Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 01:42 AM EDT

PDB ID	:	2D74
Title	:	Crystal structure of translation initiation factor aIF2betagamma heterodimer
Authors	:	Sokabe, M.; Yao, M.; Sakai, N.; Toya, S.; Tanaka, I.
Deposited on	:	2005-11-16
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

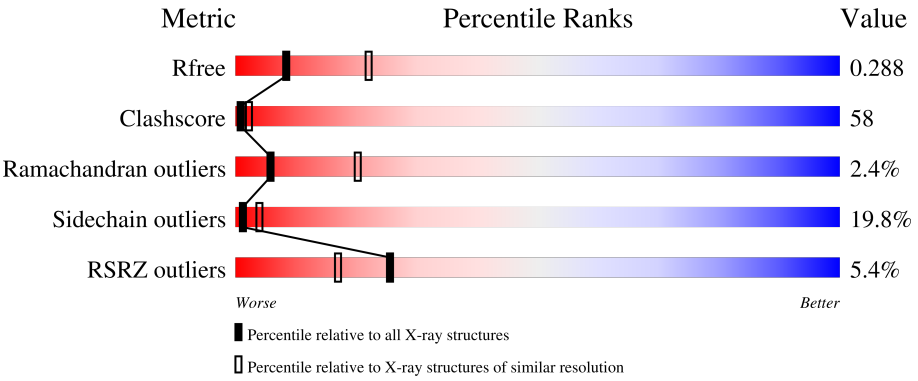
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 40% 45% 10%
2	B	148	8% 22% 45% 23% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4398 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	403	3098	1968	544	572	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 mutation	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	HIS	-	expression tag	UNP Q8U3I5

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

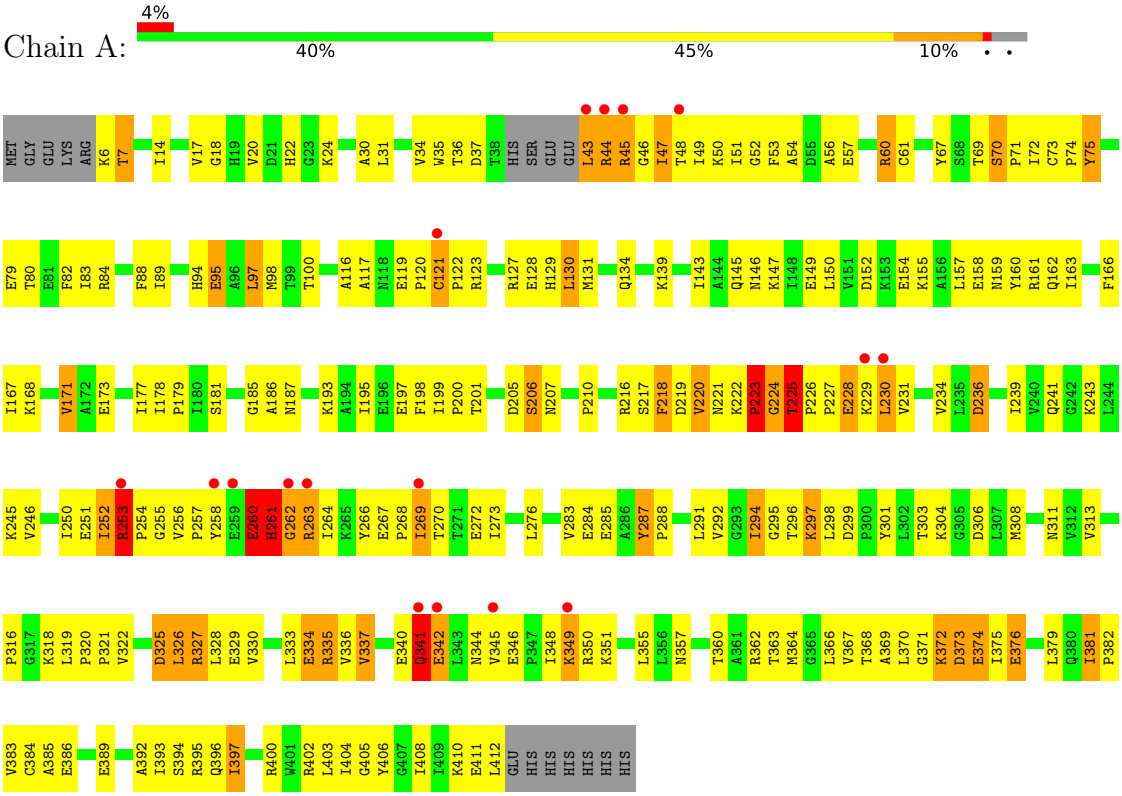
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	128	Total O 128 128	0	0
4	B	52	Total O 52 52	0	0

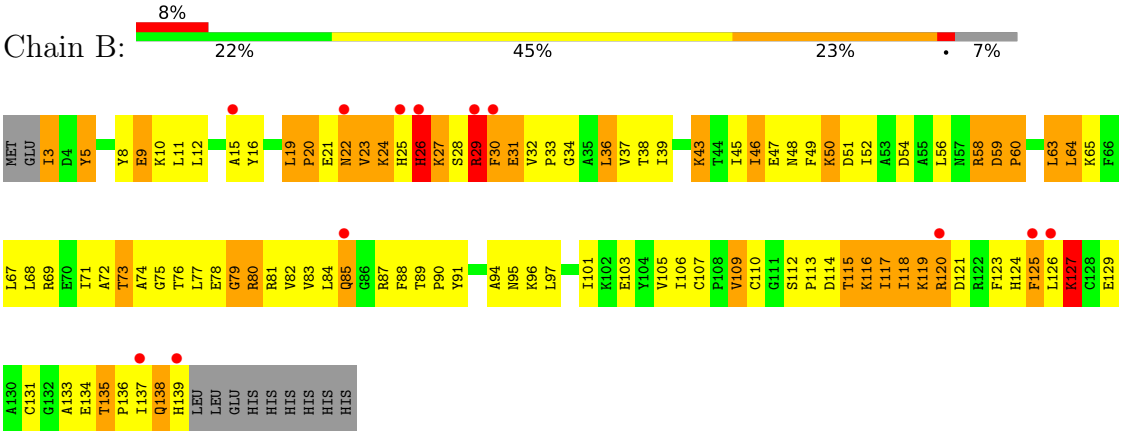
3 Residue-property plots (i)

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

• Molecule 1: 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	68.47Å 76.18Å 98.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 49.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.80) 98.0 (49.11-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.290 0.241 , 0.288	Depositor DCC
R_{free} test set	969 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4398	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN

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	0/3151	0.78	6/4265 (0.1%)
2	B	0.40	0/1142	0.88	4/1540 (0.3%)
All	All	0.35	0/4293	0.81	10/5805 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	29	ARG	N-CA-C	-9.68	84.86	111.00
1	A	262	GLY	N-CA-C	-8.53	91.78	113.10
1	A	224	GLY	N-CA-C	-7.82	93.54	113.10
2	B	125	PHE	N-CA-C	-7.41	90.99	111.00
1	A	225	THR	N-CA-C	6.23	127.83	111.00
1	A	261	HIS	N-CA-C	-6.17	94.35	111.00
2	B	127	LYS	N-CA-C	6.04	127.30	111.00
1	A	253	ARG	N-CA-C	5.69	126.35	111.00
2	B	138	GLN	N-CA-C	-5.62	95.83	111.00
1	A	260	GLU	N-CA-C	5.24	125.15	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3098	0	3220	288	0
2	B	1118	0	1138	221	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	128	0	0	17	0
4	B	52	0	0	9	0
All	All	4398	0	4358	500	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 58.

