



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 3GJX / pdb_00003gix
Title : Crystal Structure of the Nuclear Export Complex CRM1-Snurportin1-RanGTP
Authors : Monecke, T.; Guettler, T.; Neumann, P.; Dickmanns, A.; Goerlich, D.; Ficner, R.
Deposited on : 2009-03-09
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

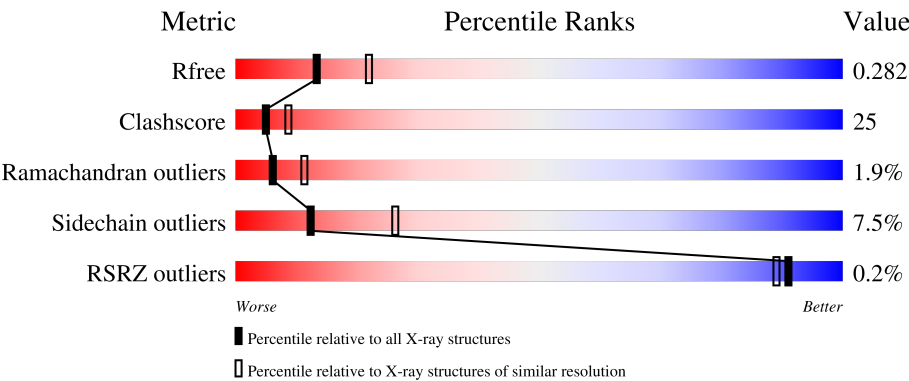
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	365	42%27%5%•25%
1	E	365	41%32%•24%
2	C	216	46%29%•21%
2	F	216	52%23%5%21%

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Mol	Chain	Length	Quality of chain
3	A	1073	54%37%6%
3	D	1073	% 53%38%6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25280 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 Snurportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	274	Total	C	N	O	S	0	2	0
			2222	1413	379	415	15			
1	E	279	Total	C	N	O	S	0	8	0
			2303	1466	394	427	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP O95149
B	-3	PRO	-	expression tag	UNP O95149
B	-2	LEU	-	expression tag	UNP O95149
B	-1	GLY	-	expression tag	UNP O95149
B	0	SER	-	expression tag	UNP O95149
E	-4	GLY	-	expression tag	UNP O95149
E	-3	PRO	-	expression tag	UNP O95149
E	-2	LEU	-	expression tag	UNP O95149
E	-1	GLY	-	expression tag	UNP O95149
E	0	SER	-	expression tag	UNP O95149

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	S	0	1	0
			1399	910	246	238	5			
2	F	171	Total	C	N	O	S	0	0	0
			1389	904	243	237	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	engineered mutation	UNP P62826
F	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1041	Total	C	N	O	S	0	5	0
			8456	5424	1421	1557	54			
3	D	1041	Total	C	N	O	S	0	8	0
			8483	5438	1427	1564	54			

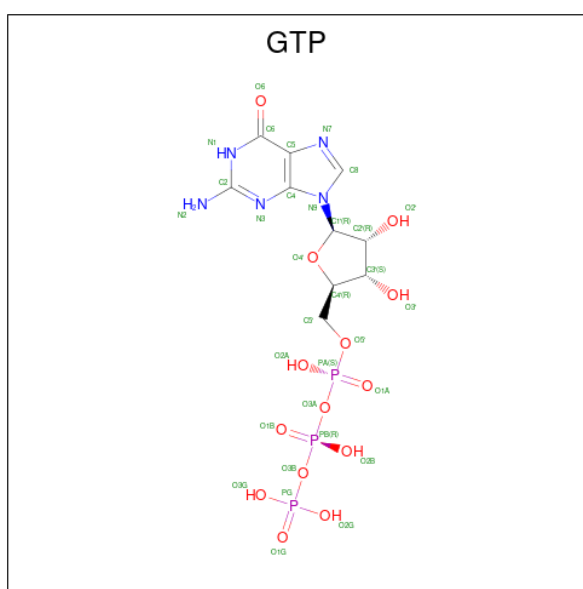
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6P5F9
A	0	SER	-	expression tag	UNP Q6P5F9
D	-1	GLY	-	expression tag	UNP Q6P5F9
D	0	SER	-	expression tag	UNP Q6P5F9

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	E	1	Total	Na	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Cl	0	0
			1	1		

