Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:30 AM GMT

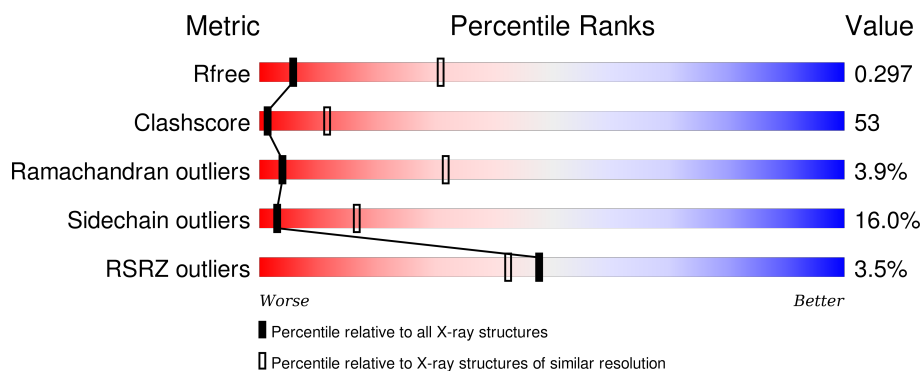|		
PDB ID	:	2DCU
Title	:	Crystal structure of translation initiation factor aIF2betagamma heterodimer with GDP
Authors	:	Sokabe, M.; Yao, M.; Sakai, N.; Toya, S.; Tanaka, I.
Deposited on	:	2006-01-16
Resolution	:	3.40 Å(reported)

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1 Overall quality at a glance ⓘ

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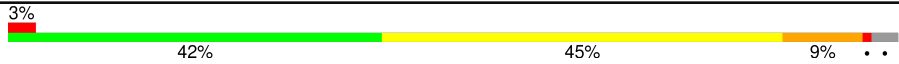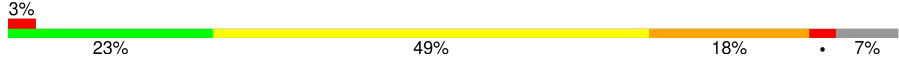*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.297
Clashscore		53
Ramachandran outliers		3.9%
Sidechain outliers		16.0%
RSRZ outliers		3.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	419	3% / 42% / 45% / 9% · ·
2	B	148	3% / 23% / 49% / 18% · 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4389 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 Translation initiation factor 2 gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3132	1987	550	581	14	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ASP	GLY	ENGINEERED	UNP Q8U082
A	412	LEU	-	EXPRESSION TAG	UNP Q8U082
A	413	GLU	-	EXPRESSION TAG	UNP Q8U082
A	414	HIS	-	EXPRESSION TAG	UNP Q8U082
A	415	HIS	-	EXPRESSION TAG	UNP Q8U082
A	416	HIS	-	EXPRESSION TAG	UNP Q8U082
A	417	HIS	-	EXPRESSION TAG	UNP Q8U082
A	418	HIS	-	EXPRESSION TAG	UNP Q8U082
A	419	HIS	-	EXPRESSION TAG	UNP Q8U082

- Molecule 2 is a protein called Translation initiation factor 2 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	137	1118	720	194	200	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	141	LEU	-	EXPRESSION TAG	UNP Q8U3I5
B	142	GLU	-	EXPRESSION TAG	UNP Q8U3I5
B	143	HIS	-	EXPRESSION TAG	UNP Q8U3I5
B	144	HIS	-	EXPRESSION TAG	UNP Q8U3I5
B	145	HIS	-	EXPRESSION TAG	UNP Q8U3I5
B	146	HIS	-	EXPRESSION TAG	UNP Q8U3I5
B	147	HIS	-	EXPRESSION TAG	UNP Q8U3I5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	148	HIS	-	EXPRESSION TAG	UNP Q8U3I5

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	28	10	5	11	2	0	0

- Molecule 6 is water.
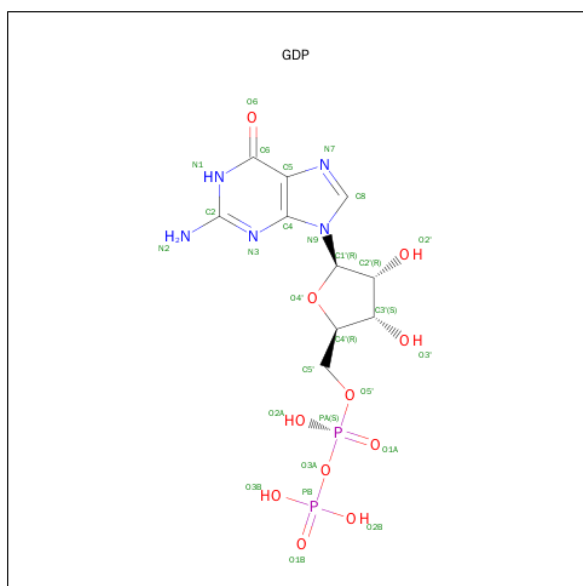
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total 85	O 85	0	0
6	B	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Translation initiation factor 2 gamma subunit
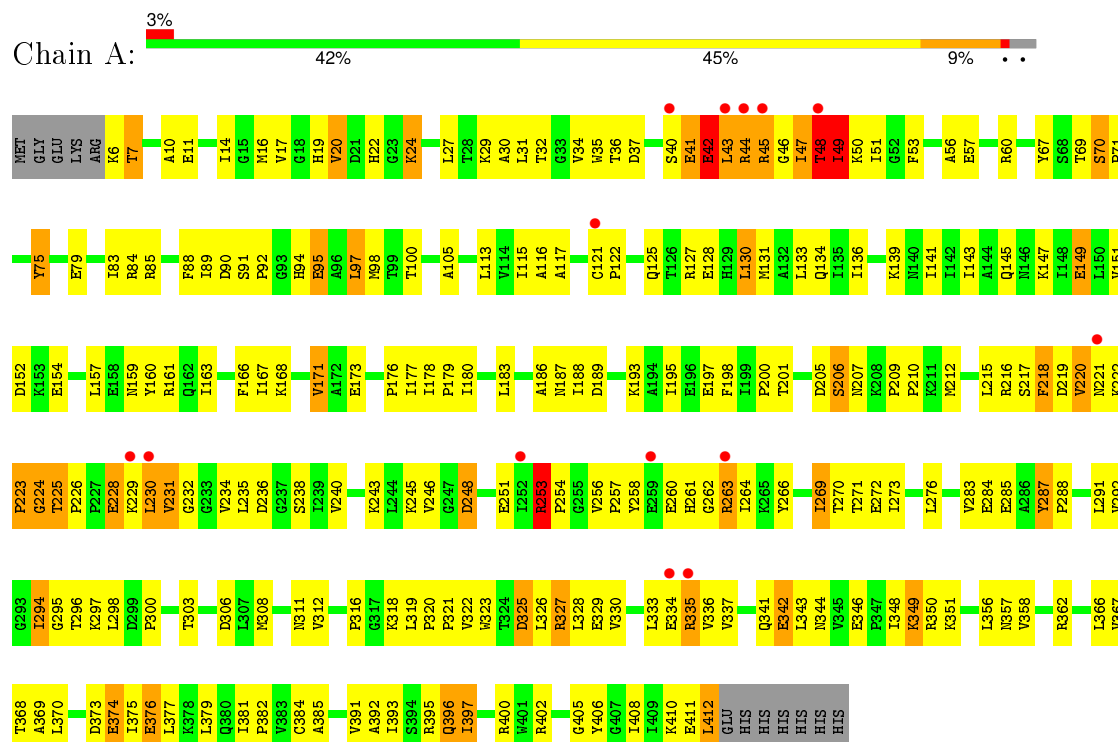
- Molecule 2: Translation initiation factor 2 beta subunit
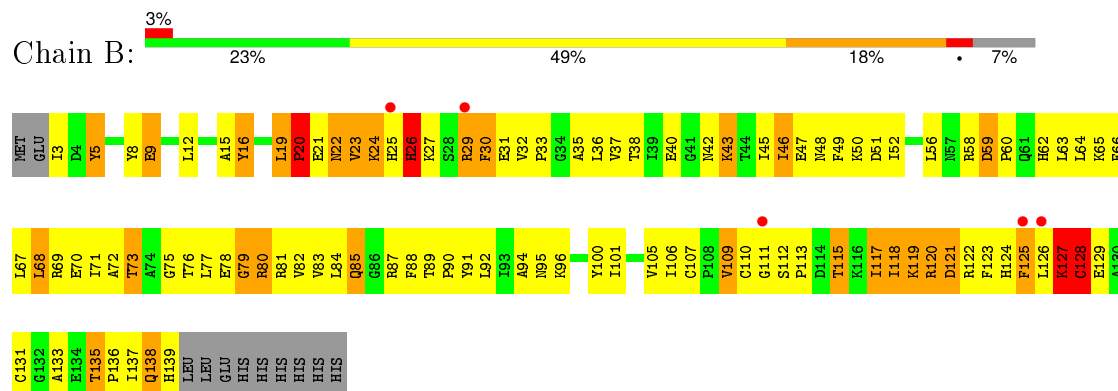
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.20Å 76.56Å 97.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 45.46 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.40) 97.0 (45.46-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	1.45 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.298 0.239 , 0.297	Depositor DCC
R_{free} test set	560 reflections (7.55%)	DCC
Wilson B-factor (Å^2)	76.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.42$, $<L^2> = 0.25$	Xtriage
Outliers	0 of 8006 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4389	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ZN, MG