All (500) 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:B:22:ASN:HB3	2:B:29:ARG:NH1	1.58	1.16
1:A:350:ARG:HG3	1:A:370:LEU:HD13	1.21	1.15
1:A:253:ARG:HG3	1:A:384:CYS:HB2	1.15	1.14
1:A:226:PRO:O	1:A:230:LEU:HG	1.54	1.07
2:B:46:ILE:HD11	2:B:49:PHE:CD1	1.92	1.05
1:A:253:ARG:CG	1:A:384:CYS:HB2	1.88	1.03
2:B:29:ARG:NH1	2:B:29:ARG:HB3	1.73	1.03
1:A:272:GLU:HB3	1:A:297:LYS:HD2	1.38	1.02
2:B:22:ASN:HB2	2:B:29:ARG:O	1.59	1.01
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.22	0.99
1:A:120:PRO:HB2	4:A:1101:HOH:O	1.61	0.99
1:A:257:PRO:HG3	1:A:266:TYR:CE1	1.99	0.98
2:B:50:LYS:HD2	2:B:80:ARG:NE	1.78	0.98
1:A:303:THR:HG22	1:A:308:MET:HG3	1.46	0.96
1:A:369:ALA:HB3	1:A:376:GLU:HB2	1.49	0.95
1:A:253:ARG:HG3	1:A:384:CYS:CB	1.97	0.95
1:A:253:ARG:HG2	1:A:384:CYS:SG	2.07	0.94
2:B:126:LEU:HD22	2:B:137:ILE:HD11	1.49	0.94
2:B:46:ILE:HD11	2:B:49:PHE:HD1	1.28	0.94
1:A:45:ARG:O	1:A:50:LYS:HA	1.67	0.93
1:A:253:ARG:HB3	1:A:254:PRO:HD3	1.48	0.93
2:B:22:ASN:HB3	2:B:29:ARG:HH12	1.34	0.92
2:B:36:LEU:HD22	2:B:47:GLU:HG3	1.54	0.90
2:B:107:CYS:SG	2:B:109:VAL:HG23	2.12	0.90
1:A:222:LYS:O	1:A:224:GLY:N	2.05	0.89
1:A:400:ARG:NH1	1:A:400:ARG:HA	1.90	0.87
1:A:121:CYS:HB3	1:A:122:PRO:HD3	1.57	0.86
1:A:224:GLY:O	1:A:226:PRO:HD3	1.74	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ILE:HA	2:B:126:LEU:HB3	1.57	0.86
2:B:118:ILE:H	2:B:126:LEU:HA	1.38	0.85
1:A:253:ARG:HD2	1:A:253:ARG:C	1.95	0.85
2:B:22:ASN:ND2	2:B:23:VAL:HG12	1.92	0.85
1:A:256:VAL:HG23	1:A:269:ILE:HG21	1.59	0.84
2:B:79:GLY:C	2:B:80:ARG:HG2	1.95	0.84
1:A:294:ILE:HD11	1:A:296:THR:CG2	2.07	0.84
1:A:219:ASP:OD1	1:A:221:ASN:HB2	1.77	0.84
1:A:269:ILE:HD11	1:A:298:LEU:HD11	1.59	0.83
2:B:46:ILE:HG12	2:B:46:ILE:O	1.78	0.83
1:A:294:ILE:HD11	1:A:296:THR:HG22	1.60	0.83
1:A:253:ARG:HH21	1:A:322:VAL:N	1.76	0.83
1:A:327:ARG:HG2	1:A:410:LYS:HB2	1.61	0.82
2:B:110:CYS:SG	2:B:131:CYS:HB3	2.18	0.82
2:B:29:ARG:HH21	2:B:105:VAL:HG12	1.45	0.82
2:B:95:ASN:ND2	2:B:96:LYS:HE3	1.95	0.82
2:B:117:ILE:HB	2:B:126:LEU:HD23	1.60	0.81
1:A:252:ILE:HD12	1:A:308:MET:HE1	1.62	0.81
2:B:22:ASN:HB3	2:B:29:ARG:HH11	1.43	0.81
1:A:253:ARG:CG	1:A:384:CYS:CB	2.56	0.81
1:A:342:GLU:HG3	1:A:397:ILE:HG21	1.63	0.81
1:A:253:ARG:HG2	1:A:384:CYS:HG	1.45	0.81
1:A:257:PRO:HG3	1:A:266:TYR:HE1	1.44	0.81
2:B:126:LEU:C	2:B:127:LYS:HE2	2.02	0.80
1:A:60:ARG:HB2	1:A:83:ILE:HD11	1.63	0.80
1:A:396:GLN:HG3	1:A:400:ARG:O	1.82	0.79
2:B:36:LEU:C	2:B:36:LEU:HD23	2.04	0.78
2:B:36:LEU:CD2	2:B:47:GLU:HG3	2.13	0.78
2:B:39:ILE:HG21	2:B:87:ARG:HD3	1.65	0.78
2:B:22:ASN:CB	2:B:29:ARG:NH1	2.45	0.78
1:A:326:LEU:HD22	1:A:379:LEU:HD11	1.67	0.77
1:A:333:LEU:HG	1:A:405:GLY:HA2	1.64	0.77
1:A:397:ILE:HD12	1:A:402:ARG:HD3	1.66	0.77
2:B:126:LEU:HD22	2:B:137:ILE:CD1	2.14	0.77
1:A:60:ARG:CB	1:A:83:ILE:HD11	2.14	0.77
1:A:349:LYS:HB2	1:A:349:LYS:NZ	1.98	0.76
1:A:272:GLU:CB	1:A:297:LYS:HD2	2.15	0.76
1:A:17:VAL:HG12	1:A:97:LEU:HD13	1.66	0.76
2:B:125:PHE:C	2:B:126:LEU:HD12	2.07	0.75
1:A:95:GLU:OE2	1:A:402:ARG:HA	1.87	0.75
2:B:29:ARG:HB3	2:B:29:ARG:HH11	1.50	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:OE1	1:A:335:ARG:NH1	2.20	0.75
1:A:350:ARG:HG3	1:A:370:LEU:CD1	2.10	0.75
2:B:117:ILE:HA	2:B:126:LEU:CB	2.16	0.74
2:B:45:ILE:HD13	4:B:1035:HOH:O	1.86	0.74
2:B:50:LYS:HG3	2:B:51:ASP:N	2.01	0.74
1:A:252:ILE:HD12	1:A:308:MET:CE	2.17	0.74
2:B:58:ARG:NH2	2:B:115:THR:OG1	2.21	0.73
1:A:253:ARG:NH2	1:A:322:VAL:HB	2.03	0.73