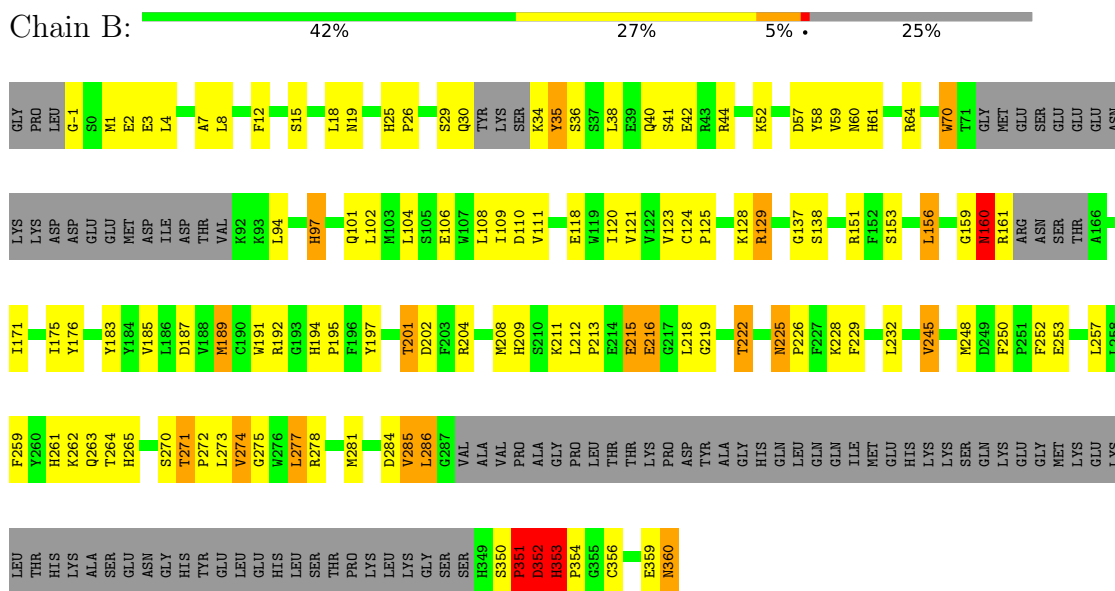
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	134	Total	O	0	0
			134	134		
8	C	58	Total	O	0	0
			58	58		
8	A	258	Total	O	0	0
			258	258		
8	E	130	Total	O	0	0
			130	130		
8	F	46	Total	O	0	0
			46	46		
8	D	333	Total	O	0	0
			333	333		

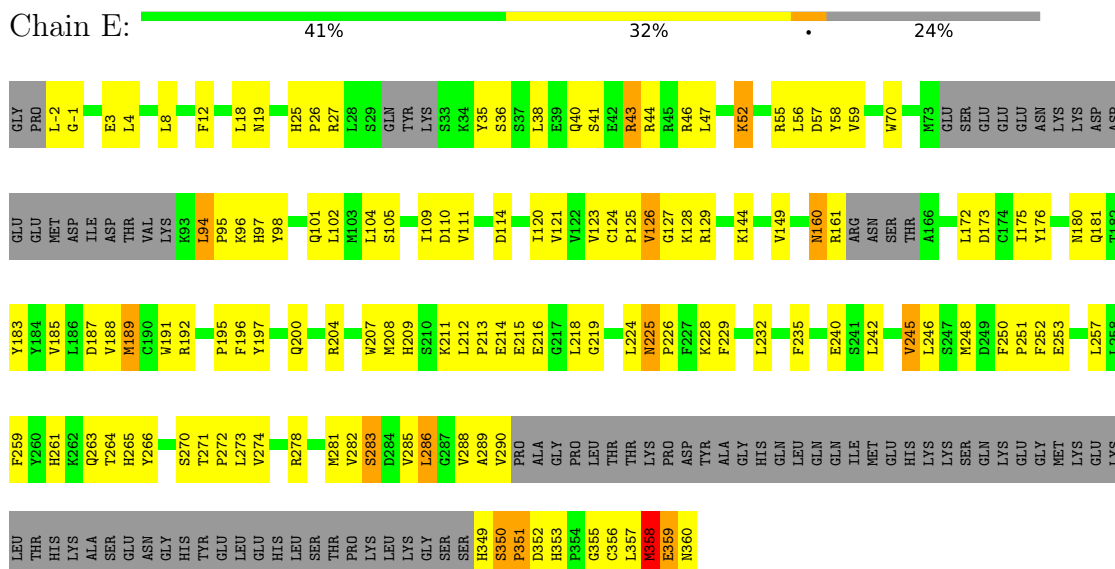
3 Residue-property plots

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.