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	0.33	0/3187	0.75	8/4315 (0.2%)
2	B	0.33	0/1142	0.79	5/1540 (0.3%)
All	All	0.33	0/4329	0.76	13/5855 (0.2%)

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
2	B	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	GLY	N-CA-C	11.15	140.97	113.10
2	B	29	ARG	N-CA-C	-8.80	87.24	111.00
1	A	42	GLU	N-CA-C	8.54	134.05	111.00
1	A	261	HIS	N-CA-C	-7.15	91.70	111.00
1	A	262	GLY	N-CA-C	-6.92	95.79	113.10
1	A	41	GLU	N-CA-C	-6.87	92.45	111.00
1	A	49	ILE	N-CA-C	-6.77	92.72	111.00
2	B	127	LYS	N-CA-C	6.56	128.72	111.00
1	A	224	GLY	N-CA-C	-6.14	97.75	113.10
2	B	125	PHE	N-CA-C	-5.64	95.78	111.00
2	B	138	GLN	N-CA-C	-5.29	96.70	111.00
1	A	48	THR	CA-CB-CG2	-5.03	105.36	112.40
2	B	128	CYS	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	TYR	Sidechain

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	3132	0	3245	289	0
2	B	1118	0	1138	196	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	12	3	0
6	A	85	0	0	9	0
6	B	23	0	0	9	0
All	All	4389	0	4395	461	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 53.