1:A:84:ARG:HH12	1:A:200:PRO:HA	1.52	0.73
2:B:80:ARG:HG3	2:B:80:ARG:NH1	2.02	0.73
1:A:263:ARG:HH11	1:A:263:ARG:CG	2.01	0.73
1:A:45:ARG:HG2	1:A:46:GLY:O	1.89	0.73
1:A:253:ARG:HB3	1:A:254:PRO:CD	2.19	0.73
1:A:397:ILE:O	1:A:397:ILE:HG22	1.88	0.73
2:B:38:THR:O	2:B:45:ILE:HG22	1.89	0.72
2:B:95:ASN:HD22	2:B:96:LYS:HE3	1.50	0.72
1:A:272:GLU:HB3	1:A:297:LYS:CD	2.16	0.72
2:B:119:LYS:HD3	2:B:124:HIS:CD2	2.25	0.72
1:A:218:PHE:N	1:A:218:PHE:CD1	2.57	0.72
2:B:126:LEU:CD2	2:B:137:ILE:HD11	2.19	0.72
1:A:51:ILE:HD12	1:A:100:THR:HG21	1.72	0.71
1:A:329:GLU:HB3	1:A:408:ILE:HB	1.72	0.71
2:B:34:GLY:HA2	4:B:1037:HOH:O	1.88	0.71
2:B:117:ILE:HB	2:B:126:LEU:CD2	2.20	0.71
2:B:20:PRO:O	2:B:24:LYS:HB2	1.89	0.71
2:B:103:GLU:HB2	2:B:139:HIS:O	1.90	0.71
2:B:127:LYS:HG2	2:B:135:THR:N	2.06	0.71
1:A:34:VAL:HG23	2:B:87:ARG:HB3	1.72	0.71
1:A:45:ARG:HD3	1:A:216:ARG:NH2	2.06	0.71
1:A:400:ARG:HA	1:A:400:ARG:HH11	1.54	0.71
1:A:357:ASN:HB2	1:A:392:ALA:HB3	1.72	0.71
1:A:139:LYS:HG2	1:A:171:VAL:HG12	1.72	0.70
2:B:107:CYS:HB3	2:B:110:CYS:O	1.89	0.70
2:B:50:LYS:HD2	2:B:80:ARG:HE	1.56	0.70
1:A:245:LYS:HD2	1:A:285:GLU:OE2	1.91	0.70
1:A:369:ALA:O	1:A:370:LEU:HD12	1.91	0.70
1:A:45:ARG:C	1:A:50:LYS:HA	2.10	0.69
1:A:294:ILE:HD12	1:A:295:GLY:N	2.07	0.69
1:A:395:ARG:HG3	4:A:1109:HOH:O	1.93	0.69
2:B:29:ARG:HB2	2:B:113:PRO:CG	2.23	0.69
2:B:38:THR:HB	2:B:45:ILE:HG23	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HD11	1:A:298:LEU:CD1	2.22	0.68
1:A:217:SER:CB	1:A:308:MET:HB2	2.23	0.68
1:A:253:ARG:CZ	1:A:322:VAL:HB	2.24	0.68
1:A:253:ARG:C	1:A:253:ARG:CD	2.60	0.68
2:B:127:LYS:HG2	2:B:135:THR:H	1.58	0.68
1:A:403:LEU:HG	4:A:1128:HOH:O	1.94	0.68
2:B:125:PHE:O	2:B:126:LEU:HD12	1.93	0.68
2:B:29:ARG:HB3	2:B:29:ARG:CZ	2.24	0.67
1:A:48:THR:HG21	1:A:360:THR:O	1.94	0.67
1:A:139:LYS:HG2	1:A:171:VAL:CG1	2.25	0.67
2:B:117:ILE:HG13	2:B:126:LEU:HG	1.77	0.67
1:A:43:LEU:HD11	1:A:54:ALA:HB2	1.77	0.67
2:B:45:ILE:HD11	2:B:81:ARG:NE	2.10	0.67
2:B:80:ARG:HG3	2:B:80:ARG:HH11	1.60	0.67
2:B:126:LEU:O	2:B:127:LYS:HE2	1.95	0.67
2:B:64:LEU:CD1	2:B:68:LEU:HD11	2.25	0.66
2:B:118:ILE:O	2:B:125:PHE:O	2.13	0.66
2:B:16:TYR:O	2:B:19:LEU:HB2	1.95	0.66
2:B:126:LEU:HD22	2:B:137:ILE:CG1	2.26	0.66
2:B:105:VAL:O	2:B:115:THR:HG23	1.95	0.66
2:B:118:ILE:CG2	2:B:125:PHE:O	2.43	0.65
1:A:287:TYR:CD1	1:A:287:TYR:N	2.64	0.65
1:A:45:ARG:HD3	1:A:216:ARG:HH22	1.61	0.65
2:B:29:ARG:HH21	2:B:105:VAL:CG1	2.10	0.65
1:A:363:THR:OG1	1:A:381:ILE:HG13	1.97	0.65
1:A:157:LEU:O	1:A:161:ARG:HD3	1.97	0.64
2:B:121:ASP:C	2:B:123:PHE:N	2.49	0.64
1:A:122:PRO:HB2	1:A:127:ARG:NH1	2.12	0.64
1:A:168:LYS:HA	1:A:173:GLU:HG3	1.80	0.64
2:B:29:ARG:HD2	2:B:32:VAL:HG13	1.78	0.64
1:A:355:LEU:HD13	1:A:364:MET:CE	2.28	0.64
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.02	0.63
1:A:355:LEU:HB3	1:A:394:SER:HB2	1.79	0.63
2:B:38:THR:HB	2:B:45:ILE:CG2	2.29	0.63
2:B:27:LYS:O	2:B:27:LYS:HG2	1.97	0.63
1:A:253:ARG:O	1:A:254:PRO:C	2.34	0.62
1:A:330:VAL:CG2	1:A:375:ILE:HG12	2.29	0.62
2:B:45:ILE:HD11	2:B:81:ARG:HE	1.63	0.62
1:A:350:ARG:HD3	1:A:370:LEU:HD22	1.82	0.62
2:B:75:GLY:HA2	2:B:83:VAL:O	1.99	0.62
2:B:36:LEU:HD22	2:B:47:GLU:CG	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ILE:HG22	2:B:125:PHE:O	1.98	0.62
2:B:37:VAL:HG21	2:B:90:PRO:HA	1.82	0.62
2:B:127:LYS:CG	2:B:135:THR:H	2.12	0.62
1:A:17:VAL:HG12	1:A:97:LEU:CD1	2.30	0.62
1:A:266:TYR:CE2	1:A:382:PRO:HD2	2.34	0.62
2:B:126:LEU:O	2:B:127:LYS:CB	2.46	0.62