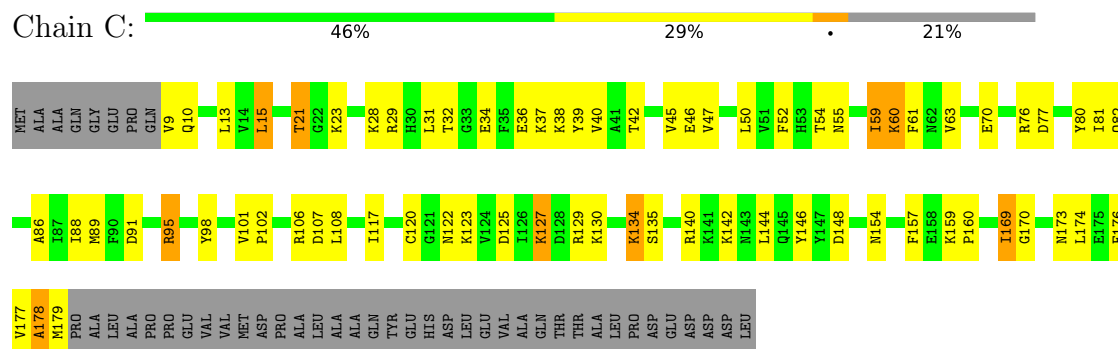
• Molecule 1: Snurportin-1



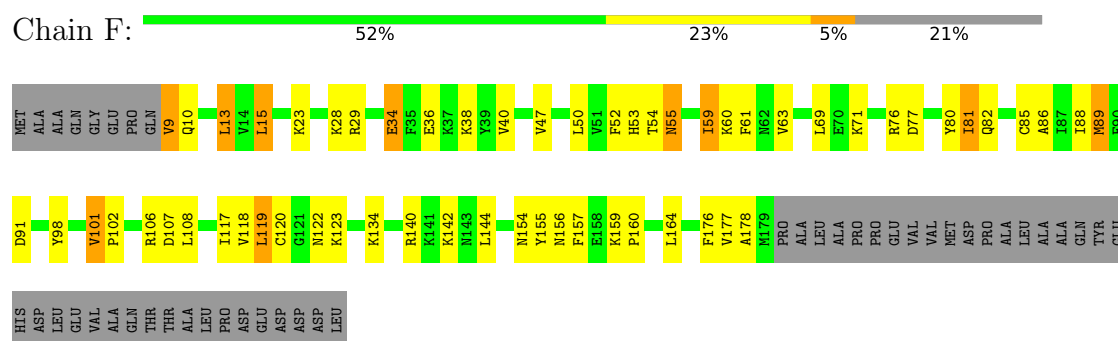
• Molecule 1: Snurportin-1



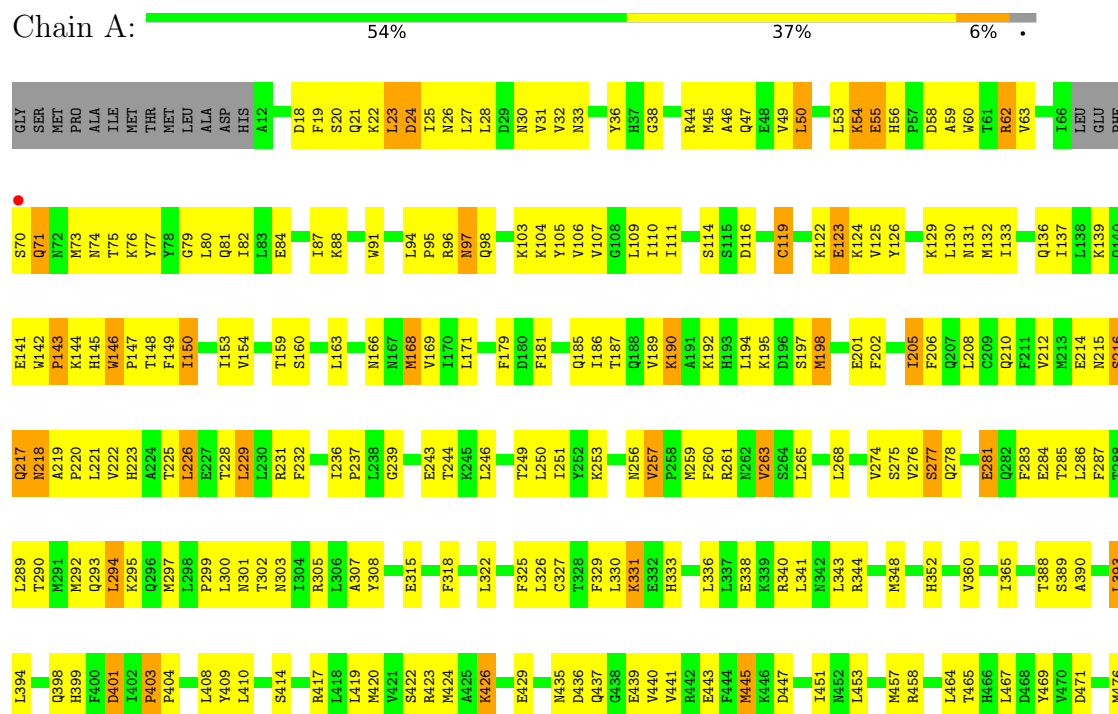
- Molecule 2: GTP-binding nuclear protein Ran

