Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID	:	4GVL
Title	:	Crystal Structure of the GsuK RCK domain
Authors	:	Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.
Deposited on	:	2012-08-30
Resolution	:	3.00 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:

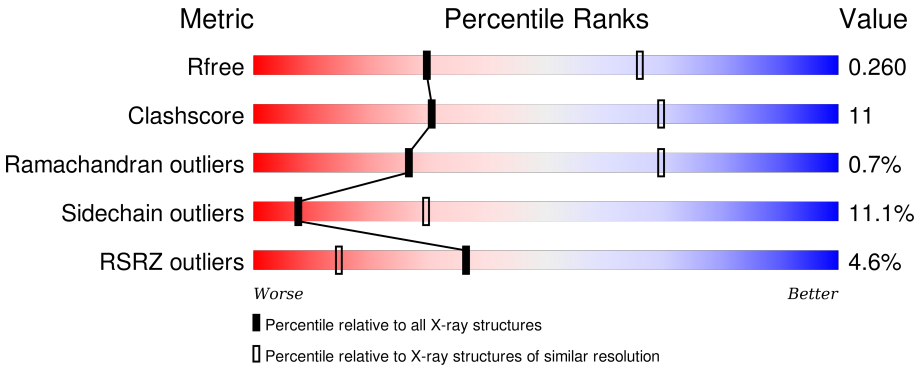
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	462	68% 26% 5%
1	B	462	69% 25%
1	C	462	13% 78% 18%
1	D	462	4% 68% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	C	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13940 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	B	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	C	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			
1	D	455	Total	C	N	O	S	0	0	0
			3460	2183	620	648	9			

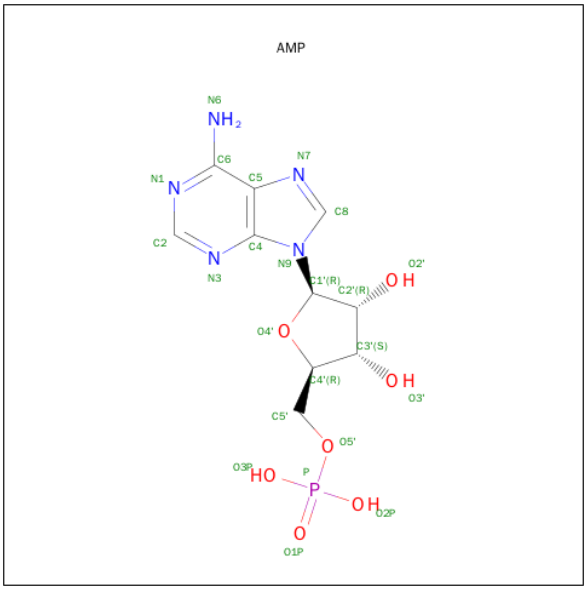
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
A	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
A	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
A	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
B	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
B	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
B	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
B	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
C	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
C	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
C	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
C	568	ARG	-	EXPRESSION TAG	UNP Q74FS9
D	565	LEU	-	EXPRESSION TAG	UNP Q74FS9
D	566	VAL	-	EXPRESSION TAG	UNP Q74FS9
D	567	PRO	-	EXPRESSION TAG	UNP Q74FS9
D	568	ARG	-	EXPRESSION TAG	UNP Q74FS9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0
3	B	1	Total C N O P 23 10 5 7 1	0	0
3	C	1	Total C N O P 23 10 5 7 1	0	0
3	D	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	2	Total Ca 2 2	0	0

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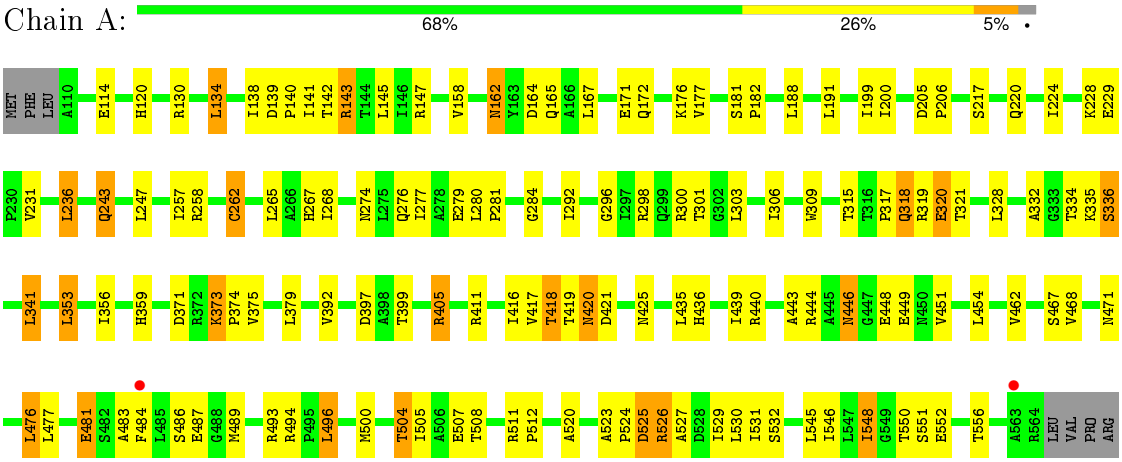
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	C	1	1	1	0	0

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 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.

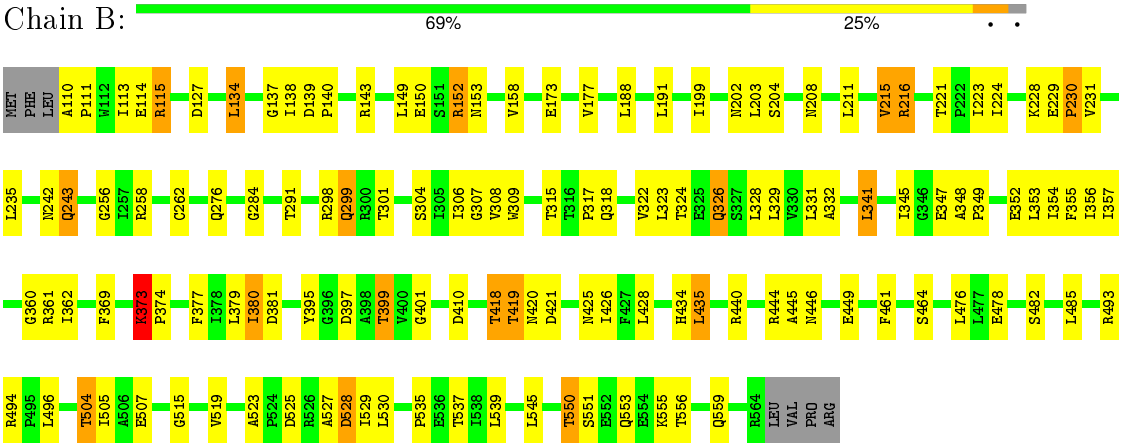
- Molecule 1: TrkA domain protein

Chain A:



