56	0.42
1:B:152:PHE:CE2	1:B:223:GLY:C	2.93	0.42
1:A:171:ASN:HB3	1:A:224:ILE:O	2.18	0.42
1:B:158:ALA:HB2	1:B:217:THR:HA	2.01	0.42
1:B:367:ASN:N	1:B:367:ASN:HD22	2.18	0.42
1:A:163:ILE:HG22	1:A:164:GLN:N	2.34	0.42
1:B:338:VAL:CG1	1:B:339:ALA:H	2.33	0.42
1:B:173:TYR:CD2	1:B:173:TYR:N	2.87	0.42
1:A:118:LYS:NZ	1:A:149:ASP:HA	2.35	0.42
1:B:140:ASP:O	1:B:141:ASP:C	2.58	0.42
1:A:352:ARG:HB2	1:A:352:ARG:NH1	2.35	0.42
1:B:184:VAL:O	1:B:187:GLU:HB2	2.20	0.42
1:B:255:GLU:C	1:B:257:LEU:H	2.23	0.41
1:B:298:ALA:HA	1:B:340:ARG:CB	2.49	0.41
1:B:152:PHE:HE2	1:B:223:GLY:C	2.23	0.41
1:B:226:ARG:CG	1:B:227:ASP:N	2.82	0.41
1:A:266:ALA:O	1:A:269:LEU:HG	2.20	0.41
1:B:274:PHE:CD2	1:B:280:ILE:HG12	2.55	0.41
1:B:281:VAL:H	1:B:338:VAL:CG2	2.33	0.41
1:B:120:TYR:O	1:B:121:LYS:C	2.57	0.41
1:B:188:TRP:CG	1:B:189:ALA:N	2.87	0.41
1:B:172:PHE:CD1	1:B:229:TYR:CD1	3.09	0.41
1:B:197:SER:O	1:B:198:PHE:HB3	2.19	0.41
1:A:121:LYS:NZ	1:B:145:SER:CB	2.83	0.41
1:B:165:GLN:HA	1:B:165:GLN:HE21	1.86	0.41
1:A:274:PHE:CE2	1:A:280:ILE:HG12	2.55	0.41
1:A:300:VAL:HG12	1:A:301:LEU:H	1.86	0.41
1:B:172:PHE:HB3	1:B:224:ILE:HG23	2.01	0.41
1:A:247:PHE:C	1:A:247:PHE:CD2	2.94	0.41
1:B:190:THR:HG23	1:B:191:SER:H	1.86	0.41
1:B:164:GLN:O	1:B:165:GLN:C	2.59	0.41
1:A:116:ILE:O	1:A:118:LYS:NZ	2.53	0.40
1:A:325:ILE:HG23	1:A:329:MET:HG3	2.03	0.40
1:B:278:GLN:HE21	1:B:278:GLN:HB2	1.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:PHE:HE2	1:B:224:ILE:N	2.19	0.40
1:B:325:ILE:HB	2:B:402:CMP:P	2.62	0.40
1:B:182:VAL:HG12	1:B:189:ALA:HB3	2.03	0.40
1:B:337:VAL:HB	1:B:338:VAL:H	1.74	0.40
1:A:352:ARG:CB	1:A:352:ARG:HH11	2.34	0.40
1:B:134:VAL:CG2	1:B:267:ASP:O	2.69	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	270/379 (71%)	203 (75%)	44 (16%)	23 (8%)	1 17
1	B	267/379 (70%)	197 (74%)	49 (18%)	21 (8%)	1 19
All	All	537/758 (71%)	400 (74%)	93 (17%)	44 (8%)	1 18

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	TYR
1	A	112	VAL
1	A	141	ASP
1	A	272	VAL
1	A	275	GLU
1	A	300	VAL
1	A	301	LEU
1	A	302	GLN
1	A	349	ASP
1	A	375	VAL
1	B	141	ASP
1	B	153	PRO