1:A:210:PRO:HA	1:A:241:GLN:O	1.99	0.62
2:B:9:GLU:HA	2:B:9:GLU:OE1	1.99	0.62
2:B:22:ASN:HD21	2:B:23:VAL:HG12	1.63	0.62
2:B:29:ARG:HB2	2:B:113:PRO:HB3	1.80	0.62
1:A:253:ARG:CB	1:A:254:PRO:HD3	2.26	0.62
1:A:349:LYS:HB2	1:A:349:LYS:HZ2	1.62	0.62
2:B:112:SER:O	2:B:115:THR:HG22	2.00	0.62
2:B:110:CYS:SG	2:B:110:CYS:O	2.57	0.61
1:A:276:LEU:HD23	1:A:294:ILE:HA	1.82	0.61
2:B:50:LYS:CG	2:B:80:ARG:HB3	2.30	0.61
2:B:107:CYS:SG	2:B:109:VAL:CG2	2.88	0.61
1:A:134:GLN:HA	1:A:171:VAL:HG21	1.82	0.61
1:A:297:LYS:HZ2	1:A:297:LYS:HB3	1.65	0.61
2:B:29:ARG:HB2	2:B:113:PRO:CB	2.29	0.61
2:B:119:LYS:HD3	2:B:124:HIS:HD2	1.64	0.61
2:B:139:HIS:HA	4:B:1003:HOH:O	1.99	0.61
1:A:217:SER:HB3	1:A:308:MET:HB2	1.83	0.61
1:A:269:ILE:HD11	1:A:298:LEU:HD21	1.83	0.61
2:B:50:LYS:HB3	2:B:80:ARG:HB3	1.82	0.61
2:B:22:ASN:OD1	2:B:32:VAL:HG21	2.01	0.60
2:B:121:ASP:C	2:B:123:PHE:H	2.03	0.60
1:A:7:THR:HG21	1:A:283:VAL:HG11	1.82	0.60
2:B:22:ASN:CB	2:B:29:ARG:HH11	2.10	0.60
1:A:245:LYS:HD2	1:A:285:GLU:CD	2.22	0.60
2:B:28:SER:O	2:B:30:PHE:CD2	2.55	0.60
2:B:88:PHE:HA	4:B:1008:HOH:O	2.01	0.60
2:B:127:LYS:CB	2:B:134:GLU:HA	2.32	0.60
2:B:22:ASN:ND2	2:B:32:VAL:HG22	2.16	0.60
2:B:117:ILE:HA	2:B:126:LEU:CG	2.32	0.60
1:A:294:ILE:HD11	1:A:296:THR:HG23	1.82	0.59
1:A:320:PRO:HB2	1:A:384:CYS:SG	2.42	0.59
2:B:120:ARG:HH12	2:B:134:GLU:HB2	1.67	0.59
2:B:126:LEU:O	2:B:127:LYS:CG	2.51	0.59
2:B:135:THR:HG22	2:B:136:PRO:HD2	1.84	0.59
1:A:44:ARG:HB2	1:A:46:GLY:H	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:O	1:A:131:MET:HB3	2.01	0.59
1:A:253:ARG:HG2	1:A:384:CYS:CB	2.30	0.59
2:B:117:ILE:HD11	4:B:1040:HOH:O	2.02	0.59
1:A:31:LEU:HA	1:A:69:THR:HG21	1.84	0.59
1:A:181:SER:O	1:A:185:GLY:N	2.34	0.59
2:B:36:LEU:CD2	2:B:47:GLU:CG	2.81	0.59
2:B:64:LEU:HD12	2:B:68:LEU:HD11	1.85	0.59
1:A:355:LEU:HD13	1:A:364:MET:HE1	1.85	0.59
2:B:120:ARG:HH12	2:B:134:GLU:CB	2.16	0.59
2:B:116:LYS:O	2:B:127:LYS:N	2.35	0.58
2:B:39:ILE:HD11	2:B:88:PHE:O	2.03	0.58
1:A:186:ALA:O	1:A:187:ASN:HB2	2.04	0.58
2:B:78:GLU:O	2:B:79:GLY:C	2.42	0.58
1:A:206:SER:HB2	1:A:243:LYS:HE2	1.84	0.58
1:A:51:ILE:CG1	1:A:89:ILE:HG23	2.34	0.58
2:B:78:GLU:O	2:B:80:ARG:N	2.37	0.58
1:A:226:PRO:HB2	1:A:230:LEU:HD21	1.86	0.58
2:B:126:LEU:O	2:B:127:LYS:CE	2.51	0.58
1:A:179:PRO:HG3	2:B:8:TYR:CE2	2.39	0.58
1:A:221:ASN:C	1:A:222:LYS:HG3	2.25	0.58
2:B:117:ILE:CA	2:B:126:LEU:HG	2.34	0.58
1:A:143:ILE:HD11	1:A:167:ILE:HG21	1.85	0.57
1:A:123:ARG:CD	4:A:1101:HOH:O	2.53	0.57
1:A:273:ILE:HG12	1:A:294:ILE:HD13	1.87	0.57
1:A:35:TRP:CD1	1:A:56:ALA:HA	2.39	0.57
2:B:127:LYS:HB3	2:B:133:ALA:O	2.05	0.57
1:A:73:CYS:SG	1:A:75:TYR:HD1	2.28	0.57
2:B:80:ARG:HH11	2:B:80:ARG:CG	2.17	0.57
2:B:137:ILE:HG13	2:B:137:ILE:O	2.04	0.57
1:A:53:PHE:CG	1:A:291:LEU:HD13	2.40	0.57
1:A:123:ARG:HD2	4:A:1101:HOH:O	2.04	0.57
1:A:268:PRO:HD3	4:A:1116:HOH:O	2.04	0.56
1:A:18:GLY:H	1:A:129:HIS:CD2	2.23	0.56
1:A:255:GLY:HA3	1:A:267:GLU:O	2.05	0.56
2:B:68:LEU:O	2:B:71:ILE:O	2.23	0.56
1:A:261:HIS:HD1	1:A:261:HIS:N	2.03	0.56
2:B:22:ASN:ND2	2:B:32:VAL:CG2	2.68	0.56
1:A:341:GLN:C	1:A:341:GLN:CD	2.64	0.56
1:A:260:GLU:HG3	1:A:260:GLU:O	2.06	0.56
2:B:3:ILE:HD12	2:B:10:LYS:HB3	1.87	0.56
1:A:128:GLU:CD	1:A:337:VAL:HG12	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HB3	1:A:320:PRO:CD	2.36	0.56
2:B:37:VAL:HB	2:B:90:PRO:HG3	1.88	0.56
1:A:128:GLU:CD	1:A:337:VAL:CG1	2.75	0.56
2:B:75:GLY:CA	2:B:83:VAL:O	2.54	0.56
2:B:118:ILE:HG22	2:B:126:LEU:HA	1.88	0.55
1:A:327:ARG:HG3	1:A:328:LEU:N	2.13	0.55