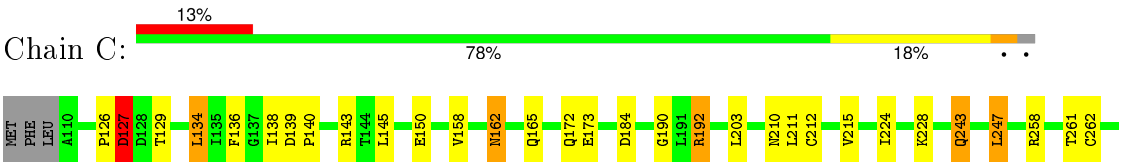
- Molecule 1: TrkA domain protein

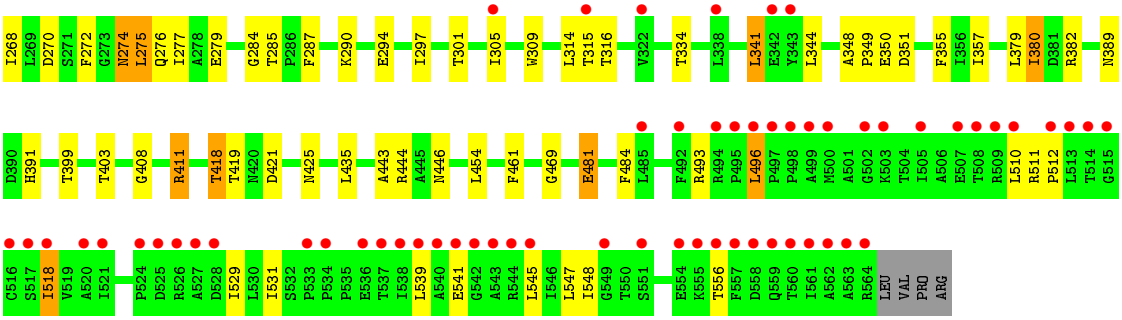
Chain B:



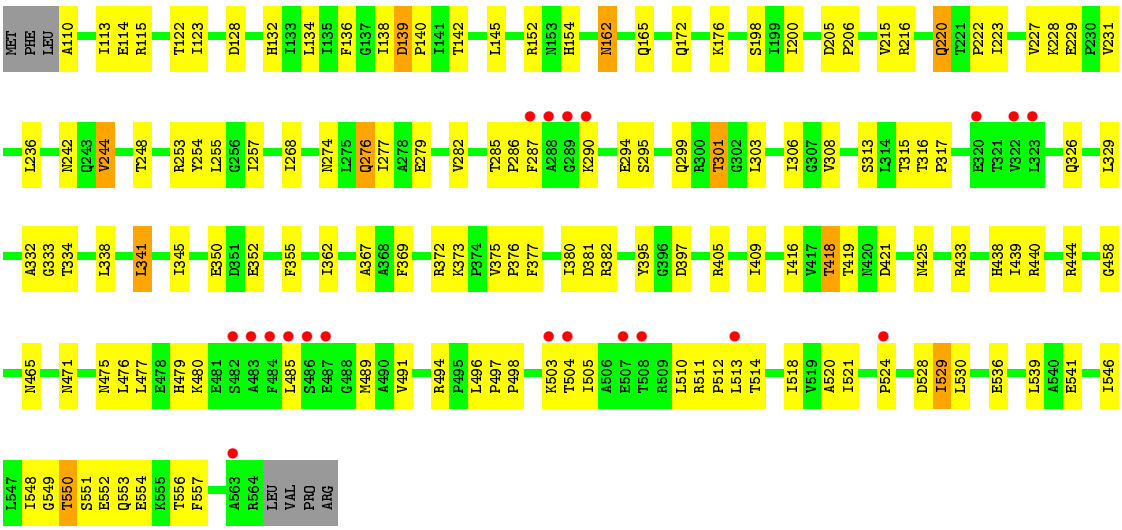
- Molecule 1: TrkA domain protein

Chain C:





- Molecule 1: TrkA domain protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.65Å 161.69Å 310.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 3.00 37.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-3.00) 98.6 (37.77-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.262 0.224 , 0.260	Depositor DCC
R_{free} test set	1128 reflections (2.08%)	DCC
Wilson B-factor (Å^2)	100.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 55352 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13940	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: AMP, ZN, CA

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	0.45	0/3521	0.65	2/4796 (0.0%)
1	B	0.45	0/3521	0.64	0/4796
1	C	0.47	4/3521 (0.1%)	0.56	0/4796
1	D	0.55	5/3521 (0.1%)	0.66	2/4796 (0.0%)
All	All	0.48	9/14084 (0.1%)	0.63	4/19184 (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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	216	ARG	CZ-NH2	16.15	1.54	1.33
1	C	126	PRO	C-N	8.02	1.52	1.34
1	C	190	GLY	C-O	7.78	1.36	1.23
1	D	216	ARG	CZ-NH1	7.12	1.42	1.33
1	D	220	GLN	CD-OE1	6.64	1.38	1.24
1	C	129	THR	CB-OG1	5.98	1.55	1.43
1	C	127	ASP	C-N	5.81	1.47	1.34
1	D	220	GLN	C-O	5.65	1.34	1.23
1	D	220	GLN	CD-NE2	5.58	1.46	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	216	ARG	NE-CZ-NH1	-18.05	111.28	120.30
1	D	216	ARG	NH1-CZ-NH2	6.87	126.95	119.40
1	A	353	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	496	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	LYS	Peptide

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	3460	0	3518	94	0
1	B	3460	0	3518	81	0
1	C	3460	0	3518	58	0
1	D	3460	0	3518	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	12	1	0
3	B	23	0	12	2	0
3	C	23	0	12	2	0
3	D	23	0	12	2	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	13940	0	14120	309	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 11.