All (461) 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:48:THR:HG21	1:A:362:ARG:CD	1.56	1.32
1:A:44:ARG:HD2	1:A:44:ARG:O	1.37	1.19
1:A:42:GLU:O	1:A:43:LEU:HD23	1.41	1.19
2:B:15:ALA:O	2:B:19:LEU:HD23	1.49	1.13
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.05	1.12
1:A:29:LYS:HG2	1:A:43:LEU:HG	1.19	1.11
1:A:253:ARG:HG3	1:A:384:CYS:HB2	1.23	1.10
1:A:48:THR:HG21	1:A:362:ARG:HD2	1.09	1.08
2:B:22:ASN:HB2	2:B:29:ARG:O	1.55	1.06
1:A:44:ARG:HD2	1:A:44:ARG:C	1.77	1.03
1:A:350:ARG:HG3	1:A:370:LEU:HD13	1.40	1.03
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:CG2	1:A:362:ARG:HD2	1.93	0.98
1:A:357:ASN:HB2	1:A:392:ALA:HB3	1.49	0.94
1:A:42:GLU:O	1:A:43:LEU:CD2	2.14	0.94
1:A:303:THR:HG22	1:A:308:MET:HG3	1.47	0.93
2:B:110:CYS:SG	2:B:131:CYS:HB3	2.08	0.93
1:A:226:PRO:O	1:A:230:LEU:HG	1.70	0.92
2:B:15:ALA:O	2:B:19:LEU:CD2	2.17	0.92
1:A:253:ARG:HB3	1:A:254:PRO:HD3	1.52	0.92
1:A:121:CYS:HB3	1:A:122:PRO:HD3	1.50	0.92
1:A:257:PRO:HG3	1:A:266:TYR:CE1	2.07	0.89
1:A:48:THR:HG21	1:A:362:ARG:HD3	1.52	0.89
1:A:139:LYS:HG2	1:A:171:VAL:HG12	1.53	0.88
1:A:45:ARG:NH1	1:A:45:ARG:HG3	1.83	0.88
1:A:369:ALA:HB3	1:A:376:GLU:HB2	1.56	0.87
2:B:20:PRO:O	2:B:24:LYS:HB2	1.74	0.87
1:A:333:LEU:HG	1:A:405:GLY:HA2	1.56	0.87
1:A:253:ARG:CG	1:A:384:CYS:HB2	2.05	0.86
2:B:22:ASN:HB3	2:B:29:ARG:NH1	1.90	0.86
2:B:50:LYS:HG3	2:B:51:ASP:N	1.89	0.86
2:B:22:ASN:ND2	2:B:23:VAL:HG12	1.92	0.85
2:B:20:PRO:HB2	2:B:23:VAL:HG13	1.56	0.84
2:B:50:LYS:HD2	2:B:80:ARG:NE	1.93	0.84
1:A:37:ASP:HA	2:B:87:ARG:HH22	1.41	0.83
2:B:118:ILE:HG22	2:B:126:LEU:HA	1.59	0.83
2:B:95:ASN:ND2	2:B:96:LYS:HE3	1.94	0.82
2:B:118:ILE:HG12	2:B:119:LYS:H	1.43	0.82
1:A:187:ASN:ND2	2:B:15:ALA:HB2	1.93	0.82
1:A:37:ASP:HA	2:B:87:ARG:NH2	1.94	0.82
2:B:118:ILE:HG23	2:B:125:PHE:O	1.80	0.82
2:B:29:ARG:HB3	2:B:29:ARG:NH1	1.96	0.81
1:A:219:ASP:OD1	1:A:221:ASN:HB2	1.81	0.81
1:A:45:ARG:HB3	1:A:92:PRO:HD2	1.63	0.81
1:A:222:LYS:O	1:A:224:GLY:N	2.14	0.79
1:A:253:ARG:HH21	1:A:322:VAL:N	1.80	0.79
1:A:400:ARG:NH1	1:A:400:ARG:HA	1.99	0.78
2:B:126:LEU:HD22	2:B:137:ILE:HD11	1.65	0.78
2:B:36:LEU:HD22	2:B:47:GLU:HG3	1.66	0.78
1:A:29:LYS:CG	1:A:43:LEU:HG	2.10	0.77
1:A:84:ARG:HH12	1:A:200:PRO:HA	1.49	0.77
1:A:327:ARG:HG2	1:A:410:LYS:HB2	1.65	0.77
2:B:118:ILE:HG12	2:B:119:LYS:N	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HG2	1:A:384:CYS:SG	2.26	0.75
1:A:253:ARG:HB3	1:A:254:PRO:CD	2.17	0.75
1:A:294:ILE:HD11	1:A:296:THR:HG22	1.68	0.75
1:A:31:LEU:HA	1:A:69:THR:HG21	1.68	0.75
2:B:29:ARG:HH21	2:B:105:VAL:HG12	1.51	0.75
1:A:45:ARG:HG2	1:A:92:PRO:HG2	1.69	0.75
1:A:273:ILE:HG12	1:A:294:ILE:HD13	1.69	0.75
2:B:46:ILE:HD11	2:B:49:PHE:CD1	2.22	0.74
2:B:117:ILE:HA	2:B:126:LEU:HB3	1.69	0.74
1:A:253:ARG:HG3	1:A:384:CYS:CB	2.11	0.74
1:A:37:ASP:CA	2:B:87:ARG:HH22	1.99	0.74
1:A:272:GLU:HB3	1:A:297:LYS:HD2	1.70	0.74
1:A:95:GLU:OE2	1:A:402:ARG:HA	1.87	0.73
2:B:46:ILE:O	2:B:46:ILE:HG12	1.88	0.73
2:B:95:ASN:HD22	2:B:96:LYS:HE3	1.51	0.73
1:A:36:THR:CG2	1:A:40:SER:O	2.36	0.73
2:B:20:PRO:O	2:B:24:LYS:CB	2.36	0.73
1:A:350:ARG:O	1:A:351:LYS:HB2	1.90	0.72
1:A:329:GLU:HB3	1:A:408:ILE:HB	1.71	0.72
1:A:60:ARG:HB2	1:A:83:ILE:HD11	1.72	0.72
1:A:34:VAL:HG23	2:B:87:ARG:HB3	1.72	0.71
1:A:49:ILE:HD11	1:A:100:THR:HA	1.71	0.71
1:A:49:ILE:C	1:A:51:ILE:H	1.90	0.71
1:A:186:ALA:O	1:A:187:ASN:HB2	1.89	0.71
1:A:149:GLU:HB3	2:B:19:LEU:CD1	2.20	0.71
1:A:44:ARG:NH2	6:A:3044:HOH:O	2.22	0.71
1:A:224:GLY:O	1:A:226:PRO:HD3	1.90	0.71
2:B:12:LEU:HG	2:B:16:TYR:CE2	2.26	0.70
1:A:139:LYS:HG2	1:A:171:VAL:CG1	2.21	0.69
1:A:49:ILE:HG23	1:A:51:ILE:HB	1.74	0.69
1:A:269:ILE:HD11	1:A:298:LEU:HD21	1.74	0.69
1:A:263:ARG:NH1	1:A:263:ARG:HG2	2.04	0.69
1:A:226:PRO:HB2	1:A:230:LEU:HD21	1.75	0.69
1:A:36:THR:H	2:B:87:ARG:HH12	1.40	0.69
1:A:349:LYS:HB2	1:A:349:LYS:NZ	2.06	0.68
1:A:326:LEU:HD22	1:A:379:LEU:HD11	1.75	0.68
2:B:58:ARG:NH2	2:B:115:THR:OG1	2.26	0.68
1:A:35:TRP:CD1	1:A:56:ALA:HA	2.29	0.68
1:A:128:GLU:OE1	1:A:335:ARG:NH1	2.26	0.68
1:A:44:ARG:NE	6:A:3044:HOH:O	2.09	0.68
1:A:122:PRO:HB2	1:A:127:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:HG2	2:B:40:GLU:OE2	1.94	0.68
1:A:342:GLU:HG3	1:A:397:ILE:HG21	1.77	0.67
1:A:276:LEU:HD23	1:A:294:ILE:HA	1.76	0.67
1:A:36:THR:HG22	1:A:40:SER:O	1.93	0.67
1:A:253:ARG:HH21	1:A:322:VAL:H	1.40	0.67
2:B:126:LEU:O	2:B:127:LYS:CB	2.43	0.67
1:A:272:GLU:HB3	1:A:297:LYS:CD	2.25	0.66
2:B:91:TYR:HA	2:B:94:ALA:HB3	1.77	0.66
1:A:44:ARG:C	1:A:44:ARG:CD	2.60	0.66
1:A:257:PRO:HG3	1:A:266:TYR:HE1	1.59	0.66
1:A:400:ARG:HH11	1:A:400:ARG:HA	1.61	0.66
2:B:12:LEU:HG	2:B:16:TYR:HE2	1.61	0.66
1:A:49:ILE:O	1:A:51:ILE:N	2.28	0.66
1:A:51:ILE:HG13	1:A:89:ILE:HG23	1.77	0.66
1:A:24:LYS:HG3	5:A:2001:GDP:O2B	1.96	0.66
1:A:266:TYR:CE2	1:A:382:PRO:HD2	2.31	0.66
2:B:22:ASN:HB3	2:B:29:ARG:HH12	1.58	0.65
2:B:29:ARG:HB2	2:B:113:PRO:CG	2.26	0.65
1:A:149:GLU:HB3	2:B:19:LEU:HD11	1.79	0.65
2:B:117:ILE:HB	2:B:126:LEU:HD23	1.78	0.65
2:B:107:CYS:SG	2:B:109:VAL:HG23	2.37	0.65