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Mol	Chain	Res	Type
1	B	271	PRO
1	B	275	GLU
1	B	301	LEU
1	B	302	GLN
1	B	332	PRO
1	B	338	VAL
1	B	339	ALA
1	A	167	ASP
1	A	186	ASN
1	A	194	GLU
1	A	348	LEU
1	B	154	VAL
1	B	194	GLU
1	B	304	ARG
1	B	326	ALA
1	B	340	ARG
1	B	362	ASP
1	A	185	ASN
1	A	305	SER
1	A	307	ASN
1	B	272	VAL
1	B	363	ILE
1	A	245	GLU
1	A	154	VAL
1	A	309	GLU
1	B	259	LYS
1	A	209	ARG
1	A	332	PRO
1	B	209	ARG
1	B	300	VAL
1	A	224	ILE
1	B	224	ILE

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	209/324 (64%)	164 (78%)	45 (22%)	1 10
1	B	209/324 (64%)	164 (78%)	45 (22%)	1 10
All	All	418/648 (64%)	328 (78%)	90 (22%)	1 10

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	120	TYR
1	A	130	ILE
1	A	131	GLU
1	A	134	VAL
1	A	135	LEU
1	A	137	SER
1	A	138	HIS
1	A	140	ASP
1	A	142	ASN
1	A	154	VAL
1	A	164	GLN
1	A	165	GLN
1	A	168	GLU
1	A	171	ASN
1	A	188	TRP
1	A	190	THR
1	A	192	VAL
1	A	201	LEU
1	A	217	THR
1	A	221	LEU
1	A	224	ILE
1	A	226	ARG
1	A	232	ILE
1	A	236	SER
1	A	238	LEU
1	A	242	LYS
1	A	248	LEU
1	A	253	ILE
1	A	254	LEU
1	A	259	LYS
1	A	265	VAL
1	A	272	VAL
1	A	278	GLN
1	A	292	ILE

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Mol	Chain	Res	Type
1	A	293	ILE
1	A	310	PHE
1	A	346	VAL
1	A	348	LEU
1	A	356	VAL
1	A	357	LEU
1	A	363	ILE
1	A	366	ARG
1	A	372	ASN
1	A	374	PHE
1	B	118	LYS
1	B	121	LYS
1	B	131	GLU
1	B	135	LEU
1	B	137	SER
1	B	138	HIS
1	B	140	ASP
1	B	147	ILE
1	B	151	MET
1	B	152	PHE
1	B	164	GLN
1	B	165	GLN
1	B	171	ASN
1	B	172	PHE
1	B	182	VAL
1	B	188	TRP
1	B	190	THR
1	B	191	SER
1	B	192	VAL
1	B	194	GLU
1	B	200	GLU
1	B	201	LEU
1	B	207	THR
1	B	217	THR
1	B	224	ILE
1	B	226	ARG
1	B	232	ILE
1	B	239	ARG
1	B	242	LYS
1	B	243	MET
1	B	248	LEU
1	B	253	ILE

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Mol	Chain	Res	Type
1	B	257	LEU
1	B	259	LYS
1	B	278	GLN
1	B	279	LYS
1	B	292	ILE
1	B	293	ILE
1	B	324	GLU
1	B	348	LEU
1	B	353	PHE
1	B	357	LEU
1	B	360	CYS
1	B	365	LYS
1	B	372	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	218	ASN
1	A	278	GLN
1	A	372	ASN
1	B	185	ASN
1	B	218	ASN
1	B	278	GLN
1	B	367	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	$\#\|Z\| > 2$
2	CMP	A	401	-	19,25,25	1.65	4 (21%)	18,39,39	2.70	6 (33%)
2	CMP	A	402	-	19,25,25	1.47	3 (15%)	18,39,39	2.16	2 (11%)
2	CMP	B	401	-	19,25,25	1.39	5 (26%)	18,39,39	2.69	6 (33%)
2	CMP	B	402	-	19,25,25	1.43	3 (15%)	18,39,39	2.30	2 (11%)