All (309) 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:A:143:ARG:NH1	1:A:172:GLN:HG2	1.58	1.16
1:B:355:PHE:CZ	1:B:380:ILE:HD11	1.89	1.06
1:A:143:ARG:HH12	1:A:172:GLN:HG2	1.20	1.00
1:D:419:THR:HG22	1:D:421:ASP:H	1.28	0.97
1:A:301:THR:CG2	1:A:303:LEU:HG	1.95	0.97
1:A:419:THR:HG22	1:A:421:ASP:H	1.30	0.96
1:A:436:HIS:HB3	1:A:439:ILE:HD12	1.47	0.96
1:C:418:THR:HG22	1:C:444:ARG:HH11	1.32	0.94
1:C:419:THR:HB	1:C:425:ASN:HD21	1.31	0.92
1:C:419:THR:HB	1:C:425:ASN:ND2	1.87	0.89
1:A:306:ILE:HD11	1:A:332:ALA:HB2	1.58	0.86
1:B:444:ARG:HE	1:B:446:ASN:HD21	1.25	0.85
1:D:553:GLN:HA	1:D:556:THR:HB	1.58	0.85
1:A:301:THR:HG21	1:A:303:LEU:HG	1.60	0.82
1:D:444:ARG:HE	1:D:465:ASN:HD21	1.22	0.82
1:D:551:SER:HA	1:D:554:GLU:HB3	1.60	0.82
1:B:419:THR:HG22	1:B:421:ASP:H	1.44	0.81
1:C:419:THR:HG22	1:C:421:ASP:H	1.46	0.80
1:A:334:THR:HG22	1:A:336:SER:H	1.46	0.80
1:A:301:THR:HG22	1:A:303:LEU:HG	1.64	0.78
1:B:419:THR:HB	1:B:425:ASN:OD1	1.84	0.78
1:A:258:ARG:O	1:A:440:ARG:NH1	2.16	0.78
1:B:299:GLN:H	1:B:299:GLN:HE21	1.30	0.77
1:D:475:ASN:O	1:D:479:HIS:HB2	1.84	0.77
1:A:138:ILE:HD11	1:A:143:ARG:HG3	1.64	0.76
1:A:143:ARG:HH12	1:A:172:GLN:CG	2.00	0.74
1:A:397:ASP:OD1	1:A:399:THR:HB	1.88	0.74
1:A:309:TRP:HB2	1:A:328:LEU:HB3	1.67	0.74
1:B:550:THR:HG22	1:B:553:GLN:H	1.53	0.74
1:A:268:ILE:HD11	1:A:279:GLU:HG3	1.69	0.74
1:D:308:VAL:HG22	1:D:329:LEU:HD23	1.71	0.73
1:A:134:LEU:CD1	1:A:199:ILE:HG12	2.19	0.72
1:C:268:ILE:HD11	1:C:279:GLU:HG3	1.72	0.71
1:B:262:CYS:HA	1:B:284:GLY:HA3	1.72	0.71
1:D:419:THR:H	1:D:425:ASN:HD21	1.39	0.70
1:A:243:GLN:HA	1:A:243:GLN:HE21	1.57	0.69
1:C:444:ARG:HH21	1:C:446:ASN:HD21	1.39	0.69
1:D:551:SER:HA	1:D:554:GLU:CB	2.22	0.69
1:B:306:ILE:HD11	1:B:332:ALA:HB2	1.74	0.69
1:A:504:THR:HG22	1:A:507:GLU:H	1.58	0.69
1:A:417:VAL:HG12	1:A:425:ASN:HD22	1.57	0.68
1:A:436:HIS:CB	1:A:439:ILE:HD12	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PRO:HA	1:B:114:GLU:HB3	1.74	0.68
1:A:420:ASN:H	1:A:420:ASN:HD22	1.42	0.68
1:D:419:THR:HB	1:D:425:ASN:ND2	2.08	0.68
1:B:444:ARG:HE	1:B:446:ASN:ND2	1.92	0.67
1:A:520:ALA:HB3	1:A:546:ILE:HB	1.77	0.67
1:A:143:ARG:HH11	1:A:172:GLN:HG2	1.55	0.66
1:D:550:THR:HG22	1:D:552:GLU:H	1.61	0.66
1:A:319:ARG:HG3	1:A:320:GLU:HG3	1.78	0.65
1:D:290:LYS:HB3	1:D:294:GLU:HG3	1.78	0.65
1:D:419:THR:HB	1:D:425:ASN:HD21	1.61	0.65
1:B:523:ALA:HB3	1:B:527:ALA:HB3	1.77	0.65
1:D:306:ILE:HD11	1:D:332:ALA:HB2	1.79	0.65
1:D:529:ILE:HD12	1:D:529:ILE:H	1.60	0.65
1:B:299:GLN:N	1:B:299:GLN:HE21	1.94	0.64
1:B:419:THR:CG2	1:B:421:ASP:H	2.11	0.64
1:D:162:ASN:HD22	1:D:165:GLN:H	1.44	0.64
1:C:419:THR:CB	1:C:425:ASN:HD21	2.07	0.64
1:B:360:GLY:HA3	3:B:602:AMP:O5'	1.98	0.64
1:D:268:ILE:HD12	1:D:277:ILE:HG22	1.80	0.64
1:D:110:ALA:HB1	1:D:113:ILE:HD13	1.78	0.63
1:C:444:ARG:HH21	1:C:446:ASN:ND2	1.96	0.63
1:C:262:CYS:HA	1:C:284:GLY:HA3	1.79	0.63
1:C:211:LEU:O	1:C:215:VAL:HG12	2.00	0.62
1:D:444:ARG:HE	1:D:465:ASN:ND2	1.95	0.62
1:B:354:ILE:O	1:B:377:PHE:HA	1.99	0.62
1:C:270:ASP:HA	1:C:276:GLN:HG2	1.81	0.62
1:A:301:THR:HG21	1:A:303:LEU:CG	2.26	0.62
1:A:134:LEU:HD12	1:A:199:ILE:HG12	1.82	0.62
1:A:296:GLY:O	1:A:300:ARG:HD3	2.00	0.61
1:D:489:MET:HB3	1:D:549:GLY:O	1.99	0.61
1:B:356:ILE:HB	1:B:379:LEU:HD23	1.82	0.60
1:B:418:THR:HG22	1:B:444:ARG:HH11	1.65	0.60
1:B:134:LEU:HD21	1:B:199:ILE:HG12	1.82	0.60
1:A:318:GLN:HB2	1:A:321:THR:HG23	1.83	0.60
1:A:306:ILE:O	1:A:531:ILE:HD11	2.00	0.60
1:B:326:GLN:N	1:B:326:GLN:HE21	1.99	0.60
1:D:132:HIS:CD2	1:D:132:HIS:H	2.20	0.59
1:B:299:GLN:H	1:B:299:GLN:NE2	2.01	0.59