1:A:160:TYR:CE1	1:A:177:ILE:HD12	2.42	0.55
1:A:253:ARG:HH21	1:A:322:VAL:H	1.50	0.55
2:B:16:TYR:HA	2:B:19:LEU:HG	1.88	0.55
1:A:263:ARG:CG	1:A:263:ARG:NH1	2.66	0.55
2:B:117:ILE:HD12	2:B:126:LEU:HD21	1.89	0.55
1:A:134:GLN:HA	1:A:171:VAL:CG2	2.37	0.55
1:A:226:PRO:HB2	1:A:230:LEU:HD11	1.88	0.55
2:B:125:PHE:CE1	2:B:136:PRO:HB3	2.42	0.55
2:B:29:ARG:CZ	2:B:29:ARG:CB	2.85	0.55
2:B:36:LEU:C	2:B:36:LEU:CD2	2.73	0.55
2:B:22:ASN:CB	2:B:29:ARG:O	2.44	0.55
1:A:253:ARG:CB	1:A:254:PRO:CD	2.84	0.55
1:A:350:ARG:O	1:A:351:LYS:HB2	2.07	0.55
2:B:117:ILE:HA	2:B:126:LEU:HG	1.88	0.55
1:A:325:ASP:O	1:A:326:LEU:HD13	2.08	0.54
2:B:8:TYR:CZ	2:B:12:LEU:HD13	2.42	0.54
2:B:58:ARG:HH22	2:B:115:THR:C	2.11	0.54
1:A:61:CYS:HA	1:A:80:THR:HG22	1.89	0.54
1:A:245:LYS:HG3	1:A:284:GLU:O	2.07	0.54
1:A:60:ARG:HB3	1:A:83:ILE:HD11	1.86	0.54
2:B:50:LYS:HG2	2:B:80:ARG:HB3	1.89	0.54
2:B:125:PHE:CZ	2:B:136:PRO:HB3	2.43	0.54
1:A:224:GLY:C	1:A:226:PRO:HD3	2.28	0.54
2:B:32:VAL:HG23	2:B:32:VAL:O	2.08	0.54
1:A:34:VAL:CG2	2:B:87:ARG:HB3	2.37	0.54
1:A:195:ILE:O	1:A:198:PHE:O	2.25	0.54
1:A:254:PRO:HD2	1:A:311:ASN:ND2	2.22	0.54
1:A:342:GLU:CG	1:A:397:ILE:HG21	2.34	0.54
2:B:31:GLU:O	2:B:33:PRO:HD3	2.08	0.54
1:A:318:LYS:C	1:A:319:LEU:HD12	2.27	0.53
1:A:225:THR:O	1:A:225:THR:CG2	2.57	0.53
1:A:256:VAL:HG23	1:A:269:ILE:CG2	2.34	0.53
2:B:117:ILE:CG1	2:B:126:LEU:HG	2.38	0.53
1:A:257:PRO:HG3	1:A:266:TYR:CD1	2.43	0.53
1:A:297:LYS:HB3	1:A:297:LYS:NZ	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HB3	1:A:386:GLU:OE1	2.09	0.53
2:B:109:VAL:HG21	2:B:133:ALA:CB	2.38	0.53
1:A:261:HIS:N	1:A:261:HIS:ND1	2.57	0.53
1:A:373:ASP:OD1	1:A:373:ASP:N	2.42	0.53
2:B:60:PRO:HD2	4:B:1025:HOH:O	2.08	0.53
1:A:95:GLU:HG2	4:A:1071:HOH:O	2.09	0.53
1:A:152:ASP:OD1	1:A:155:LYS:HD2	2.09	0.53
2:B:43:LYS:CB	2:B:43:LYS:NZ	2.72	0.53
2:B:126:LEU:O	2:B:127:LYS:HG2	2.09	0.53
1:A:51:ILE:HG13	1:A:89:ILE:HG23	1.90	0.53
2:B:20:PRO:O	2:B:24:LYS:CB	2.57	0.53
2:B:73:THR:HG21	2:B:88:PHE:HE2	1.73	0.52
1:A:158:GLU:O	1:A:162:GLN:HG3	2.09	0.52
2:B:105:VAL:HG12	2:B:105:VAL:O	2.09	0.52
1:A:253:ARG:HD2	1:A:254:PRO:N	2.24	0.52
1:A:163:ILE:O	1:A:167:ILE:HG12	2.10	0.52
1:A:321:PRO:HD2	1:A:385:ALA:O	2.09	0.52
1:A:217:SER:OG	1:A:306:ASP:HA	2.09	0.52
2:B:120:ARG:NH1	2:B:125:PHE:CD2	2.78	0.52
1:A:94:HIS:NE2	1:A:337:VAL:HG11	2.25	0.52
1:A:45:ARG:C	1:A:46:GLY:O	2.45	0.52
2:B:120:ARG:NH1	2:B:125:PHE:HD2	2.07	0.52
1:A:225:THR:O	1:A:227:PRO:HD3	2.10	0.52
1:A:269:ILE:HD11	1:A:298:LEU:CD2	2.40	0.52
1:A:146:ASN:OD1	1:A:147:LYS:N	2.42	0.51
2:B:117:ILE:CB	2:B:126:LEU:HG	2.41	0.51
2:B:126:LEU:HB2	2:B:137:ILE:HG12	1.92	0.51
2:B:50:LYS:HD2	2:B:80:ARG:CZ	2.39	0.51
2:B:50:LYS:CB	2:B:80:ARG:HB3	2.40	0.51
1:A:49:ILE:HG13	1:A:51:ILE:HG22	1.93	0.51
1:A:393:ILE:O	4:A:1128:HOH:O	2.19	0.51
1:A:269:ILE:HG13	1:A:270:THR:N	2.24	0.50
1:A:230:LEU:N	1:A:230:LEU:CD2	2.74	0.50
1:A:239:ILE:O	1:A:288:PRO:HB3	2.11	0.50
1:A:197:GLU:HG2	2:B:5:TYR:CE1	2.46	0.50
1:A:329:GLU:CD	1:A:408:ILE:HD12	2.31	0.50
2:B:118:ILE:HG23	2:B:125:PHE:O	2.10	0.50
1:A:36:THR:O	2:B:87:ARG:NH2	2.42	0.50
1:A:333:LEU:HD21	1:A:406:TYR:HD1	1.76	0.50
2:B:136:PRO:O	2:B:136:PRO:HG2	2.11	0.50
1:A:254:PRO:HD2	1:A:311:ASN:CG	2.33	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:HIS:HB3	2:B:26:HIS:ND1	2.27	0.50
2:B:49:PHE:HE1	2:B:63:LEU:HD22	1.76	0.50
2:B:64:LEU:HD12	2:B:68:LEU:CD1	2.42	0.50
1:A:70:SER:HB2	2:B:89:THR:CG2	2.42	0.49