2:B:38:THR:O	2:B:45:ILE:HG22	1.97	0.65
1:A:253:ARG:NH2	1:A:322:VAL:H	1.95	0.65
2:B:46:ILE:HD11	2:B:49:PHE:HD1	1.62	0.65
2:B:127:LYS:NZ	2:B:137:ILE:HD13	2.11	0.64
1:A:44:ARG:O	1:A:44:ARG:CD	2.31	0.64
2:B:16:TYR:O	2:B:24:LYS:HG3	1.96	0.64
1:A:49:ILE:HG12	1:A:100:THR:HG23	1.79	0.64
2:B:117:ILE:HG13	2:B:126:LEU:HG	1.78	0.64
2:B:22:ASN:HD21	2:B:23:VAL:HG12	1.62	0.64
2:B:38:THR:HB	2:B:45:ILE:HG23	1.80	0.64
1:A:206:SER:HB2	1:A:243:LYS:HE2	1.79	0.63
2:B:126:LEU:O	2:B:127:LYS:HB2	1.99	0.63
1:A:45:ARG:CB	1:A:92:PRO:HD2	2.28	0.63
1:A:217:SER:OG	1:A:306:ASP:HA	1.98	0.63
1:A:20:VAL:HB	1:A:125:GLN:OE1	1.98	0.63
1:A:47:ILE:HG13	1:A:48:THR:N	2.13	0.63
2:B:119:LYS:HD3	2:B:124:HIS:CD2	2.33	0.63
1:A:49:ILE:CG2	1:A:51:ILE:CG2	2.76	0.62
1:A:121:CYS:CB	1:A:122:PRO:HD3	2.25	0.62
2:B:50:LYS:CG	2:B:80:ARG:HB3	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:CB	1:A:83:ILE:HD11	2.29	0.62
2:B:110:CYS:SG	2:B:131:CYS:CB	2.81	0.62
2:B:29:ARG:HB3	2:B:29:ARG:HH11	1.64	0.62
1:A:218:PHE:N	1:A:218:PHE:CD1	2.67	0.62
1:A:253:ARG:HD2	1:A:253:ARG:C	2.19	0.62
1:A:128:GLU:CD	1:A:337:VAL:HG12	2.20	0.62
1:A:20:VAL:HG13	1:A:20:VAL:O	1.99	0.62
1:A:294:ILE:HD12	1:A:295:GLY:N	2.15	0.61
1:A:253:ARG:O	1:A:254:PRO:C	2.37	0.61
1:A:217:SER:HB3	1:A:308:MET:HB2	1.82	0.61
1:A:397:ILE:HD12	1:A:402:ARG:HD3	1.81	0.61
2:B:112:SER:O	2:B:115:THR:HG22	1.99	0.61
2:B:20:PRO:HB2	2:B:23:VAL:CG1	2.29	0.61
1:A:294:ILE:HD11	1:A:296:THR:CG2	2.31	0.61
2:B:37:VAL:HB	2:B:90:PRO:HG3	1.83	0.60
2:B:9:GLU:HA	2:B:9:GLU:OE1	2.01	0.60
2:B:115:THR:HB	2:B:127:LYS:HD2	1.83	0.60
2:B:50:LYS:HG3	2:B:51:ASP:H	1.64	0.60
2:B:127:LYS:HE2	2:B:137:ILE:HG21	1.82	0.60
1:A:19:HIS:CD2	1:A:125:GLN:HB2	2.36	0.60
1:A:369:ALA:O	1:A:370:LEU:HD12	2.02	0.60
2:B:79:GLY:C	2:B:80:ARG:HG2	2.22	0.60
1:A:45:ARG:CG	1:A:92:PRO:HD2	2.31	0.60
1:A:49:ILE:HG22	1:A:51:ILE:HG22	1.84	0.60
2:B:50:LYS:HG2	2:B:80:ARG:HB3	1.83	0.59
1:A:327:ARG:HG3	1:A:328:LEU:N	2.17	0.59
2:B:32:VAL:HG23	2:B:32:VAL:O	2.03	0.59
2:B:118:ILE:CG2	2:B:125:PHE:O	2.49	0.59
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.58	0.59
2:B:37:VAL:HG21	2:B:90:PRO:HA	1.85	0.59
2:B:137:ILE:O	2:B:137:ILE:HG13	2.02	0.59
1:A:253:ARG:CG	1:A:384:CYS:CB	2.78	0.59
2:B:25:HIS:HB2	2:B:26:HIS:ND1	2.18	0.59
2:B:70:GLU:HB3	2:B:96:LYS:HD2	1.84	0.59
1:A:36:THR:C	2:B:87:ARG:HH22	2.05	0.58
2:B:105:VAL:O	2:B:105:VAL:HG12	2.02	0.58
1:A:45:ARG:HG2	1:A:92:PRO:CG	2.31	0.58
1:A:223:PRO:HA	6:A:3041:HOH:O	2.01	0.58
1:A:197:GLU:HB3	1:A:198:PHE:CD1	2.39	0.58
2:B:106:ILE:HD13	6:B:3022:HOH:O	2.03	0.58
2:B:80:ARG:HG3	2:B:80:ARG:NH1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG13	1:A:294:ILE:O	2.03	0.57
1:A:256:VAL:HG23	1:A:269:ILE:HG21	1.86	0.57
2:B:46:ILE:CG1	2:B:46:ILE:O	2.52	0.57
1:A:90:ASP:OD1	1:A:91:SER:N	2.37	0.57
1:A:37:ASP:CA	2:B:87:ARG:NH2	2.64	0.57
2:B:38:THR:HB	2:B:45:ILE:CG2	2.34	0.57
1:A:287:TYR:HB3	1:A:288:PRO:HD2	1.85	0.57
1:A:45:ARG:HG2	1:A:92:PRO:CD	2.34	0.57
2:B:50:LYS:HE3	2:B:80:ARG:HH21	1.68	0.57
1:A:22:HIS:CG	1:A:116:ALA:H	2.22	0.57
2:B:26:HIS:ND1	2:B:26:HIS:N	2.52	0.56
2:B:126:LEU:O	2:B:127:LYS:CG	2.53	0.56
1:A:49:ILE:CG2	1:A:51:ILE:HG22	2.34	0.56
2:B:126:LEU:HD22	2:B:137:ILE:CD1	2.35	0.56
1:A:187:ASN:HD21	2:B:15:ALA:HB2	1.65	0.56
2:B:110:CYS:SG	2:B:110:CYS:O	2.63	0.56
1:A:143:ILE:HD11	1:A:167:ILE:HG21	1.86	0.56
1:A:51:ILE:CG1	1:A:89:ILE:HG23	2.36	0.56
2:B:22:ASN:HB3	2:B:29:ARG:HH11	1.71	0.56
1:A:269:ILE:HD11	1:A:298:LEU:CD2	2.35	0.56
1:A:24:LYS:HB2	1:A:24:LYS:NZ	2.21	0.56
2:B:117:ILE:HA	2:B:126:LEU:CB	2.36	0.55
1:A:224:GLY:C	1:A:226:PRO:HD3	2.27	0.55
1:A:45:ARG:H	1:A:45:ARG:NH1	2.04	0.55
1:A:34:VAL:O	1:A:34:VAL:HG22	2.07	0.55
1:A:243:LYS:HD2	1:A:285:GLU:OE2	2.07	0.55
2:B:31:GLU:O	2:B:33:PRO:HD3	2.07	0.55
2:B:45:ILE:HD11	2:B:81:ARG:HE	1.71	0.55
2:B:36:LEU:C	2:B:36:LEU:HD23	2.26	0.55
2:B:88:PHE:HD1	2:B:92:LEU:HD13	1.72	0.54
2:B:119:LYS:HA	6:B:3017:HOH:O	2.07	0.54
2:B:36:LEU:HB3	2:B:48:ASN:HB2	1.89	0.54
1:A:49:ILE:HG23	1:A:51:ILE:CB	2.37	0.54
1:A:121:CYS:SG	1:A:163:ILE:HA	2.47	0.54
1:A:348:ILE:HA	1:A:395:ARG:HH21	1.71	0.54
1:A:253:ARG:CZ	1:A:322:VAL:HB	2.38	0.54
2:B:50:LYS:HE3	2:B:80:ARG:NH2	2.23	0.54
1:A:236:ASP:HA	1:A:292:VAL:O	2.08	0.54
1:A:238:SER:O	1:A:240:VAL:HG13	2.07	0.54
1:A:70:SER:HB2	2:B:89:THR:CG2	2.38	0.53
1:A:269:ILE:HG13	1:A:270:THR:N	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ILE:HD11	2:B:81:ARG:NE	2.22	0.53
2:B:80:ARG:HH11	2:B:80:ARG:HG3	1.74	0.53
1:A:49:ILE:C	1:A:51:ILE:N	2.61	0.53
1:A:160:TYR:CE1	1:A:177:ILE:HD12	2.43	0.53
1:A:321:PRO:HD2	1:A:385:ALA:O	2.08	0.53
1:A:149:GLU:H	1:A:149:GLU:CD	2.11	0.53
1:A:44:ARG:H	1:A:44:ARG:HH11	1.57	0.53
1:A:49:ILE:CG2	1:A:49:ILE:O	2.56	0.53
1:A:396:GLN:O	1:A:397:ILE:HB	2.09	0.53
1:A:263:ARG:CG	1:A:263:ARG:HH11	2.11	0.52
1:A:49:ILE:HG22	1:A:49:ILE:O	2.08	0.52
2:B:71:ILE:HG22	2:B:72:ALA:N	2.25	0.52
2:B:105:VAL:O	2:B:115:THR:HG23	2.09	0.52
2:B:66:PHE:CE2	2:B:100:TYR:HB2	2.44	0.52
2:B:126:LEU:HB2	2:B:137:ILE:HG12	1.91	0.52