1:A:268:ILE:HD12	1:A:277:ILE:HG22	1.84	0.59
1:C:274:ASN:HD22	1:C:275:LEU:H	1.51	0.59
1:D:418:THR:HG22	1:D:444:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG21	1:A:303:LEU:CD1	2.33	0.58
1:A:262:CYS:HA	1:A:284:GLY:HA3	1.85	0.58
1:B:152:ARG:H	1:B:152:ARG:HD2	1.68	0.58
1:A:420:ASN:HB3	3:A:602:AMP:H5'1	1.85	0.58
1:C:243:GLN:HA	1:C:243:GLN:HE21	1.69	0.58
1:D:369:PHE:HA	1:D:372:ARG:HH11	1.69	0.57
1:B:138:ILE:HD11	1:B:143:ARG:HG3	1.86	0.57
1:B:309:TRP:HB2	1:B:328:LEU:HB3	1.84	0.57
1:A:267:HIS:HE1	1:A:276:GLN:NE2	2.03	0.57
1:D:205:ASP:HB2	1:D:206:PRO:HD3	1.87	0.57
1:D:496:LEU:HD11	1:D:539:LEU:HB3	1.86	0.56
1:A:243:GLN:HA	1:A:243:GLN:NE2	2.20	0.56
1:C:162:ASN:ND2	1:C:165:GLN:H	2.03	0.56
1:B:258:ARG:O	1:B:440:ARG:NH1	2.38	0.56
1:B:139:ASP:HB2	1:B:140:PRO:CD	2.36	0.56
1:D:489:MET:HB2	1:D:548:ILE:HG22	1.87	0.56
1:D:139:ASP:HB2	1:D:140:PRO:HD2	1.88	0.56
1:A:419:THR:H	1:A:425:ASN:HD21	1.54	0.56
1:B:397:ASP:OD1	1:B:399:THR:HB	2.06	0.56
1:B:444:ARG:NE	1:B:446:ASN:HD21	1.97	0.56
1:A:373:LYS:O	1:A:375:VAL:N	2.39	0.55
1:B:152:ARG:HH12	1:B:478:GLU:HG3	1.71	0.55
1:D:200:ILE:HD11	1:D:477:LEU:HD11	1.87	0.55
1:A:257:ILE:HG23	1:A:281:PRO:HG3	1.88	0.55
1:A:550:THR:HG22	1:A:552:GLU:H	1.72	0.55
1:B:355:PHE:CE2	1:B:380:ILE:HD11	2.41	0.54
1:D:491:VAL:HG13	1:D:548:ILE:HG12	1.90	0.54
1:C:444:ARG:NH2	1:C:446:ASN:HD21	2.03	0.54
1:A:265:LEU:HD23	1:A:280:LEU:HB2	1.89	0.54
1:D:397:ASP:OD1	3:D:602:AMP:N6	2.41	0.53
1:C:408:GLY:O	1:C:411:ARG:HG3	2.07	0.53
1:A:529:ILE:HD12	1:A:529:ILE:H	1.72	0.53
1:D:476:LEU:O	1:D:480:LYS:HB2	2.07	0.53
1:A:224:ILE:HD12	1:A:477:LEU:HD23	1.89	0.53
1:C:355:PHE:HD2	1:C:380:ILE:HD11	1.74	0.53
1:A:526:ARG:HH11	1:A:526:ARG:HA	1.74	0.53
1:A:444:ARG:HH21	1:A:446:ASN:HD22	1.57	0.53
1:A:444:ARG:NH2	1:A:446:ASN:HD22	2.07	0.53
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.91	0.53
1:B:224:ILE:HG23	1:B:243:GLN:HB3	1.90	0.53
1:C:136:PHE:HB3	1:C:203:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:GLN:O	1:D:557:PHE:HB2	2.08	0.52
1:C:224:ILE:HG23	1:C:243:GLN:HB3	1.90	0.52
1:B:505:ILE:HD12	1:B:537:THR:HB	1.90	0.52
1:A:493:ARG:O	1:A:494:ARG:HD2	2.10	0.52
1:B:326:GLN:H	1:B:326:GLN:HE21	1.58	0.52
1:B:349:PRO:HG2	1:B:352:GLU:HB3	1.92	0.51
1:D:301:THR:HG21	1:D:341:LEU:HB2	1.93	0.51
1:A:419:THR:N	1:A:425:ASN:HD21	2.07	0.51
1:C:162:ASN:HD22	1:C:165:GLN:H	1.59	0.51
1:B:529:ILE:H	1:B:529:ILE:HD12	1.75	0.51
1:B:449:GLU:HG3	1:C:184:ASP:OD2	2.10	0.51
1:B:496:LEU:HD11	1:B:539:LEU:HB3	1.92	0.51
1:A:205:ASP:HB2	1:A:206:PRO:HD3	1.93	0.51
1:D:152:ARG:HD3	1:D:154:HIS:CE1	2.46	0.51
1:B:515:GLY:HA3	1:B:553:GLN:NE2	2.26	0.51
1:A:359:HIS:O	1:A:359:HIS:CG	2.63	0.50
1:B:528:ASP:N	1:B:528:ASP:OD1	2.43	0.50
1:B:515:GLY:HA3	1:B:553:GLN:HE22	1.75	0.50
1:B:134:LEU:CD2	1:B:199:ILE:HG12	2.41	0.49
1:A:523:ALA:HB3	1:A:527:ALA:HB3	1.94	0.49
1:C:511:ARG:HB3	1:C:512:PRO:HD3	1.94	0.49
1:C:357:ILE:HG12	1:C:380:ILE:HD12	1.92	0.49
1:D:419:THR:HG23	3:D:602:AMP:C8	2.47	0.49
1:C:382:ARG:HG3	3:C:602:AMP:C2	2.47	0.49
1:A:229:GLU:HG3	1:A:231:VAL:HG22	1.94	0.49
1:B:216:ARG:NH1	1:B:221:THR:O	2.38	0.49
1:A:243:GLN:CA	1:A:243:GLN:HE21	2.20	0.49
1:B:211:LEU:O	1:B:215:VAL:HG13	2.12	0.49
1:D:520:ALA:HB3	1:D:546:ILE:HB	1.94	0.49
1:D:419:THR:HG22	1:D:421:ASP:N	2.12	0.49
1:D:444:ARG:NE	1:D:465:ASN:HD21	2.02	0.49
1:D:405:ARG:HA	1:D:409:ILE:HG22	1.95	0.49
1:C:419:THR:HG22	1:C:421:ASP:N	2.20	0.49
1:B:215:VAL:CG2	1:B:223:ILE:HD11	2.43	0.49
1:C:127:ASP:OD2	1:C:192:ARG:NH2	2.46	0.48
1:A:188:LEU:HA	1:A:191:LEU:HD12	1.95	0.48
1:C:341:LEU:HA	1:C:344:LEU:HD12	1.94	0.48