1:A:139:LYS:CG	1:A:171:VAL:HG12	2.42	0.49
1:A:217:SER:C	1:A:218:PHE:CD1	2.86	0.49
1:A:346:GLU:O	1:A:395:ARG:NH1	2.44	0.49
1:A:266:TYR:HD2	1:A:382:PRO:HG2	1.77	0.49
1:A:149:GLU:HG2	1:A:150:LEU:HD13	1.94	0.49
1:A:344:ASN:ND2	4:A:1003:HOH:O	2.46	0.49
1:A:327:ARG:CG	1:A:410:LYS:HB2	2.40	0.49
2:B:64:LEU:HD11	2:B:68:LEU:HD11	1.93	0.49
2:B:127:LYS:HG3	2:B:133:ALA:O	2.13	0.48
2:B:22:ASN:O	2:B:28:SER:HB3	2.13	0.48
2:B:26:HIS:ND1	2:B:26:HIS:N	2.60	0.48
2:B:127:LYS:HE2	2:B:127:LYS:HA	1.95	0.48
2:B:21:GLU:HG2	4:B:1032:HOH:O	2.13	0.48
2:B:91:TYR:HA	2:B:94:ALA:HB3	1.94	0.48
2:B:126:LEU:O	2:B:127:LYS:HB2	2.14	0.48
2:B:71:ILE:HG22	2:B:72:ALA:N	2.29	0.48
1:A:45:ARG:O	1:A:50:LYS:HD2	2.14	0.48
1:A:230:LEU:N	1:A:230:LEU:HD23	2.28	0.47
2:B:127:LYS:HB2	2:B:134:GLU:HA	1.96	0.47
1:A:145:GLN:NE2	1:A:159:ASN:HB3	2.29	0.47
2:B:36:LEU:HD23	2:B:36:LEU:O	2.14	0.47
2:B:127:LYS:CG	2:B:134:GLU:HA	2.45	0.47
2:B:71:ILE:CG2	2:B:73:THR:OG1	2.62	0.47
1:A:48:THR:HG22	1:A:362:ARG:HB3	1.97	0.47
2:B:49:PHE:CE1	2:B:63:LEU:HD22	2.49	0.47
2:B:127:LYS:CE	2:B:127:LYS:HA	2.44	0.47
1:A:51:ILE:HG13	1:A:89:ILE:CG2	2.44	0.47
1:A:386:GLU:HB2	1:A:389:GLU:OE2	2.15	0.47
2:B:20:PRO:HB2	2:B:23:VAL:HG13	1.96	0.47
1:A:236:ASP:HA	1:A:292:VAL:O	2.15	0.47
1:A:404:ILE:N	4:A:1128:HOH:O	2.48	0.47
2:B:68:LEU:HD22	2:B:74:ALA:HA	1.96	0.47
1:A:220:VAL:HG23	1:A:220:VAL:O	2.15	0.47
1:A:350:ARG:CG	1:A:370:LEU:HD13	2.16	0.47
2:B:43:LYS:NZ	2:B:43:LYS:HB3	2.29	0.46
1:A:61:CYS:CA	1:A:80:THR:HG22	2.45	0.46
1:A:330:VAL:HG21	1:A:375:ILE:HG12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:VAL:O	2:B:105:VAL:CG1	2.62	0.46
1:A:44:ARG:HG2	1:A:52:GLY:HA2	1.97	0.46
1:A:49:ILE:HD12	1:A:100:THR:HG23	1.97	0.46
1:A:95:GLU:O	1:A:98:MET:HB2	2.15	0.46
1:A:329:GLU:OE2	1:A:408:ILE:HD12	2.16	0.46
1:A:371:GLY:HA3	1:A:374:GLU:OE1	2.15	0.46
1:A:74:PRO:HD2	1:A:75:TYR:CE1	2.51	0.46
1:A:253:ARG:NH2	1:A:322:VAL:H	2.14	0.46
1:A:396:GLN:O	1:A:397:ILE:HB	2.16	0.46
2:B:71:ILE:CG2	2:B:72:ALA:N	2.78	0.46
1:A:45:ARG:O	1:A:46:GLY:C	2.54	0.46
2:B:67:LEU:C	2:B:69:ARG:H	2.19	0.46
1:A:130:LEU:HD22	1:A:130:LEU:O	2.16	0.46
2:B:105:VAL:O	2:B:115:THR:CG2	2.62	0.46
2:B:112:SER:C	2:B:114:ASP:H	2.19	0.46
1:A:342:GLU:HA	1:A:397:ILE:HD13	1.98	0.46
1:A:348:ILE:CG2	1:A:367:VAL:HG21	2.45	0.46
1:A:117:ALA:HB2	1:A:145:GLN:HG2	1.98	0.46
2:B:118:ILE:HG22	2:B:126:LEU:CA	2.46	0.46
1:A:299:ASP:OD1	1:A:301:TYR:HB2	2.15	0.45
1:A:405:GLY:N	4:A:1128:HOH:O	2.27	0.45
2:B:59:ASP:OD1	2:B:59:ASP:N	2.49	0.45
1:A:366:LEU:O	1:A:368:THR:HG23	2.16	0.45
1:A:383:VAL:HG23	1:A:383:VAL:O	2.15	0.45
2:B:22:ASN:CG	2:B:32:VAL:HG21	2.36	0.45
2:B:67:LEU:C	2:B:69:ARG:N	2.70	0.45
1:A:250:ILE:HD12	1:A:313:VAL:HG11	1.99	0.45
1:A:330:VAL:HG23	1:A:375:ILE:HG12	1.98	0.45
1:A:45:ARG:HB2	1:A:50:LYS:HE3	1.98	0.45
1:A:334:GLU:O	1:A:334:GLU:HG3	2.16	0.45
1:A:346:GLU:O	1:A:395:ARG:NH2	2.44	0.45
2:B:125:PHE:C	2:B:126:LEU:CD1	2.82	0.45
1:A:266:TYR:CD2	1:A:382:PRO:HD2	2.52	0.45
1:A:349:LYS:NZ	1:A:349:LYS:CB	2.76	0.45
1:A:269:ILE:CD1	1:A:298:LEU:HD21	2.46	0.44
1:A:218:PHE:N	1:A:218:PHE:HD1	2.11	0.44
2:B:127:LYS:HE2	2:B:127:LYS:CA	2.47	0.44
1:A:216:ARG:HB3	1:A:218:PHE:CZ	2.53	0.44
2:B:64:LEU:O	2:B:68:LEU:HG	2.16	0.44
1:A:121:CYS:CB	1:A:122:PRO:HD3	2.33	0.44
1:A:403:LEU:CG	4:A:1128:HOH:O	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HD2	1:A:229:LYS:HA	1.38	0.44
2:B:48:ASN:O	2:B:51:ASP:HB2	2.18	0.44
1:A:49:ILE:HA	4:A:1124:HOH:O	2.18	0.44