1:A:49:ILE:O	1:A:51:ILE:HG22	2.10	0.52
2:B:127:LYS:HZ3	2:B:137:ILE:HD13	1.74	0.52
2:B:58:ARG:NH1	2:B:115:THR:O	2.39	0.52
1:A:134:GLN:HA	1:A:171:VAL:HG21	1.90	0.52
1:A:358:VAL:HB	1:A:391:VAL:HG22	1.92	0.52
1:A:48:THR:CG2	1:A:362:ARG:CD	2.53	0.52
2:B:35:ALA:HB3	6:B:3020:HOH:O	2.09	0.52
1:A:183:LEU:HB2	5:A:2001:GDP:C6	2.44	0.52
2:B:117:ILE:HA	2:B:126:LEU:CG	2.40	0.51
2:B:118:ILE:H	2:B:126:LEU:HA	1.74	0.51
2:B:115:THR:CB	2:B:127:LYS:HD2	2.40	0.51
2:B:48:ASN:O	2:B:51:ASP:HB2	2.10	0.51
1:A:396:GLN:HG3	1:A:400:ARG:O	2.10	0.51
1:A:178:ILE:HG22	1:A:180:ILE:CG2	2.39	0.51
1:A:320:PRO:HB2	1:A:384:CYS:SG	2.50	0.51
2:B:68:LEU:O	2:B:71:ILE:O	2.29	0.51
1:A:253:ARG:NH2	1:A:322:VAL:N	2.51	0.51
2:B:58:ARG:NH2	2:B:115:THR:HG1	2.08	0.51
1:A:350:ARG:HD3	1:A:370:LEU:HD22	1.93	0.51
2:B:105:VAL:CG1	2:B:105:VAL:O	2.59	0.50
1:A:287:TYR:CD1	1:A:287:TYR:N	2.79	0.50
1:A:37:ASP:N	2:B:87:ARG:HH22	2.09	0.50
2:B:119:LYS:CA	6:B:3017:HOH:O	2.58	0.50
2:B:8:TYR:HE1	2:B:12:LEU:HD22	1.77	0.50
1:A:36:THR:HG21	1:A:42:GLU:HA	1.92	0.50
2:B:29:ARG:HB2	2:B:113:PRO:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	1:A:51:ILE:CG2	2.40	0.50
1:A:217:SER:CB	1:A:308:MET:HB2	2.41	0.50
2:B:67:LEU:C	2:B:69:ARG:N	2.65	0.50
2:B:36:LEU:HD22	2:B:47:GLU:CG	2.41	0.50
1:A:195:ILE:O	1:A:198:PHE:O	2.30	0.50
2:B:27:LYS:HG2	2:B:111:GLY:O	2.12	0.49
2:B:68:LEU:HD22	2:B:73:THR:O	2.11	0.49
1:A:246:VAL:CG2	1:A:284:GLU:HA	2.42	0.49
1:A:179:PRO:HG3	2:B:8:TYR:CE2	2.47	0.49
1:A:19:HIS:HD2	1:A:125:GLN:HB2	1.78	0.49
2:B:80:ARG:HH11	2:B:80:ARG:CG	2.24	0.49
2:B:67:LEU:O	2:B:69:ARG:N	2.46	0.49
1:A:318:LYS:C	1:A:319:LEU:HD12	2.33	0.49
1:A:245:LYS:HB3	1:A:248:ASP:OD1	2.12	0.49
2:B:121:ASP:O	6:B:3017:HOH:O	2.20	0.49
1:A:186:ALA:HB2	2:B:19:LEU:CD2	2.43	0.48
1:A:327:ARG:CG	1:A:410:LYS:HB2	2.39	0.48
2:B:21:GLU:O	2:B:23:VAL:N	2.46	0.48
2:B:50:LYS:CG	2:B:51:ASP:N	2.70	0.48
2:B:94:ALA:HB2	6:B:3020:HOH:O	2.13	0.48
1:A:412:LEU:HB2	6:A:3084:HOH:O	2.12	0.48
1:A:232:GLY:HA2	1:A:300:PRO:HG3	1.94	0.48
1:A:366:LEU:O	1:A:368:THR:HG23	2.13	0.48
1:A:128:GLU:O	1:A:131:MET:HB3	2.14	0.48
1:A:20:VAL:O	5:A:2001:GDP:O1B	2.32	0.48
1:A:198:PHE:N	1:A:198:PHE:CD1	2.80	0.48
1:A:133:LEU:HD13	1:A:141:ILE:CD1	2.44	0.48
1:A:53:PHE:CG	1:A:291:LEU:HD13	2.49	0.48
2:B:120:ARG:N	6:B:3017:HOH:O	2.45	0.48
1:A:115:ILE:HA	6:A:3068:HOH:O	2.13	0.48
2:B:29:ARG:NH2	2:B:105:VAL:HG12	2.25	0.48
2:B:58:ARG:HH22	2:B:115:THR:C	2.17	0.48
1:A:266:TYR:CD2	1:A:382:PRO:HD2	2.49	0.48
1:A:36:THR:O	2:B:87:ARG:NH2	2.47	0.47
1:A:16:MET:HE1	1:A:27:LEU:HD23	1.96	0.47
1:A:57:GLU:HG3	1:A:85:ARG:HD2	1.95	0.47
1:A:183:LEU:HD23	6:A:3060:HOH:O	2.14	0.47
1:A:147:LYS:HA	1:A:149:GLU:OE2	2.14	0.47
2:B:22:ASN:CB	2:B:29:ARG:O	2.46	0.47
1:A:212:MET:CE	1:A:292:VAL:HB	2.45	0.47
1:A:257:PRO:HG3	1:A:266:TYR:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:HIS:NE2	1:A:337:VAL:HG11	2.30	0.47
2:B:29:ARG:HB2	2:B:113:PRO:HB3	1.95	0.47
2:B:121:ASP:C	2:B:123:PHE:N	2.68	0.47
2:B:21:GLU:HA	2:B:21:GLU:OE1	2.15	0.47
1:A:45:ARG:H	1:A:45:ARG:HH11	1.61	0.47
1:A:67:TYR:CE2	1:A:83:ILE:HD12	2.49	0.47
1:A:51:ILE:HD12	1:A:100:THR:HG21	1.96	0.47
1:A:51:ILE:HG13	1:A:89:ILE:CG2	2.44	0.47
1:A:10:ALA:HA	1:A:85:ARG:O	2.15	0.47
1:A:36:THR:H	2:B:87:ARG:NH1	2.11	0.47
2:B:119:LYS:HD3	2:B:124:HIS:HD2	1.80	0.47
2:B:78:GLU:O	2:B:79:GLY:C	2.53	0.47
1:A:349:LYS:HZ2	1:A:349:LYS:HB2	1.78	0.47
1:A:70:SER:HB2	2:B:89:THR:HG23	1.97	0.47
1:A:117:ALA:HA	1:A:159:ASN:ND2	2.30	0.47
2:B:56:LEU:CD2	2:B:101:ILE:HG12	2.45	0.47
1:A:367:VAL:HA	1:A:376:GLU:O	2.15	0.47
2:B:52:ILE:HD12	2:B:52:ILE:N	2.30	0.47
1:A:36:THR:N	2:B:87:ARG:HH12	2.11	0.46
2:B:121:ASP:C	2:B:123:PHE:H	2.18	0.46
1:A:253:ARG:NH2	1:A:322:VAL:HB	2.31	0.46
2:B:50:LYS:HG3	2:B:51:ASP:OD1	2.15	0.46
2:B:66:PHE:HE2	2:B:96:LYS:O	1.98	0.46
1:A:245:LYS:HD2	1:A:285:GLU:OE2	2.15	0.46
2:B:67:LEU:C	2:B:69:ARG:H	2.19	0.46
1:A:205:ASP:OD1	1:A:207:ASN:HB2	2.15	0.46
2:B:126:LEU:HD22	2:B:137:ILE:CG1	2.45	0.46
1:A:45:ARG:HD2	1:A:92:PRO:HB2	1.95	0.46
1:A:75:TYR:N	1:A:75:TYR:CD1	2.84	0.46
1:A:253:ARG:CB	1:A:254:PRO:CD	2.90	0.46
1:A:168:LYS:HA	1:A:173:GLU:HG3	1.97	0.46
2:B:127:LYS:N	2:B:127:LYS:HD3	2.28	0.46
2:B:21:GLU:OE1	2:B:24:LYS:NZ	2.49	0.46
2:B:29:ARG:HD2	2:B:32:VAL:HG13	1.98	0.46
1:A:17:VAL:O	1:A:113:LEU:HD12	2.15	0.46
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.79	0.46
2:B:45:ILE:HG23	2:B:45:ILE:O	2.16	0.46
2:B:75:GLY:HA2	2:B:83:VAL:O	2.15	0.46
2:B:49:PHE:HE1	2:B:63:LEU:HD22	1.81	0.46
2:B:19:LEU:O	2:B:24:LYS:HE3	2.16	0.45
2:B:22:ASN:ND2	2:B:32:VAL:CG2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASP:OD1	1:A:373:ASP:N	2.50	0.45
1:A:51:ILE:CG2	1:A:215:LEU:HD11	2.47	0.45
1:A:17:VAL:HG23	1:A:113:LEU:HD13	1.99	0.45
2:B:124:HIS:HB3	2:B:126:LEU:HD11	1.97	0.45
2:B:50:LYS:HD2	2:B:80:ARG:CZ	2.44	0.45
1:A:251:GLU:O	1:A:319:LEU:HD21	2.17	0.45
1:A:75:TYR:OH	1:A:189:ASP:HB3	2.16	0.45
2:B:8:TYR:CE1	2:B:12:LEU:HD22	2.51	0.45
2:B:29:ARG:HB3	2:B:29:ARG:CZ	2.46	0.45