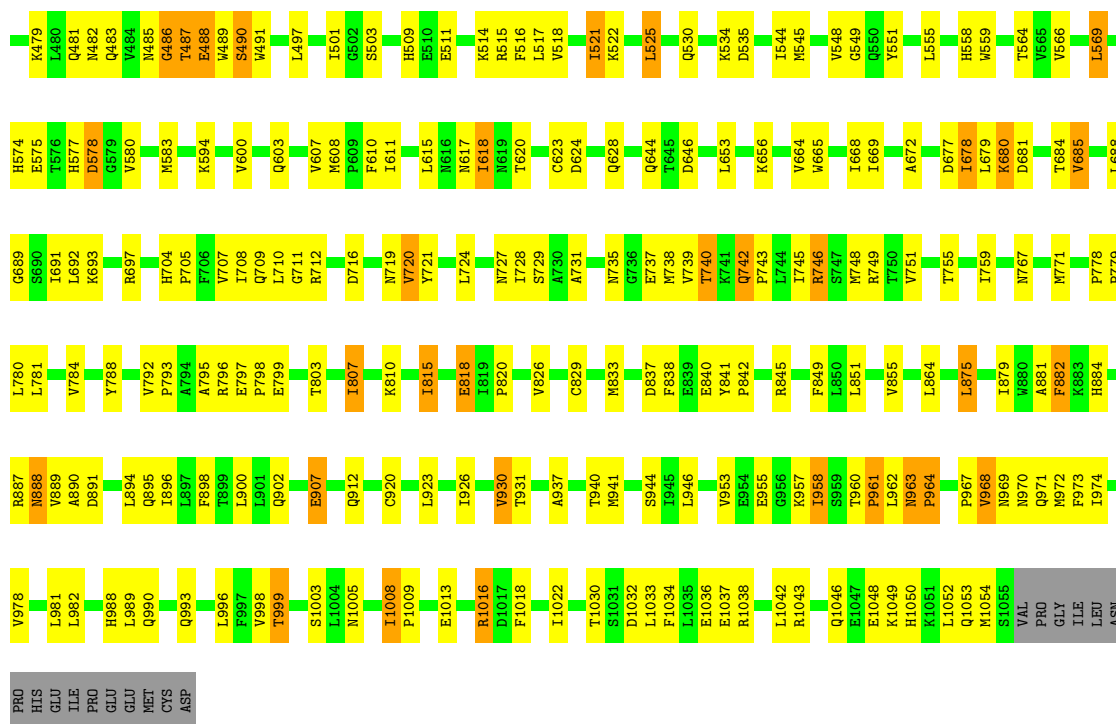


- Molecule 2: GTP-binding nuclear protein Ran

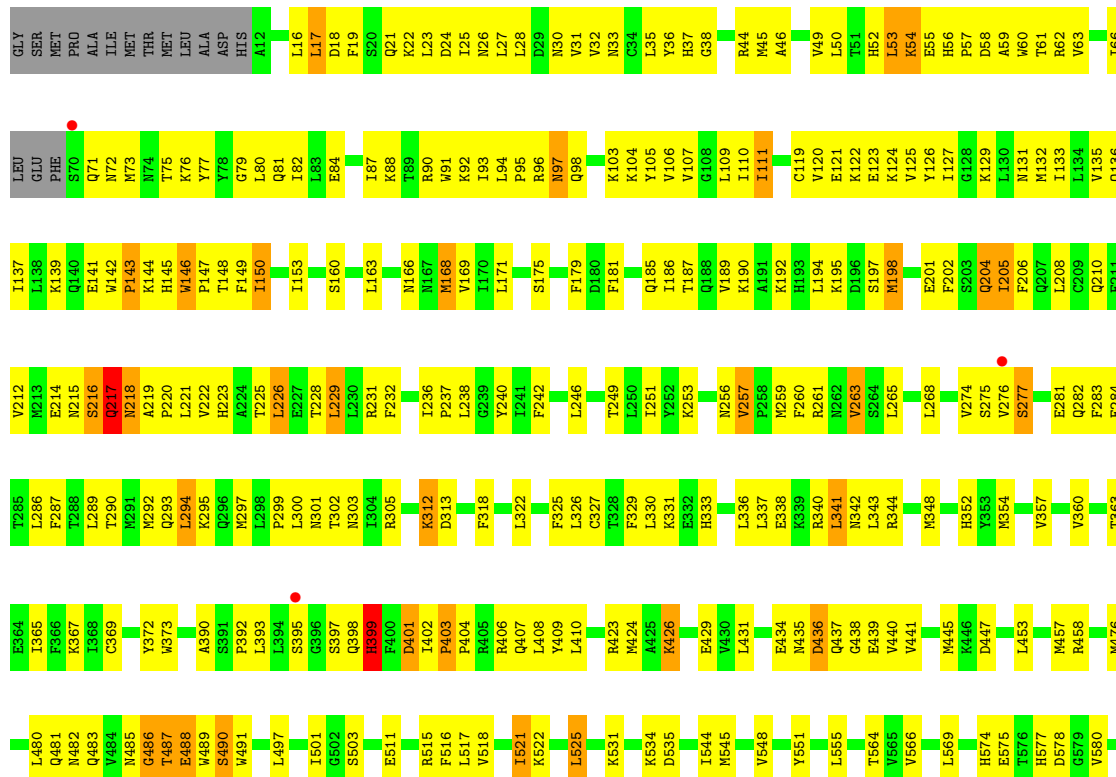


- Molecule 3: Exportin-1





• Molecule 3: Exportin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.17Å 225.74Å 163.45Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	38.84 – 2.50 38.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.84-2.50) 86.9 (38.84-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.51Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, R_{free}	0.244 , 0.281 0.246 , 0.282	Depositor DCC
R_{free} test set	8606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25280	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, GTP, 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	B	0.53	0/2283	1.12	17/3090 (0.6%)
1	E	0.51	0/2364	0.95	11/3202 (0.3%)
2	C	0.45	0/1434	0.78	0/1936
2	F	0.44	0/1423	0.85	2/1921 (0.1%)
3	A	0.47	0/8628	0.84	8/11687 (0.1%)
3	D	0.47	0/8656	0.83	11/11724 (0.1%)
All	All	0.48	0/24788	0.87	49/33560 (0.1%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASP	N-CA-C	14.40	128.97	110.24
1	B	351	PRO	CA-N-CD	-11.30	96.18	112.00
1	B	350	SER	CA-C-N	10.38	132.81	119.84
1	B	350	SER	C-N-CA	10.38	132.81	119.84
3	A	488	GLU	N-CA-C	-9.45	101.95	112.72
3	D	488	GLU	N-CA-C	-9.44	101.96	112.72
1	B	353	HIS	CA-C-N	8.56	128.32	119.76
1	B	353	HIS	C-N-CA	8.56	128.32	119.76
1	B	70	TRP	N-CA-C	8.27	122.92	109.85
2	F	76	ARG	CB-CA-C	-8.10	107.22	116.54
1	B	351	PRO	CA-C-N	8.03	132.62	120.82
1	B	351	PRO	C-N-CA	8.03	132.62	120.82
1	E	94	LEU	CA-C-N	7.93	128.42	119.93
1	E	94	LEU	C-N-CA	7.93	128.42	119.93
3	A	38	GLY	N-CA-C	7.75	117.27	110.21
3	D	38	GLY	N-CA-C	7.68	117.20	110.21
3	A	742	GLN	CA-C-N	6.79	128.32	119.84