1:A:219:ASP:CB	1:A:304:LYS:HG3	2.48	0.44
1:A:304:LYS:NZ	4:A:1050:HOH:O	2.51	0.44
2:B:43:LYS:HD3	2:B:83:VAL:HG22	2.00	0.44
1:A:147:LYS:HA	1:A:149:GLU:OE2	2.18	0.44
1:A:243:LYS:HD2	1:A:285:GLU:OE2	2.17	0.44
2:B:36:LEU:CD2	2:B:36:LEU:O	2.66	0.44
1:A:119:GLU:O	1:A:120:PRO:C	2.54	0.44
1:A:128:GLU:CG	1:A:337:VAL:HG12	2.48	0.44
1:A:355:LEU:HD13	1:A:364:MET:HE2	2.00	0.44
2:B:30:PHE:CD1	2:B:30:PHE:N	2.86	0.44
2:B:64:LEU:CD1	2:B:68:LEU:CD1	2.96	0.44
1:A:128:GLU:HG3	1:A:337:VAL:HG12	1.99	0.43
2:B:112:SER:HA	2:B:113:PRO:HD3	1.80	0.43
1:A:197:GLU:HB3	1:A:198:PHE:CD1	2.53	0.43
1:A:18:GLY:N	1:A:129:HIS:CD2	2.85	0.43
1:A:117:ALA:HB2	1:A:145:GLN:CG	2.48	0.43
2:B:73:THR:HG21	2:B:88:PHE:CE2	2.52	0.43
1:A:178:ILE:HA	1:A:179:PRO:HD3	1.66	0.43
2:B:36:LEU:HD21	2:B:47:GLU:CG	2.48	0.43
2:B:67:LEU:O	2:B:69:ARG:N	2.51	0.43
2:B:79:GLY:O	2:B:80:ARG:HG2	2.17	0.43
2:B:95:ASN:ND2	2:B:96:LYS:CE	2.73	0.43
1:A:397:ILE:O	1:A:397:ILE:CG2	2.61	0.43
2:B:58:ARG:HD2	2:B:58:ARG:HA	1.71	0.43
1:A:335:ARG:HG3	4:A:1090:HOH:O	2.18	0.43
2:B:22:ASN:CG	2:B:32:VAL:CG2	2.86	0.43
2:B:50:LYS:O	2:B:54:ASP:HB2	2.19	0.43
2:B:109:VAL:HG21	2:B:133:ALA:HB2	2.00	0.43
2:B:127:LYS:HE2	2:B:127:LYS:N	2.33	0.43
1:A:225:THR:O	1:A:225:THR:HG22	2.18	0.43
2:B:112:SER:C	2:B:114:ASP:N	2.72	0.43
1:A:205:ASP:OD1	1:A:207:ASN:HB2	2.18	0.43
1:A:251:GLU:OE1	1:A:316:PRO:HA	2.18	0.43
1:A:397:ILE:CD1	1:A:402:ARG:HD3	2.43	0.43
2:B:52:ILE:N	2:B:52:ILE:HD12	2.34	0.43
1:A:14:ILE:O	1:A:88:PHE:HA	2.19	0.43
1:A:70:SER:HB2	2:B:89:THR:HG21	2.00	0.43
1:A:229:LYS:HD3	4:A:1038:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:HG23	1:A:284:GLU:HA	2.01	0.42
1:A:260:GLU:C	1:A:262:GLY:O	2.57	0.42
1:A:261:HIS:C	1:A:262:GLY:O	2.57	0.42
1:A:299:ASP:OD1	1:A:301:TYR:CB	2.67	0.42
2:B:101:ILE:HA	2:B:105:VAL:HB	2.00	0.42
2:B:21:GLU:HB3	2:B:106:ILE:CD1	2.50	0.42
1:A:218:PHE:CE1	1:A:236:ASP:OD1	2.72	0.42
1:A:335:ARG:NH2	1:A:402:ARG:NH1	2.67	0.42
1:A:348:ILE:HD13	1:A:375:ILE:HD13	2.01	0.42
1:A:372:LYS:HE3	1:A:372:LYS:HB3	1.81	0.42
2:B:121:ASP:O	2:B:123:PHE:N	2.52	0.42
2:B:48:ASN:OD1	2:B:51:ASP:HB2	2.20	0.42
1:A:70:SER:OG	1:A:72:ILE:O	2.37	0.42
2:B:58:ARG:NH2	2:B:115:THR:C	2.73	0.42
1:A:70:SER:HA	1:A:71:PRO:HD3	1.79	0.42
1:A:47:ILE:CG2	1:A:48:THR:N	2.83	0.42
1:A:75:TYR:CD1	1:A:75:TYR:N	2.84	0.42
1:A:345:VAL:HG22	1:A:346:GLU:O	2.20	0.42
1:A:345:VAL:HG23	1:A:395:ARG:NH1	2.35	0.42
2:B:85:GLN:HE21	2:B:85:GLN:HB3	1.52	0.42
2:B:106:ILE:CG2	2:B:107:CYS:N	2.83	0.42
1:A:22:HIS:CG	1:A:116:ALA:H	2.37	0.42
1:A:334:GLU:O	1:A:334:GLU:CG	2.68	0.42
2:B:45:ILE:HG13	2:B:82:VAL:O	2.19	0.41
2:B:21:GLU:O	2:B:23:VAL:N	2.54	0.41
1:A:130:LEU:HD12	1:A:166:PHE:CZ	2.55	0.41
1:A:152:ASP:OD2	1:A:154:GLU:HB3	2.21	0.41
1:A:335:ARG:NE	1:A:403:LEU:O	2.53	0.41
2:B:11:LEU:O	2:B:15:ALA:HB2	2.21	0.41
2:B:36:LEU:HB3	2:B:48:ASN:HB2	2.02	0.41
1:A:57:GLU:OE2	1:A:82:PHE:CD2	2.73	0.41
1:A:60:ARG:HB2	1:A:83:ILE:CD1	2.43	0.41
1:A:221:ASN:C	1:A:222:LYS:CG	2.87	0.41
2:B:28:SER:O	2:B:30:PHE:CE2	2.73	0.41
2:B:139:HIS:HA	4:B:1051:HOH:O	2.21	0.41
1:A:228:GLU:HB2	1:A:229:LYS:H	1.35	0.41
1:A:320:PRO:CB	1:A:386:GLU:OE1	2.68	0.41
2:B:9:GLU:OE1	2:B:9:GLU:CA	2.68	0.41
2:B:126:LEU:CD1	2:B:126:LEU:N	2.83	0.41
1:A:121:CYS:CB	1:A:122:PRO:CD	2.97	0.41
1:A:234:VAL:HG13	1:A:294:ILE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:HB1	2:B:91:TYR:CZ	2.55	0.41
1:A:222:LYS:O	1:A:223:PRO:C	2.57	0.41
1:A:45:ARG:O	1:A:46:GLY:O	2.39	0.41
1:A:67:TYR:CE2	1:A:83:ILE:HD12	2.55	0.41