1:B:308:VAL:HG22	1:B:329:LEU:HD23	1.95	0.48
1:B:426:ILE:HD12	1:C:210:ASN:ND2	2.29	0.48
1:C:139:ASP:HB2	1:C:140:PRO:HD2	1.95	0.48
1:C:270:ASP:C	1:C:272:PHE:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:THR:HG22	1:A:336:SER:N	2.23	0.48
1:D:367:ALA:HB1	1:D:377:PHE:CE1	2.49	0.48
1:C:290:LYS:HB3	1:C:294:GLU:HG3	1.95	0.47
1:B:115:ARG:O	1:B:115:ARG:HG2	2.14	0.47
1:D:255:LEU:HD22	1:D:416:ILE:HG23	1.97	0.47
1:C:243:GLN:HA	1:C:243:GLN:NE2	2.28	0.47
1:A:224:ILE:HD13	1:A:476:LEU:HB3	1.97	0.47
1:A:525:ASP:C	1:A:527:ALA:H	2.18	0.47
1:D:162:ASN:ND2	1:D:165:GLN:H	2.10	0.47
1:D:303:LEU:HD23	1:D:333:GLY:HA3	1.97	0.47
1:B:445:ALA:HB3	1:B:464:SER:HA	1.97	0.47
1:C:418:THR:HG22	1:C:444:ARG:HD3	1.97	0.47
1:D:513:LEU:HD23	1:D:514:THR:HG23	1.97	0.47
1:B:215:VAL:HG21	1:B:223:ILE:HD11	1.96	0.47
1:D:134:LEU:HD13	1:D:136:PHE:CE2	2.49	0.46
1:C:529:ILE:H	1:C:529:ILE:HD12	1.80	0.46
1:C:309:TRP:CE2	1:C:314:LEU:HD13	2.50	0.46
1:D:438:HIS:CD2	1:D:439:ILE:HG13	2.50	0.46
1:A:139:ASP:HB2	1:A:140:PRO:CD	2.45	0.46
1:B:496:LEU:CD1	1:B:539:LEU:HB3	2.46	0.46
1:B:381:ASP:O	1:B:395:TYR:HA	2.15	0.46
1:B:355:PHE:HZ	1:B:380:ILE:HD11	1.69	0.46
1:D:505:ILE:HD11	1:D:521:ILE:HD11	1.98	0.46
1:A:162:ASN:ND2	1:A:165:GLN:H	2.13	0.46
1:A:138:ILE:HD12	1:A:142:THR:OG1	2.16	0.46
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.98	0.46
1:C:496:LEU:HD21	1:C:539:LEU:HD13	1.96	0.46
1:A:417:VAL:HG12	1:A:425:ASN:ND2	2.28	0.46
1:D:223:ILE:N	1:D:242:ASN:OD1	2.49	0.46
1:B:229:GLU:CG	1:B:361:ARG:HH21	2.28	0.46
1:A:489:MET:HE1	1:A:548:ILE:HG23	1.98	0.46
1:D:138:ILE:H	1:D:138:ILE:HG13	1.54	0.45
1:B:504:THR:HG22	1:B:507:GLU:H	1.81	0.45
1:D:198:SER:HB3	1:D:222:PRO:HG2	1.98	0.45
1:D:362:ILE:HG22	1:D:418:THR:HG21	1.99	0.45
1:D:285:THR:HB	1:D:286:PRO:HD2	1.98	0.45
1:A:120:HIS:CE1	1:D:115:ARG:HG2	2.50	0.45
1:A:356:ILE:HG12	1:A:416:ILE:HD12	1.98	0.45
1:A:416:ILE:HG22	1:A:418:THR:OG1	2.17	0.45
1:B:110:ALA:HB3	1:B:113:ILE:HD12	1.99	0.45
1:B:341:LEU:HD13	1:B:345:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:THR:HG22	1:C:316:THR:H	1.81	0.45
1:B:348:ALA:HB1	1:B:349:PRO:HD2	1.98	0.45
1:C:350:GLU:HG3	1:C:351:ASP:H	1.82	0.45
1:A:443:ALA:HB1	1:A:454:LEU:HD22	1.98	0.45
1:C:510:LEU:HD12	1:C:518:ILE:HD11	1.98	0.45
1:D:227:VAL:HG12	1:D:229:GLU:H	1.81	0.45
1:B:229:GLU:O	1:B:230:PRO:C	2.55	0.44
1:A:493:ARG:HA	1:A:545:LEU:O	2.17	0.44
1:A:419:THR:CG2	1:A:420:ASN:N	2.80	0.44
1:C:139:ASP:HB2	1:C:140:PRO:CD	2.47	0.44
1:A:267:HIS:CE1	1:A:276:GLN:NE2	2.84	0.44
1:C:493:ARG:HA	1:C:545:LEU:O	2.18	0.44
1:B:551:SER:O	1:B:555:LYS:HG3	2.17	0.44
1:B:307:GLY:HA2	1:B:317:PRO:HD3	1.99	0.44
1:B:362:ILE:HD12	1:B:444:ARG:CZ	2.48	0.44
1:B:276:GLN:O	1:B:332:ALA:HA	2.17	0.44
1:A:523:ALA:HB1	1:A:524:PRO:HD2	2.00	0.44
1:B:229:GLU:HA	1:B:230:PRO:HD2	1.84	0.44
1:C:443:ALA:HB1	1:C:454:LEU:HD22	1.98	0.44
1:D:514:THR:HG21	1:D:557:PHE:CD1	2.53	0.44
1:B:256:GLY:HA3	1:B:369:PHE:CD2	2.53	0.44
1:C:138:ILE:HD13	1:C:158:VAL:HG11	2.00	0.44
1:A:162:ASN:C	1:A:162:ASN:HD22	2.21	0.44
1:A:483:ALA:O	1:A:486:SER:HB2	2.18	0.44
1:C:518:ILE:HD13	1:C:545:LEU:HD22	2.00	0.43
1:A:504:THR:HG23	1:A:505:ILE:N	2.33	0.43
1:D:381:ASP:OD2	1:D:382:ARG:N	2.52	0.43
1:D:306:ILE:CD1	1:D:332:ALA:HB2	2.48	0.43
1:B:137:GLY:HA3	1:B:202:ASN:O	2.19	0.43
1:C:419:THR:HG23	3:C:602:AMP:C8	2.54	0.43
1:D:491:VAL:HG22	1:D:548:ILE:HG23	2.01	0.43
1:A:418:THR:HG22	1:A:444:ARG:HH11	1.84	0.43
1:C:379:LEU:HD12	1:C:391:HIS:HB3	2.00	0.43
1:A:471:ASN:OD1	1:A:471:ASN:C	2.57	0.43
1:C:247:LEU:HD21	1:C:469:GLY:HA2	1.99	0.43