1:A:121:CYS:CB	1:A:122:PRO:CD	2.94	0.45
2:B:139:HIS:ND1	2:B:139:HIS:C	2.69	0.45
2:B:30:PHE:CD1	2:B:30:PHE:N	2.84	0.45
2:B:117:ILE:HB	2:B:126:LEU:CD2	2.47	0.45
2:B:22:ASN:ND2	2:B:32:VAL:HG22	2.31	0.45
1:A:157:LEU:O	1:A:161:ARG:HD3	2.17	0.45
2:B:126:LEU:C	2:B:127:LYS:HD3	2.36	0.45
2:B:126:LEU:CD2	2:B:137:ILE:HD11	2.41	0.45
1:A:397:ILE:HG22	1:A:397:ILE:O	2.15	0.45
2:B:125:PHE:C	2:B:126:LEU:HD12	2.38	0.45
2:B:56:LEU:HD21	2:B:101:ILE:HG12	1.99	0.45
1:A:329:GLU:CD	1:A:408:ILE:HD12	2.37	0.45
1:A:329:GLU:OE2	1:A:408:ILE:HD12	2.17	0.45
1:A:133:LEU:HD13	1:A:141:ILE:HD13	1.99	0.45
1:A:130:LEU:HD12	1:A:166:PHE:CZ	2.51	0.45
1:A:49:ILE:HG12	1:A:100:THR:CG2	2.46	0.44
1:A:326:LEU:HD12	6:A:3059:HOH:O	2.18	0.44
1:A:326:LEU:O	1:A:377:LEU:N	2.49	0.44
1:A:356:LEU:CD2	1:A:393:ILE:HG12	2.47	0.44
2:B:135:THR:HG22	2:B:136:PRO:HD2	1.99	0.44
1:A:253:ARG:CG	1:A:384:CYS:SG	3.01	0.44
1:A:51:ILE:HG21	1:A:215:LEU:HD11	1.98	0.44
1:A:197:GLU:HG2	2:B:5:TYR:CE1	2.52	0.44
2:B:16:TYR:HA	2:B:19:LEU:HB2	1.99	0.44
1:A:45:ARG:CD	1:A:92:PRO:HB2	2.47	0.44
2:B:107:CYS:HB3	2:B:110:CYS:O	2.17	0.44
1:A:374:GLU:HG2	1:A:375:ILE:N	2.33	0.44
1:A:246:VAL:HG23	1:A:284:GLU:HA	1.98	0.44
1:A:134:GLN:HA	1:A:171:VAL:CG2	2.48	0.44
1:A:176:PRO:HG2	1:A:198:PHE:CZ	2.52	0.44
1:A:346:GLU:O	1:A:395:ARG:NH1	2.50	0.44
1:A:271:THR:CB	1:A:298:LEU:HG	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLY:CA	2:B:83:VAL:O	2.66	0.44
1:A:209:PRO:HA	1:A:210:PRO:HD3	1.83	0.44
1:A:32:THR:HG22	1:A:56:ALA:HB2	1.98	0.44
2:B:45:ILE:HG13	2:B:82:VAL:O	2.17	0.44
2:B:125:PHE:HA	2:B:136:PRO:HA	1.99	0.43
2:B:29:ARG:CZ	2:B:29:ARG:CB	2.95	0.43
1:A:396:GLN:O	1:A:400:ARG:O	2.35	0.43
1:A:321:PRO:O	1:A:323:TRP:CD1	2.71	0.43
1:A:49:ILE:HG12	1:A:100:THR:OG1	2.19	0.43
2:B:136:PRO:HG2	2:B:136:PRO:O	2.19	0.43
1:A:45:ARG:HG2	1:A:92:PRO:HD2	1.97	0.43
1:A:312:VAL:HG21	1:A:384:CYS:SG	2.58	0.43
1:A:152:ASP:OD2	1:A:154:GLU:HB3	2.19	0.43
2:B:29:ARG:HH21	2:B:105:VAL:CG1	2.24	0.43
1:A:333:LEU:HD21	1:A:406:TYR:HD1	1.84	0.43
1:A:348:ILE:HA	1:A:395:ARG:NH2	2.32	0.43
2:B:43:LYS:NZ	2:B:43:LYS:HB3	2.33	0.43
1:A:45:ARG:CG	1:A:92:PRO:HG2	2.45	0.43
1:A:330:VAL:CG2	1:A:375:ILE:HG12	2.49	0.43
2:B:138:GLN:HB2	6:B:3025:HOH:O	2.18	0.43
1:A:225:THR:CG2	1:A:225:THR:O	2.67	0.43
1:A:245:LYS:O	1:A:248:ASP:OD1	2.37	0.43
1:A:220:VAL:O	1:A:220:VAL:HG23	2.19	0.43
2:B:85:GLN:HB3	2:B:85:GLN:HE21	1.62	0.43
2:B:101:ILE:HA	2:B:105:VAL:HB	2.00	0.43
1:A:235:LEU:O	1:A:294:ILE:HG23	2.18	0.43
1:A:30:ALA:HB1	2:B:91:TYR:CZ	2.54	0.43
1:A:14:ILE:O	1:A:88:PHE:HA	2.18	0.42
1:A:263:ARG:NH1	1:A:263:ARG:CG	2.73	0.42
1:A:45:ARG:H	1:A:45:ARG:HG3	1.61	0.42
1:A:326:LEU:N	1:A:377:LEU:O	2.50	0.42
1:A:325:ASP:O	1:A:326:LEU:HD13	2.18	0.42
1:A:349:LYS:HZ3	1:A:349:LYS:HB2	1.84	0.42
2:B:82:VAL:HG12	2:B:84:LEU:HD13	2.00	0.42
1:A:228:GLU:HB2	1:A:229:LYS:H	1.50	0.42
2:B:12:LEU:HD12	2:B:12:LEU:HA	1.93	0.42
1:A:151:VAL:HG23	1:A:151:VAL:O	2.19	0.42
1:A:230:LEU:N	1:A:230:LEU:CD2	2.83	0.42
1:A:212:MET:HE2	1:A:292:VAL:HB	2.00	0.42
1:A:251:GLU:OE1	1:A:316:PRO:HA	2.20	0.42
1:A:180:ILE:HA	1:A:186:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:CG2	1:A:362:ARG:HD3	2.37	0.41
1:A:186:ALA:CB	2:B:19:LEU:HD21	2.50	0.41
1:A:188:ILE:HG13	2:B:91:TYR:CE2	2.54	0.41
2:B:66:PHE:CD2	2:B:100:TYR:HB2	2.54	0.41
1:A:346:GLU:O	1:A:395:ARG:NH2	2.50	0.41
1:A:49:ILE:CD1	1:A:100:THR:HA	2.45	0.41
1:A:215:LEU:O	1:A:216:ARG:HG2	2.21	0.41
1:A:323:TRP:CE3	1:A:326:LEU:CD1	3.03	0.41
2:B:107:CYS:O	2:B:111:GLY:HA2	2.20	0.41
1:A:44:ARG:CZ	6:A:3044:HOH:O	2.49	0.41
1:A:35:TRP:CZ2	1:A:57:GLU:HB2	2.56	0.41
1:A:128:GLU:CD	1:A:337:VAL:CG1	2.87	0.41
1:A:70:SER:HA	1:A:71:PRO:HD3	1.81	0.41
2:B:59:ASP:HB2	2:B:62:HIS:HB2	2.01	0.41
2:B:124:HIS:HB3	2:B:126:LEU:CD1	2.50	0.41
2:B:3:ILE:HG22	6:B:3018:HOH:O	2.20	0.41
1:A:45:ARG:CG	1:A:92:PRO:CD	2.97	0.41
2:B:127:LYS:HB3	2:B:133:ALA:O	2.20	0.41
2:B:29:ARG:HB2	2:B:113:PRO:HG2	2.03	0.41
1:A:311:ASN:HD22	1:A:311:ASN:N	2.18	0.41
1:A:253:ARG:CB	1:A:254:PRO:HD3	2.35	0.41
1:A:95:GLU:O	1:A:98:MET:HB2	2.20	0.41
1:A:366:LEU:O	1:A:377:LEU:HA	2.21	0.41
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.79	0.41
1:A:225:THR:HG22	1:A:225:THR:O	2.19	0.41
2:B:122:ARG:HG2	2:B:122:ARG:NH1	2.36	0.41
2:B:36:LEU:CD2	2:B:47:GLU:HG3	2.43	0.40
1:A:117:ALA:HB2	1:A:145:GLN:CG	2.51	0.40
1:A:11:GLU:HB3	1:A:201:THR:OG1	2.21	0.40
1:A:197:GLU:HB3	1:A:198:PHE:CE1	2.55	0.40
1:A:105:ALA:HB1	1:A:136:ILE:HB	2.03	0.40
2:B:42:ASN:HA	2:B:42:ASN:HD22	1.72	0.40
2:B:50:LYS:HB3	2:B:80:ARG:HB3	2.03	0.40
1:A:127:ARG:HD2	6:A:3023:HOH:O	2.20	0.40
1:A:24:LYS:HB2	1:A:24:LYS:HZ3	1.85	0.40
1:A:7:THR:HG21	1:A:283:VAL:HG11	2.03	0.40
2:B:120:ARG:NE	2:B:125:PHE:CE2	2.90	0.40
1:A:395:ARG:HG2	1:A:396:GLN:N	2.37	0.40
2:B:71:ILE:CG2	2:B:72:ALA:N	2.85	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	405/419 (97%)	352 (87%)	40 (10%)	13 (3%)	5	38
2	B	135/148 (91%)	109 (81%)	18 (13%)	8 (6%)	2	19
All	All	540/567 (95%)	461 (85%)	58 (11%)	21 (4%)	4	32