3	A	742	GLN	C-N-CA	6.79	128.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	742	GLN	CA-C-N	6.56	128.04	119.84
3	D	742	GLN	C-N-CA	6.56	128.04	119.84
1	E	357	LEU	N-CA-C	6.46	120.35	109.76
1	B	215	GLU	N-CA-C	-6.29	97.00	108.02
1	E	350	SER	CA-C-N	6.18	127.56	119.84
1	E	350	SER	C-N-CA	6.18	127.56	119.84
3	D	680	LYS	N-CA-C	-5.92	105.80	114.39
1	E	55	ARG	N-CA-C	-5.83	107.16	114.56
1	E	111	VAL	CB-CA-C	-5.74	104.08	110.68
1	B	160	ASN	CA-CB-CG	-5.72	106.88	112.60
1	E	225	ASN	CA-C-N	5.65	125.50	119.28
1	E	225	ASN	C-N-CA	5.65	125.50	119.28
1	B	160	ASN	CA-C-N	5.57	131.72	121.70
1	B	160	ASN	C-N-CA	5.57	131.72	121.70
1	B	350	SER	N-CA-C	5.49	118.43	110.14
3	A	680	LYS	N-CA-C	-5.41	106.55	114.39
1	E	160	ASN	N-CA-C	5.38	117.58	109.41
1	B	225	ASN	CA-C-N	5.35	125.16	119.28
1	B	225	ASN	C-N-CA	5.35	125.16	119.28
3	A	784	VAL	N-CA-C	5.33	115.83	111.62
1	B	160	ASN	N-CA-C	5.27	122.03	110.80
2	F	101	VAL	CB-CA-C	-5.21	108.75	113.70
1	E	358	MET	N-CA-C	5.10	121.66	110.80
3	D	403	PRO	CA-C-N	5.05	124.66	119.05
3	D	403	PRO	C-N-CA	5.05	124.66	119.05
3	D	986	PHE	CA-C-N	5.05	124.84	119.28
3	D	986	PHE	C-N-CA	5.05	124.84	119.28
3	A	403	PRO	CA-C-N	5.04	124.65	119.05
3	A	403	PRO	C-N-CA	5.04	124.65	119.05
3	D	783	ALA	CA-C-N	-5.04	117.82	123.16
3	D	783	ALA	C-N-CA	-5.04	117.82	123.16

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	B	2222	0	2151	113	0
1	E	2303	0	2223	116	0
2	C	1399	0	1425	62	0
2	F	1389	0	1419	55	0
3	A	8456	0	8516	447	0
3	D	8483	0	8530	448	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	32	0	12	3	0
5	F	32	0	12	2	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
7	E	1	0	0	1	0
8	A	258	0	0	15	0
8	B	134	0	0	8	0
8	C	58	0	0	3	0
8	D	333	0	0	9	0
8	E	130	0	0	7	0
8	F	46	0	0	2	0
All	All	25280	0	24288	1214	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 25.