1:C:315:THR:HG22	1:C:316:THR:N	2.34	0.43
1:B:360:GLY:HA3	3:B:602:AMP:P	2.59	0.42
1:B:258:ARG:HG2	1:B:461:PHE:CG	2.54	0.42
1:B:304:SER:OG	1:B:493:ARG:NH1	2.48	0.42
1:C:258:ARG:HG3	1:C:461:PHE:CD1	2.54	0.42
1:B:203:LEU:HB2	1:B:208:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:GLU:HA	1:C:484:PHE:HD2	1.82	0.42
1:D:248:THR:HG22	1:D:362:ILE:HG13	2.01	0.42
1:A:451:VAL:HG13	1:A:462:VAL:HG11	2.02	0.42
1:B:291:THR:HG22	1:B:322:VAL:HG22	2.01	0.42
1:A:334:THR:HG22	1:A:335:LYS:N	2.34	0.42
1:B:258:ARG:HG2	1:B:461:PHE:CD1	2.55	0.42
1:A:292:ILE:HD13	1:A:317:PRO:HB3	2.00	0.42
1:D:253:ARG:HG3	1:D:369:PHE:CE1	2.54	0.42
1:C:481:GLU:HA	1:C:484:PHE:CD2	2.53	0.42
1:D:254:TYR:HA	1:D:257:ILE:HD12	2.01	0.42
1:D:355:PHE:HD2	1:D:380:ILE:HD11	1.83	0.42
1:D:510:LEU:HD13	1:D:518:ILE:HD11	2.02	0.42
1:B:357:ILE:HG21	1:B:428:LEU:HD13	2.01	0.42
1:C:134:LEU:HD13	1:C:136:PHE:CE2	2.55	0.42
1:D:511:ARG:N	1:D:512:PRO:HD2	2.35	0.42
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.92	0.42
1:A:143:ARG:HH21	1:A:147:ARG:HH21	1.68	0.42
1:B:204:SER:HA	1:B:228:LYS:HE2	2.00	0.42
1:A:481:GLU:HG3	1:A:481:GLU:H	1.59	0.42
1:C:285:THR:C	1:C:287:PHE:H	2.23	0.42
1:D:355:PHE:CD2	1:D:380:ILE:HD11	2.54	0.41
1:A:511:ARG:HB3	1:A:512:PRO:HD3	2.02	0.41
1:A:265:LEU:HD21	1:A:341:LEU:CD1	2.50	0.41
1:B:529:ILE:N	1:B:529:ILE:HD12	2.35	0.41
1:D:352:GLU:O	1:D:376:PRO:HG2	2.19	0.41
1:D:550:THR:HB	1:D:552:GLU:HB2	2.02	0.41
1:D:276:GLN:HB2	1:D:338:LEU:HD11	2.02	0.41
1:D:373:LYS:O	1:D:375:VAL:N	2.54	0.41
1:A:298:ARG:HD3	1:A:526:ARG:HH22	1.86	0.41
1:D:287:PHE:HD2	1:D:295:SER:HB2	1.85	0.41
1:A:318:GLN:HE21	1:A:318:GLN:HB2	1.56	0.41
1:A:448:GLU:O	1:A:451:VAL:HG23	2.21	0.41
1:D:497:PRO:HA	1:D:498:PRO:HD2	1.83	0.41
1:B:434:HIS:HD2	1:B:435:LEU:HD13	1.85	0.41
1:D:433:ARG:HD2	1:D:458:GLY:O	2.21	0.41
1:A:405:ARG:HE	1:A:405:ARG:HB2	1.57	0.41
1:D:282:VAL:O	1:D:282:VAL:HG12	2.21	0.41
1:B:347:GLU:OE1	1:B:347:GLU:N	2.45	0.41
1:B:152:ARG:NH1	1:B:478:GLU:HG3	2.36	0.41
1:C:518:ILE:HG23	1:C:547:LEU:HG	2.01	0.41
1:C:272:PHE:C	1:C:274:ASN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD21	1:B:199:ILE:CG1	2.49	0.41
1:A:200:ILE:HD11	1:A:477:LEU:HD11	2.03	0.41
1:A:476:LEU:HA	1:A:476:LEU:HD12	1.90	0.41
1:B:434:HIS:HD2	1:B:435:LEU:CD1	2.34	0.41
1:D:554:GLU:HA	1:D:557:PHE:HB2	2.01	0.41
1:B:505:ILE:HB	1:B:535:PRO:O	2.21	0.41
1:C:301:THR:HG21	1:C:341:LEU:HD12	2.03	0.41
1:D:227:VAL:HG21	1:D:244:VAL:HG13	2.03	0.41
1:D:341:LEU:O	1:D:345:ILE:HG12	2.22	0.40
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.89	0.40
1:A:500:MET:SD	1:A:508:THR:HG23	2.62	0.40
1:D:316:THR:HA	1:D:317:PRO:HD3	1.88	0.40
1:C:297:ILE:HB	1:C:305:ILE:HD11	2.03	0.40
1:A:181:SER:HA	1:A:182:PRO:HD2	1.89	0.40
1:D:138:ILE:HD11	1:D:165:GLN:NE2	2.36	0.40
1:B:139:ASP:HB2	1:B:140:PRO:HD3	2.03	0.40
1:A:120:HIS:HE1	1:D:115:ARG:O	2.05	0.40
1:C:348:ALA:HA	1:C:349:PRO:HD3	1.94	0.40
1:D:268:ILE:HD11	1:D:279:GLU:HG3	2.03	0.40
1:A:356:ILE:HB	1:A:379:LEU:HD23	2.03	0.40
1:D:381:ASP:O	1:D:395:TYR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/462 (98%)	413 (91%)	36 (8%)	4 (1%)	21	64
1	B	453/462 (98%)	414 (91%)	35 (8%)	4 (1%)	21	64
1	C	453/462 (98%)	408 (90%)	44 (10%)	1 (0%)	52	88
1	D	453/462 (98%)	417 (92%)	33 (7%)	3 (1%)	26	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1812/1848 (98%)	1652 (91%)	148 (8%)	12 (1%)	26 70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	GLY
1	A	467	SER
1	B	374	PRO
1	D	350	GLU
1	A	449	GLU
1	B	230	PRO
1	C	541	GLU
1	D	524	PRO
1	A	374	PRO
1	D	541	GLU
1	A	468	VAL
1	B	373	LYS