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	47	ILE
1	A	50	LYS
1	A	225	THR
1	A	228	GLU
1	A	253	ARG
2	B	20	PRO
2	B	128	CYS
1	A	231	VAL
1	A	260	GLU
1	A	343	LEU
2	B	22	ASN
2	B	79	GLY
2	B	127	LYS
1	A	223	PRO
1	A	344	ASN
2	B	26	HIS
2	B	68	LEU
1	A	396	GLN
1	A	397	ILE
2	B	60	PRO

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	342/353 (97%)	297 (87%)	45 (13%)	5	25
2	B	121/132 (92%)	92 (76%)	29 (24%)	1	4
All	All	463/485 (96%)	389 (84%)	74 (16%)	3	16

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	THR
1	A	20	VAL
1	A	24	LYS
1	A	42	GLU
1	A	43	LEU
1	A	44	ARG
1	A	45	ARG
1	A	48	THR
1	A	49	ILE
1	A	70	SER
1	A	75	TYR
1	A	79	GLU
1	A	95	GLU
1	A	97	LEU
1	A	130	LEU
1	A	149	GLU
1	A	171	VAL
1	A	193	LYS
1	A	206	SER
1	A	218	PHE
1	A	220	VAL
1	A	230	LEU
1	A	231	VAL
1	A	248	ASP
1	A	253	ARG
1	A	258	TYR