All (1214) 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)
3:A:476:MET:HE3	3:A:501:ILE:HG12	1.21	1.16
3:D:476:MET:HE3	3:D:501:ILE:HG12	1.23	1.13
2:F:54:THR:HG22	2:F:176:PHE:HB3	1.19	1.11
3:D:33:ASN:HB2	3:D:44:ARG:HG3	1.33	1.09
3:A:1008:ILE:HG23	3:A:1009:PRO:HD3	1.35	1.07
1:E:350:SER:HB3	1:E:351:PRO:HD2	1.37	1.05
1:E:351:PRO:HB3	7:E:362:CL:CL	1.97	1.01
3:A:256:ASN:HB3	3:A:293:GLN:HE21	1.22	1.00
3:D:426:LYS:H	3:D:426:LYS:HD2	1.25	0.99
3:D:131:ASN:HD21	3:D:166:ASN:HD21	1.07	0.98
3:D:960:THR:HG23	3:D:968:VAL:HG11	1.41	0.98
3:D:1008:ILE:HG23	3:D:1009:PRO:HD3	1.42	0.97
3:A:33:ASN:HB2	3:A:44:ARG:HG3	1.47	0.97
3:A:426:LYS:H	3:A:426:LYS:HD2	1.28	0.96
3:A:962:LEU:HD23	3:A:968:VAL:HG21	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:434:GLU:HG3	3:D:440:VAL:HG12	1.46	0.95
2:F:29:ARG:HB3	2:F:157:PHE:HZ	1.31	0.95
3:A:131:ASN:HD21	3:A:166:ASN:HD21	1.09	0.94
3:A:1016:ARG:HG2	3:A:1016:ARG:HH11	1.30	0.94
3:D:46:ALA:O	3:D:50:LEU:HB2	1.66	0.94
3:D:62:ARG:HB3	3:D:66:ILE:HD11	1.51	0.93
2:C:29:ARG:HB3	2:C:157:PHE:HZ	1.34	0.92
3:A:807:ILE:HD11	3:A:815:ILE:HD12	1.50	0.92
2:C:21:THR:HG23	2:C:89:MET:HG2	1.48	0.92
3:A:144:LYS:HG3	3:A:145:HIS:CD2	2.05	0.91
1:B:159:GLY:O	1:B:160:ASN:HB2	1.69	0.91
3:D:53:LEU:HD12	3:D:54:LYS:H	1.35	0.91
3:D:340:ARG:HG2	3:D:342:ASN:OD1	1.71	0.91
3:A:141:GLU:HA	3:A:144:LYS:HE2	1.54	0.90
1:E:43:ARG:HD2	1:E:46:ARG:HH12	1.35	0.89
3:A:46:ALA:O	3:A:50:LEU:HB2	1.72	0.88
3:D:770:GLN:HB3	8:D:1380:HOH:O	1.72	0.88
3:D:79:GLY:O	3:D:82:ILE:HG22	1.74	0.88
1:E:52[A]:LYS:HE3	1:E:265:HIS:H	1.39	0.87
2:C:134:LYS:HE3	2:C:135:SER:OG	1.75	0.86
3:D:63:VAL:HA	3:D:76:LYS:HG2	1.54	0.86
3:A:62:ARG:HH11	3:A:79:GLY:HA2	1.41	0.86
3:A:740:THR:HA	3:A:745[B]:ILE:HD13	1.58	0.86
3:A:53:LEU:HD12	3:A:54:LYS:H	1.41	0.85
2:F:29:ARG:HB3	2:F:157:PHE:CZ	2.11	0.85
3:A:393:LEU:HD22	3:A:398:GLN:HA	1.55	0.85
3:A:990:GLN:H	3:A:993:GLN:HE21	1.24	0.85
2:C:29:ARG:HB3	2:C:157:PHE:CZ	2.12	0.84
3:A:62:ARG:NH1	3:A:79:GLY:HA2	1.93	0.84
1:B:52:LYS:HE3	1:B:264:THR:HA	1.57	0.84
1:E:43:ARG:HD2	1:E:46:ARG:NH1	1.92	0.83
3:A:451:ILE:HG12	8:A:1203:HOH:O	1.78	0.82
3:D:393:LEU:HD12	3:D:395:SER:H	1.44	0.82
3:D:990:GLN:H	3:D:993:GLN:HE21	1.27	0.82
1:B:285:VAL:HG12	1:B:286:LEU:HD12	1.62	0.82
1:E:200:GLN:HG2	8:E:497:HOH:O	1.80	0.80
1:B:38:LEU:HG	1:B:40:GLN:H	1.46	0.80
3:A:1048:GLU:HG3	3:A:1052:LEU:HG	1.63	0.80
3:A:30:ASN:ND2	3:A:47:GLN:HE22	1.80	0.79
3:D:476:MET:HE2	3:D:516:PHE:HZ	1.46	0.79
1:B:156:LEU:HD13	1:B:218:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:LEU:HD23	3:A:95:PRO:HD2	1.65	0.79
3:D:476:MET:HE3	3:D:501:ILE:CG1	2.09	0.79
3:D:426:LYS:H	3:D:426:LYS:CD	1.94	0.79
3:A:276:VAL:HG21	3:A:336:LEU:HD22	1.64	0.79
1:B:264:THR:HG22	1:B:265:HIS:O	1.84	0.78
3:D:23:LEU:HD23	3:D:26:ASN:HB2	1.66	0.78
3:D:276:VAL:HG21	3:D:336:LEU:HD22	1.65	0.78
1:B:108:LEU:HB3	1:B:277:LEU:HD13	1.66	0.78
3:A:214:GLU:HG3	3:A:215:ASN:ND2	2.00	0.77
3:A:476:MET:HE3	3:A:501:ILE:CG1	2.09	0.77
3:A:962:LEU:HB2	3:A:973:PHE:CD2	2.19	0.77
3:A:509[B]:HIS:HD2	3:A:511:GLU:H	1.33	0.77