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	370/378 (98%)	322 (87%)	48 (13%)	5 22
1	B	370/378 (98%)	322 (87%)	48 (13%)	5 22
1	C	370/378 (98%)	338 (91%)	32 (9%)	13 44
1	D	370/378 (98%)	333 (90%)	37 (10%)	9 34
All	All	1480/1512 (98%)	1315 (89%)	165 (11%)	8 29

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	130	ARG
1	A	134	LEU

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Mol	Chain	Res	Type
1	A	141	ILE
1	A	143	ARG
1	A	145	LEU
1	A	158	VAL
1	A	162	ASN
1	A	164	ASP
1	A	167	LEU
1	A	171	GLU
1	A	176	LYS
1	A	177	VAL
1	A	217	SER
1	A	220	GLN
1	A	228	LYS
1	A	236	LEU
1	A	243	GLN
1	A	262	CYS
1	A	274	ASN
1	A	315	THR
1	A	318	GLN
1	A	320	GLU
1	A	336	SER
1	A	341	LEU
1	A	353	LEU
1	A	371	ASP
1	A	373	LYS
1	A	392	VAL
1	A	405	ARG
1	A	411	ARG
1	A	418	THR
1	A	420	ASN
1	A	435	LEU
1	A	446	ASN
1	A	476	LEU
1	A	481	GLU
1	A	484	PHE
1	A	487	GLU
1	A	496	LEU
1	A	504	THR
1	A	525	ASP
1	A	526	ARG
1	A	530	LEU
1	A	532	SER

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Mol	Chain	Res	Type
1	A	548	ILE
1	A	551	SER
1	A	556	THR
1	B	115	ARG
1	B	127	ASP
1	B	134	LEU
1	B	149	LEU
1	B	150	GLU
1	B	152	ARG
1	B	153	ASN
1	B	158	VAL
1	B	173	GLU
1	B	177	VAL
1	B	215	VAL
1	B	216	ARG
1	B	231	VAL
1	B	235	LEU
1	B	242	ASN
1	B	243	GLN
1	B	298	ARG
1	B	299	GLN
1	B	301	THR
1	B	315	THR
1	B	318	GLN
1	B	323	LEU
1	B	324	THR
1	B	326	GLN
1	B	331	LEU
1	B	341	LEU
1	B	353	LEU
1	B	373	LYS
1	B	380	ILE
1	B	399	THR
1	B	410	ASP
1	B	418	THR
1	B	419	THR
1	B	420	ASN
1	B	435	LEU
1	B	476	LEU
1	B	482	SER
1	B	485	LEU
1	B	494	ARG

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Mol	Chain	Res	Type
1	B	504	THR
1	B	519	VAL
1	B	525	ASP
1	B	528	ASP
1	B	530	LEU
1	B	545	LEU
1	B	550	THR
1	B	556	THR
1	B	559	GLN
1	C	127	ASP
1	C	134	LEU
1	C	143	ARG
1	C	145	LEU
1	C	150	GLU
1	C	162	ASN
1	C	172	GLN
1	C	173	GLU
1	C	192	ARG
1	C	212	CYS
1	C	228	LYS
1	C	243	GLN
1	C	247	LEU
1	C	261	THR
1	C	274	ASN
1	C	275	LEU
1	C	277	ILE
1	C	334	THR
1	C	341	LEU
1	C	380	ILE
1	C	389	ASN
1	C	399	THR
1	C	403	THR
1	C	411	ARG
1	C	418	THR
1	C	435	LEU
1	C	481	GLU
1	C	496	LEU
1	C	518	ILE
1	C	531	ILE
1	C	548	ILE
1	C	556	THR
1	D	114	GLU

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Mol	Chain	Res	Type
1	D	122	THR
1	D	123	ILE
1	D	128	ASP
1	D	139	ASP
1	D	142	THR
1	D	145	LEU
1	D	162	ASN
1	D	172	GLN
1	D	176	LYS
1	D	215	VAL
1	D	220	GLN
1	D	228	LYS
1	D	231	VAL
1	D	236	LEU
1	D	244	VAL
1	D	274	ASN
1	D	276	GLN
1	D	299	GLN
1	D	301	THR
1	D	313	SER
1	D	315	THR
1	D	326	GLN
1	D	334	THR
1	D	341	LEU
1	D	418	THR
1	D	440	ARG
1	D	471	ASN
1	D	485	LEU
1	D	494	ARG
1	D	503	LYS
1	D	504	THR
1	D	528	ASP
1	D	529	ILE
1	D	530	LEU
1	D	536	GLU
1	D	550	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	132	HIS

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Mol	Chain	Res	Type
1	A	162	ASN
1	A	243	GLN
1	A	267	HIS
1	A	276	GLN
1	A	318	GLN
1	A	420	ASN
1	A	425	ASN
1	B	153	ASN
1	B	243	GLN
1	B	276	GLN
1	B	299	GLN
1	B	318	GLN
1	B	326	GLN
1	B	420	ASN
1	B	446	ASN
1	B	559	GLN
1	C	162	ASN
1	C	243	GLN
1	C	274	ASN
1	C	389	ASN
1	C	425	ASN
1	C	446	ASN
1	D	132	HIS
1	D	154	HIS
1	D	162	ASN
1	D	243	GLN
1	D	274	ASN
1	D	318	GLN
1	D	389	ASN
1	D	402	GLN
1	D	425	ASN
1	D	438	HIS
1	D	446	ASN
1	D	465	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	AMP	A	602	-	20,25,25	1.17	2 (10%)	22,38,38	2.02	4 (18%)
3	AMP	B	602	-	20,25,25	1.03	1 (5%)	22,38,38	2.16	7 (31%)
3	AMP	C	602	-	20,25,25	1.11	1 (5%)	22,38,38	2.02	3 (13%)
3	AMP	D	602	-	20,25,25	1.12	2 (10%)	22,38,38	1.86	3 (13%)