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Mol	Chain	Res	Type
1	A	263	ARG
1	A	264	ILE
1	A	269	ILE
1	A	287	TYR
1	A	294	ILE
1	A	325	ASP
1	A	327	ARG
1	A	334	GLU
1	A	335	ARG
1	A	336	VAL
1	A	341	GLN
1	A	342	GLU
1	A	349	LYS
1	A	374	GLU
1	A	376	GLU
1	A	381	ILE
1	A	411	GLU
1	A	412	LEU
2	B	5	TYR
2	B	9	GLU
2	B	19	LEU
2	B	20	PRO
2	B	23	VAL
2	B	24	LYS
2	B	26	HIS
2	B	30	PHE
2	B	43	LYS
2	B	46	ILE
2	B	59	ASP
2	B	64	LEU
2	B	65	LYS
2	B	73	THR
2	B	76	THR
2	B	77	LEU
2	B	80	ARG
2	B	85	GLN
2	B	109	VAL
2	B	115	THR
2	B	117	ILE
2	B	118	ILE
2	B	119	LYS
2	B	120	ARG

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Mol	Chain	Res	Type
2	B	121	ASP
2	B	127	LYS
2	B	128	CYS
2	B	129	GLU
2	B	135	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	129	HIS
1	A	145	GLN
1	A	311	ASN
2	B	22	ASN
2	B	42	ASN
2	B	85	GLN
2	B	95	ASN
2	B	124	HIS

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)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	#$|Z| > 2$
5	GDP	A	2001	3	23,30,30	1.89	6 (26%)	30,47,47	2.63	11 (36%)

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
5	GDP	A	2001	3	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	GDP	C3'-C4'	-3.18	1.44	1.53
5	A	2001	GDP	PB-O1B	-2.44	1.43	1.51
5	A	2001	GDP	C5'-C4'	-2.23	1.44	1.51
5	A	2001	GDP	PB-O2B	3.30	1.66	1.54
5	A	2001	GDP	C6-N1	3.97	1.40	1.33
5	A	2001	GDP	O4'-C1'	4.10	1.46	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2001	GDP	C5-C6-N1	-5.85	115.58	123.59
5	A	2001	GDP	O3A-PA-O5'	-5.61	88.05	102.94
5	A	2001	GDP	C4'-O4'-C1'	-5.11	104.11	109.72
5	A	2001	GDP	C5'-C4'-C3'	-5.05	95.16	115.21
5	A	2001	GDP	N3-C2-N1	-3.74	121.75	127.44
5	A	2001	GDP	O3B-PB-O1B	-2.42	102.78	110.58
5	A	2001	GDP	C2'-C1'-N9	-2.19	110.95	114.29
5	A	2001	GDP	O3B-PB-O2B	2.40	116.51	107.38
5	A	2001	GDP	O3B-PB-O3A	2.45	116.21	105.09
5	A	2001	GDP	O4'-C4'-C3'	3.24	111.67	105.15
5	A	2001	GDP	C6-N1-C2	4.11	121.64	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	GDP	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	407/419 (97%)	0.01	14 (3%)	49	44	20, 47, 94, 95	0
2	B	137/148 (92%)	0.11	5 (3%)	46	41	20, 63, 93, 95	0
All	All	544/567 (95%)	0.03	19 (3%)	48	42	20, 51, 94, 95	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	LEU	4.1
1	A	263	ARG	4.0
1	A	45	ARG	3.4
2	B	29	ARG	3.1
1	A	335	ARG	2.8
1	A	229	LYS	2.8
1	A	48	THR	2.7
1	A	230	LEU	2.6
1	A	221	ASN	2.6
2	B	126	LEU	2.5
1	A	252	ILE	2.5
1	A	44	ARG	2.4
2	B	25	HIS	2.4
2	B	125	PHE	2.3
2	B	111	GLY	2.2
1	A	121	CYS	2.1
1	A	259	GLU	2.1
1	A	334	GLU	2.0
1	A	40	SER	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, 95th 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
5	GDP	A	2001	28/28	0.92	0.20	-0.43	21,30,34,35	0
4	ZN	A	3001	1/1	0.99	0.03	-2.11	26,26,26,26	0
4	ZN	B	3002	1/1	0.97	0.08	-4.39	61,61,61,61	0
3	MG	A	1001	1/1	0.85	0.24	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.