3:A:107:VAL:O	3:A:111:ILE:HG12	1.85	0.77
3:D:214:GLU:HG3	3:D:215:ASN:ND2	2.00	0.77
3:D:781:LEU:HD11	3:D:821:GLN:HG3	1.67	0.77
3:D:962:LEU:HB2	3:D:973:PHE:CD2	2.20	0.76
3:A:32:VAL:HG22	3:A:71:GLN:HG2	1.66	0.76
1:E:38:LEU:HG	1:E:40:GLN:H	1.48	0.76
3:A:990:GLN:HG3	3:A:993:GLN:HG3	1.68	0.76
1:B:102:LEU:HD13	1:B:129:ARG:HH11	1.51	0.76
3:A:289:LEU:O	3:A:292:MET:HG3	1.84	0.76
3:A:426:LYS:H	3:A:426:LYS:CD	1.98	0.76
3:D:990:GLN:HG3	3:D:993:GLN:HG3	1.68	0.75
1:B:359:GLU:HG2	8:B:494:HOH:O	1.84	0.75
3:D:392:PRO:HA	3:D:399:HIS:NE2	2.02	0.75
3:A:704:HIS:CD2	3:A:767[B]:ASN:H	2.05	0.74
1:B:102:LEU:HB3	1:B:129:ARG:NH1	2.02	0.74
3:A:55:GLU:HG2	3:A:56:HIS:H	1.52	0.74
3:A:476:MET:CE	3:A:501:ILE:HG12	2.12	0.74
2:F:54:THR:CG2	2:F:176:PHE:HB3	2.10	0.74
3:D:53:LEU:HD12	3:D:54:LYS:N	2.02	0.73
3:D:489:TRP:CD1	3:D:531:LYS:HZ1	2.07	0.73
3:D:56:HIS:CG	3:D:56:HIS:O	2.41	0.73
3:D:962:LEU:C	3:D:964:PRO:HD3	2.13	0.73
3:D:1033:LEU:HD12	3:D:1035:LEU:HD11	1.71	0.73
3:D:476:MET:CE	3:D:501:ILE:HG12	2.12	0.73
3:A:56:HIS:CG	3:A:56:HIS:O	2.42	0.72
3:A:476:MET:HE2	3:A:516:PHE:HZ	1.54	0.72
3:A:116:ASP:O	3:A:119:CYS:HB3	1.90	0.72
2:C:95:ARG:HD2	2:C:130:LYS:HB3	1.71	0.72
3:A:888:ASN:ND2	3:A:889:VAL:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:341:LEU:HD23	3:D:344:ARG:HD2	1.70	0.72
3:D:798:PRO:HG3	3:D:844:HIS:CE1	2.24	0.72
3:A:97:ASN:H	3:A:97:ASN:ND2	1.87	0.72
3:D:678:ILE:HD12	3:D:679:LEU:H	1.55	0.72
3:A:509[B]:HIS:CD2	3:A:511:GLU:HB3	2.24	0.71
3:A:665:TRP:O	3:A:669:ILE:HG12	1.88	0.71
3:A:509[B]:HIS:CD2	3:A:511:GLU:H	2.07	0.71
3:A:704:HIS:CD2	3:A:767[A]:ASN:H	2.09	0.71
3:D:738:MET:HG3	8:D:1269:HOH:O	1.90	0.71
3:A:739:VAL:O	3:A:745[B]:ILE:HG21	1.90	0.71
3:D:32:VAL:O	3:D:36:TYR:HD2	1.72	0.71
3:D:434:GLU:HG3	3:D:440:VAL:CG1	2.19	0.71
3:A:20:SER:HB2	3:A:22:LYS:HG3	1.72	0.71
3:D:144:LYS:HG3	3:D:145[A]:HIS:CD2	2.26	0.71
3:A:32:VAL:O	3:A:36:TYR:HD2	1.73	0.70
3:D:476:MET:HE2	3:D:516:PHE:CZ	2.24	0.70
3:D:888:ASN:ND2	3:D:889:VAL:H	1.89	0.70
3:A:1043:ARG:NH1	3:A:1046:GLN:HG2	2.06	0.70
1:B:160:ASN:CG	1:B:161:ARG:H	1.99	0.70
3:A:249:THR:O	3:A:253:LYS:HB2	1.90	0.70
3:D:672:ALA:HA	3:D:678:ILE:HD11	1.72	0.70
2:C:21:THR:HG22	2:C:23:LYS:HG3	1.72	0.70
3:D:312:LYS:HE3	3:D:312:LYS:HA	1.73	0.70
3:A:179:PHE:CE1	3:A:195:LYS:HG2	2.25	0.70
3:D:28:LEU:HD11	3:D:66:ILE:HG23	1.73	0.70
3:D:131:ASN:ND2	3:D:166:ASN:HD21	1.85	0.70
3:A:672:ALA:HA	3:A:678:ILE:HD11	1.72	0.70
3:D:249:THR:O	3:D:253:LYS:HB2	1.90	0.69
3:D:665:TRP:O	3:D:669:ILE:HG12	1.90	0.69
3:D:179:PHE:HE1	3:D:195:LYS:HE2	1.58	0.69
3:A:71:GLN:HA	3:A:74:ASN:OD1	1.92	0.69
3:A:226:LEU:HD23	3:A:263:VAL:HB	1.75	0.69
3:D:58:ASP:OD1	3:D:61:THR:HB	1.92	0.69
1:E:70:TRP:CE3	1:E:96:LYS:O	2.45	0.69
3:D:544:ILE:HG22	3:D:545:MET:HE2	1.73	0.69
1:B:159:GLY:O	1:B:160:ASN:CB	2.40	0.69
3:A:803:THR:O	3:A:807:ILE:HG23	1.92	0.69
3:D:957:LYS:NZ	3:D:961:PRO:HB3	2.07	0.69
2:C:70:GLU:O	2:C:76:ARG:NH2	2.26	0.69
3:A:53:LEU:HD12	3:A:54:LYS:N	2.06	0.69
3:D:141:GLU:HA	3:D:144:LYS:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:HIS:CD2	3:D:767:ASN:H	2.11	0.69