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	AMP	A	602	-	-	0/6/26/26	0/3/3/3
3	AMP	B	602	-	-	0/6/26/26	0/3/3/3
3	AMP	C	602	-	-	0/6/26/26	0/3/3/3
3	AMP	D	602	-	-	0/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	AMP	C2-N3	2.08	1.35	1.32
3	A	602	AMP	O4'-C1'	2.38	1.44	1.41
3	B	602	AMP	C5-C4	3.07	1.47	1.40
3	D	602	AMP	C5-C4	3.34	1.48	1.40
3	C	602	AMP	C5-C4	3.40	1.48	1.40
3	A	602	AMP	C5-C4	3.48	1.48	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	AMP	N3-C2-N1	-7.28	123.32	128.89
3	A	602	AMP	N3-C2-N1	-6.74	123.73	128.89
3	B	602	AMP	N3-C2-N1	-6.66	123.79	128.89
3	D	602	AMP	N3-C2-N1	-6.65	123.80	128.89
3	A	602	AMP	C4-C5-N7	-3.64	106.13	109.48
3	B	602	AMP	C4-C5-N7	-3.58	106.19	109.48
3	D	602	AMP	C4-C5-N7	-3.44	106.31	109.48
3	C	602	AMP	C4-C5-N7	-3.30	106.44	109.48
3	B	602	AMP	C4'-O4'-C1'	-3.14	106.27	109.72
3	B	602	AMP	C1'-N9-C4	-2.82	122.69	126.94
3	B	602	AMP	O2P-P-O5'	-2.05	100.67	106.56
3	D	602	AMP	O4'-C1'-N9	2.05	112.39	108.10
3	B	602	AMP	O2P-P-O1P	2.16	117.52	110.58
3	C	602	AMP	O3P-P-O2P	2.16	115.61	107.38
3	B	602	AMP	O3P-P-O2P	2.18	115.68	107.38
3	A	602	AMP	O3P-P-O2P	2.51	116.94	107.38
3	A	602	AMP	O4'-C1'-N9	2.85	114.07	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	AMP	1	0
3	B	602	AMP	2	0
3	C	602	AMP	2	0
3	D	602	AMP	2	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^{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	455/462 (98%)	-0.31	2 (0%) 93 80	66, 95, 148, 228	0
1	B	455/462 (98%)	-0.26	0 100 100	67, 96, 135, 169	0
1	C	455/462 (98%)	0.47	61 (13%) 4 1	95, 135, 277, 306	0
1	D	455/462 (98%)	0.07	20 (4%) 38 16	81, 129, 196, 271	0
All	All	1820/1848 (98%)	-0.01	83 (4%) 36 14	66, 113, 226, 306	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	513	LEU	9.1
1	C	497	PRO	8.7
1	D	486	SER	7.4
1	C	563	ALA	6.7
1	D	482	SER	6.5
1	C	498	PRO	6.3
1	C	533	PRO	6.1
1	C	499	ALA	6.0
1	C	516	CYS	5.9
1	C	540	ALA	5.7
1	C	564	ARG	5.6
1	C	545	LEU	5.3
1	C	528	ASP	5.3
1	C	495	PRO	5.3
1	C	526	ARG	5.3
1	D	484	PHE	5.0
1	C	537	THR	4.9
1	C	559	GLN	4.9
1	C	517	SER	4.8
1	C	542	GLY	4.7
1	C	543	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	525	ASP	4.5
1	C	496	LEU	4.3
1	D	485	LEU	4.3
1	D	289	GLY	4.3
1	D	323	LEU	4.3
1	C	507	GLU	4.2
1	C	518	ILE	4.2
1	C	505	ILE	4.1
1	D	508	THR	4.0
1	C	315	THR	3.9
1	C	541	GLU	3.8
1	C	500	MET	3.8
1	C	508	THR	3.7
1	D	483	ALA	3.7
1	C	557	PHE	3.6
1	C	485	LEU	3.6
1	C	514	THR	3.5
1	C	539	LEU	3.5
1	C	509	ARG	3.4
1	C	555	LYS	3.3
1	D	287	PHE	3.3
1	C	549	GLY	3.3
1	C	538	ILE	3.3
1	C	554	GLU	3.2
1	C	512	PRO	3.2
1	C	534	PRO	3.2
1	D	524	PRO	3.1
1	C	510	LEU	3.0
1	D	290	LYS	3.0
1	D	563	ALA	3.0
1	C	503	LYS	3.0
1	C	527	ALA	2.9
1	C	560	THR	2.9
1	C	536	GLU	2.9
1	C	524	PRO	2.9
1	A	563	ALA	2.8
1	D	507	GLU	2.8
1	C	515	GLY	2.8
1	D	504	THR	2.8
1	D	320	GLU	2.8
1	D	288	ALA	2.8
1	C	556	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	561	ILE	2.7
1	C	558	ASP	2.6
1	D	322	VAL	2.6
1	C	492	PHE	2.6
1	C	544	ARG	2.5
1	D	487	GLU	2.4
1	C	551	SER	2.4
1	C	342	GLU	2.4
1	A	484	PHE	2.4
1	C	494	ARG	2.4
1	C	502	GLY	2.4
1	C	305	ILE	2.4
1	C	338	LEU	2.3
1	D	503	LYS	2.3
1	C	322	VAL	2.3
1	C	520	ALA	2.3
1	C	343	TYR	2.2
1	C	562	ALA	2.1
1	C	521	ILE	2.1
1	D	513	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^{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
3	AMP	C	602	23/23	0.80	0.38	2.23	164,170,172,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AMP	D	602	23/23	0.86	0.25	0.98	123,126,131,134	0
3	AMP	A	602	23/23	0.86	0.22	0.58	103,105,112,113	0
3	AMP	B	602	23/23	0.95	0.15	-0.92	81,83,85,87	0
4	CA	B	603	1/1	0.97	0.11	-2.23	106,106,106,106	0
4	CA	A	603	1/1	0.98	0.09	-4.02	87,87,87,87	0
4	CA	A	604	1/1	0.97	0.08	-4.88	101,101,101,101	0
4	CA	C	603	1/1	0.97	0.07	-5.94	121,121,121,121	0
2	ZN	D	601	1/1	0.99	0.10	-	103,103,103,103	0
2	ZN	B	601	1/1	0.99	0.18	-	76,76,76,76	0
2	ZN	C	601	1/1	0.99	0.14	-	112,112,112,112	0
2	ZN	A	601	1/1	1.00	0.11	-	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.