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	CMP	A	401	-	-	0/0/31/31	0/4/4/4
2	CMP	A	402	-	-	0/0/31/31	0/4/4/4
2	CMP	B	401	-	-	0/0/31/31	0/4/4/4
2	CMP	B	402	-	-	0/0/31/31	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CMP	O3'-C3'	-3.74	1.38	1.44
2	A	401	CMP	O5'-C5'	-2.75	1.42	1.46
2	B	401	CMP	O3'-C3'	-2.54	1.40	1.44
2	B	401	CMP	O5'-C5'	-2.21	1.42	1.46
2	B	401	CMP	P-O3'	2.23	1.61	1.58
2	B	401	CMP	C5-C4	2.41	1.45	1.40
2	A	401	CMP	O4'-C1'	2.63	1.44	1.41
2	B	401	CMP	O4'-C1'	2.67	1.44	1.41
2	A	402	CMP	P-O3'	2.81	1.62	1.58
2	A	401	CMP	C5-C4	2.87	1.47	1.40
2	B	402	CMP	O4'-C1'	2.89	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	CMP	P-O3'	2.98	1.63	1.58
2	B	402	CMP	C5-C4	3.17	1.47	1.40
2	A	402	CMP	C5-C4	3.22	1.47	1.40
2	A	402	CMP	O4'-C1'	3.43	1.45	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	CMP	N3-C2-N1	-8.53	122.37	128.89
2	B	401	CMP	N3-C2-N1	-8.45	122.42	128.89
2	A	402	CMP	N3-C2-N1	-7.52	123.14	128.89
2	A	401	CMP	N3-C2-N1	-6.27	124.09	128.89
2	A	401	CMP	O3'-C3'-C4'	-5.93	105.98	110.72
2	B	401	CMP	C2'-C1'-N9	-4.20	107.88	114.29
2	A	401	CMP	C2'-C1'-N9	-3.82	108.46	114.29
2	B	401	CMP	C4'-O4'-C1'	-3.63	105.73	109.72
2	A	401	CMP	C5'-C4'-C3'	-3.45	104.96	112.62
2	A	402	CMP	C4-C5-N7	-3.24	106.50	109.48
2	B	401	CMP	C4-C5-N7	-3.12	106.61	109.48
2	B	402	CMP	C4-C5-N7	-2.62	107.06	109.48
2	A	401	CMP	C4-C5-N7	-2.27	107.39	109.48
2	B	401	CMP	O4'-C1'-N9	2.41	113.15	108.10
2	B	401	CMP	O5'-P-O3'	2.46	109.35	105.75
2	A	401	CMP	O4'-C1'-N9	4.44	117.40	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CMP	4	0
2	A	402	CMP	4	0
2	B	401	CMP	2	0
2	B	402	CMP	3	0

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^{th} 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	272/379 (71%)	0.41	21 (7%)	16	11	65, 138, 208, 241	0
1	B	269/379 (70%)	0.39	16 (5%)	26	17	68, 137, 219, 263	0
All	All	541/758 (71%)	0.40	37 (6%)	20	13	65, 137, 215, 263	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	5.3
1	A	300	VAL	4.8
1	A	253	ILE	3.6
1	A	311	VAL	3.5
1	A	312	GLU	3.5
1	A	310	PHE	3.4
1	A	316	LEU	3.4
1	B	286	PRO	3.4
1	B	287	GLY	3.2
1	A	342	PRO	3.2
1	B	280	ILE	3.0
1	B	281	VAL	3.0
1	B	310	PHE	2.9
1	A	279	LYS	2.9
1	B	301	LEU	2.9
1	A	299	ALA	2.8
1	A	280	ILE	2.8
1	A	343	LEU	2.8
1	B	313	VAL	2.7
1	A	372	ASN	2.6
1	B	334	ALA	2.6
1	A	289	GLU	2.6
1	B	373	SER	2.6
1	A	337	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	2.5
1	B	312	GLU	2.5
1	B	347	LYS	2.4
1	B	322	PHE	2.4
1	B	309	GLU	2.4
1	A	291	PHE	2.3
1	B	305	SER	2.3
1	A	322	PHE	2.3
1	A	334	ALA	2.2
1	A	290	PHE	2.2
1	B	311	VAL	2.1
1	B	374	PHE	2.1
1	A	292	ILE	2.1

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CMP	B	401	22/22	0.97	0.32	0.14	42,100,137,144	0
2	CMP	B	402	22/22	0.93	0.46	-0.07	173,202,233,237	0
2	CMP	A	402	22/22	0.91	0.47	-0.09	131,205,250,258	0
2	CMP	A	401	22/22	0.98	0.27	-0.62	55,84,108,133	0

6.5 Other polymers (i)

There are no such residues in this entry.