1:A:272:GLU:HB3	1:A:297:LYS:CG	2.50	0.41
2:B:95:ASN:HD22	2:B:96:LYS:CE	2.26	0.41
2:B:97:LEU:O	2:B:101:ILE:HG13	2.21	0.41
1:A:34:VAL:O	1:A:34:VAL:HG22	2.21	0.41
1:A:149:GLU:CB	2:B:19:LEU:CD1	2.99	0.41
1:A:117:ALA:HA	1:A:159:ASN:ND2	2.36	0.40
1:A:256:VAL:HA	1:A:257:PRO:HD3	1.74	0.40
1:A:35:TRP:CZ3	1:A:57:GLU:OE1	2.75	0.40
1:A:45:ARG:HD2	1:A:45:ARG:N	2.35	0.40
1:A:253:ARG:CG	1:A:384:CYS:SG	2.89	0.40
2:B:30:PHE:HE1	4:B:1027:HOH:O	2.03	0.40
2:B:71:ILE:HG22	2:B:73:THR:OG1	2.21	0.40
1:A:84:ARG:NH1	1:A:201:THR:H	2.19	0.40
1:A:123:ARG:HD3	4:A:1101:HOH:O	2.19	0.40
1:A:246:VAL:CG2	1:A:284:GLU:HA	2.52	0.40
2:B:52:ILE:HG22	2:B:56:LEU:HD12	2.03	0.40
1:A:181:SER:HB3	1:A:186:ALA:H	1.86	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	399/419 (95%)	360 (90%)	31 (8%)	8 (2%)	7 24
2	B	135/148 (91%)	118 (87%)	12 (9%)	5 (4%)	3 11
All	All	534/567 (94%)	478 (90%)	43 (8%)	13 (2%)	6 20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	THR
1	A	228	GLU
1	A	253	ARG
1	A	260	GLU
2	B	22	ASN
2	B	79	GLY
1	A	121	CYS
2	B	20	PRO
2	B	26	HIS
1	A	223	PRO
1	A	341	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	338/353 (96%)	284 (84%)	54 (16%)	2 7
2	B	121/132 (92%)	84 (69%)	37 (31%)	0 1
All	All	459/485 (95%)	368 (80%)	91 (20%)	1 4

All (91) 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	37	ASP
1	A	43	LEU
1	A	44	ARG
1	A	45	ARG
1	A	47	ILE
1	A	60	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	171	VAL
1	A	193	LYS
1	A	199	ILE
1	A	206	SER
1	A	218	PHE
1	A	220	VAL
1	A	223	PRO
1	A	230	LEU
1	A	231	VAL
1	A	236	ASP
1	A	252	ILE
1	A	253	ARG
1	A	258	TYR
1	A	261	HIS
1	A	263	ARG
1	A	264	ILE
1	A	269	ILE
1	A	287	TYR
1	A	294	ILE
1	A	297	LYS
1	A	325	ASP
1	A	326	LEU
1	A	327	ARG
1	A	334	GLU
1	A	335	ARG
1	A	336	VAL
1	A	337	VAL
1	A	340	GLU
1	A	341	GLN
1	A	342	GLU
1	A	349	LYS
1	A	372	LYS
1	A	373	ASP
1	A	374	GLU
1	A	376	GLU
1	A	381	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	411	GLU
1	A	412	LEU
2	B	3	ILE
2	B	5	TYR
2	B	9	GLU
2	B	19	LEU
2	B	23	VAL
2	B	24	LYS
2	B	26	HIS
2	B	27	LYS
2	B	29	ARG
2	B	30	PHE
2	B	31	GLU
2	B	36	LEU
2	B	43	LYS
2	B	46	ILE
2	B	50	LYS
2	B	58	ARG
2	B	59	ASP
2	B	63	LEU
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	84	LEU
2	B	85	GLN
2	B	109	VAL
2	B	115	THR
2	B	116	LYS
2	B	117	ILE
2	B	118	ILE
2	B	119	LYS
2	B	120	ARG
2	B	127	LYS
2	B	129	GLU
2	B	135	THR
2	B	138	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

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

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	403/419 (96%)	0.11	17 (4%) 36 26	25, 54, 95, 100	0
2	B	137/148 (92%)	0.56	12 (8%) 10 5	37, 68, 94, 99	0
All	All	540/567 (95%)	0.22	29 (5%) 25 17	25, 59, 95, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	5.3
2	B	26	HIS	5.2
1	A	349	LYS	5.2
1	A	229	LYS	4.9
2	B	125	PHE	4.7
1	A	43	LEU	4.2
2	B	30	PHE	4.0
1	A	253	ARG	3.9
1	A	263	ARG	3.9
2	B	139	HIS	3.8
1	A	121	CYS	3.8
1	A	258	TYR	3.8
1	A	44	ARG	3.7
2	B	120	ARG	3.6
1	A	259	GLU	3.5
1	A	341	GLN	3.4
2	B	85	GLN	3.3
2	B	137	ILE	3.3
2	B	25	HIS	3.1
2	B	22	ASN	2.8
2	B	29	ARG	2.7
1	A	45	ARG	2.7
1	A	269	ILE	2.7
1	A	48	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	345	VAL	2.3
2	B	126	LEU	2.3
2	B	15	ALA	2.3
1	A	230	LEU	2.2
1	A	262	GLY	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
3	ZN	B	1002	1/1	0.94	0.04	71,71,71,71	0
3	ZN	A	1001	1/1	0.97	0.08	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.