2:C:169:ILE:HG22	2:C:170:GLY:H	1.58	0.68
3:A:957:LYS:NZ	3:A:961:PRO:HB3	2.07	0.68
3:A:179:PHE:HE1	3:A:195:LYS:HE2	1.59	0.68
3:A:300:LEU:O	3:A:352:HIS:HE1	1.76	0.68
3:A:205:ILE:HD11	3:A:232:PHE:CZ	2.28	0.68
3:A:1016:ARG:HG2	3:A:1016:ARG:NH1	1.98	0.68
3:D:97:ASN:H	3:D:97:ASN:ND2	1.89	0.68
3:D:737[A]:GLU:O	3:D:740:THR:HB	1.93	0.68
3:D:759:ILE:HD13	3:D:780:LEU:HD21	1.76	0.68
3:A:399:HIS:HD2	3:A:401:ASP:HB2	1.58	0.68
3:A:704:HIS:HD2	3:A:767[B]:ASN:H	1.38	0.68
3:A:737:GLU:O	3:A:740:THR:HB	1.94	0.68
1:B:261:HIS:HD2	1:B:263:GLN:H	1.40	0.68
3:A:887:ARG:HD3	3:A:937:ALA:HB3	1.76	0.68
1:E:105:SER:HA	1:E:274:VAL:HG13	1.76	0.68
3:A:28:LEU:O	3:A:32:VAL:HG23	1.94	0.68
3:D:300:LEU:O	3:D:352:HIS:HE1	1.77	0.67
3:A:678:ILE:C	3:A:680:LYS:H	2.02	0.67
3:A:815:ILE:HG12	3:A:818:GLU:HG2	1.76	0.67
3:D:22:LYS:HG2	3:D:58:ASP:CG	2.19	0.67
2:C:38:LYS:HG2	3:A:842:PRO:HG3	1.76	0.67
1:E:43:ARG:CD	1:E:46:ARG:HH12	2.07	0.67
1:E:123:VAL:HG21	1:E:250:PHE:CZ	2.29	0.67
3:D:251:ILE:HG21	3:D:289:LEU:HB3	1.76	0.67
3:D:678:ILE:C	3:D:680:LYS:H	2.02	0.67
3:A:476:MET:HE2	3:A:516:PHE:CZ	2.29	0.67
3:A:962:LEU:HD13	3:A:973:PHE:HE2	1.60	0.67
3:D:226:LEU:HD23	3:D:263:VAL:HB	1.76	0.67
3:D:1043:ARG:NH1	3:D:1046:GLN:HG2	2.09	0.67
3:A:759:ILE:HD13	3:A:780:LEU:HD21	1.77	0.67
3:D:815:ILE:HG12	3:D:818:GLU:HG2	1.77	0.67
2:F:106:ARG:HD3	3:D:181:PHE:CE2	2.30	0.67
1:B:222:THR:HG22	1:B:225:ASN:H	1.59	0.67
2:C:21:THR:CG2	2:C:89:MET:HG2	2.24	0.67
3:A:131:ASN:ND2	3:A:166:ASN:HD21	1.87	0.67
1:E:52[A]:LYS:CE	1:E:265:HIS:H	2.08	0.66
1:E:278:ARG:HG2	1:E:281:MET:HE3	1.77	0.66
3:D:179:PHE:CE1	3:D:195:LYS:HG2	2.29	0.66
3:D:678:ILE:HD12	3:D:679:LEU:N	2.09	0.66
1:B:176:TYR:HB2	1:B:183:TYR:CE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:63:VAL:HA	3:A:76:LYS:HG2	1.76	0.66
3:D:482:ASN:HB3	3:D:488:GLU:HB2	1.76	0.66
3:D:485:ASN:C	3:D:487:THR:H	2.04	0.66
3:D:737[B]:GLU:O	3:D:740:THR:HB	1.94	0.66
1:E:176:TYR:HB2	1:E:183:TYR:CE1	2.29	0.66
2:C:37:LYS:HE3	8:A:1199:HOH:O	1.96	0.66
3:A:972:MET:HE2	3:A:972:MET:HA	1.76	0.66
1:E:207:TRP:HB3	8:E:492:HOH:O	1.95	0.66
1:E:160:ASN:O	1:E:161:ARG:HG2	1.96	0.66
3:D:435:ASN:ND2	3:D:439:GLU:HB2	2.09	0.66
3:D:887:ARG:HD3	3:D:937:ALA:HB3	1.78	0.66
3:A:482:ASN:HB3	3:A:488:GLU:HB2	1.77	0.66
3:A:388:THR:HG22	3:A:399:HIS:HE2	1.61	0.66
3:D:434:GLU:CG	3:D:440:VAL:HG12	2.25	0.66
3:D:206:PHE:CE1	3:D:240:TYR:HB3	2.31	0.66
3:D:548:VAL:HG13	3:D:555:LEU:HD21	1.78	0.66
3:D:926:ILE:HG21	3:D:946:LEU:HD11	1.77	0.66
3:A:962:LEU:HD22	3:A:968:VAL:HG11	1.77	0.65
3:D:202:PHE:O	3:D:205:ILE:HG12	1.96	0.65
1:B:4:LEU:HD11	3:A:521:ILE:HG13	1.78	0.65
3:A:962:LEU:C	3:A:964:PRO:HD3	2.22	0.65
3:A:485:ASN:C	3:A:487:THR:H	2.05	0.65
3:A:887:ARG:HH21	3:A:891:ASP:HB3	1.61	0.65
3:A:729:SER:OG	3:A:792:VAL:HG22	1.97	0.65
3:D:28:LEU:O	3:D:32:VAL:HG23	1.96	0.65
2:C:55:ASN:OD1	2:C:174:LEU:HD12	1.97	0.65
1:E:127:GLY:HA2	8:E:549:HOH:O	1.97	0.65
3:D:33:ASN:HB2	3:D:44:ARG:CG	2.18	0.65
1:E:95:PRO:HB2	1:E:101:GLN:NE2	2.12	0.65
3:A:171:LEU:HD13	3:A:205:ILE:HD12	1.79	0.65
2:C:106:ARG:HD3	3:A:181:PHE:CE2	2.32	0.64
3:D:489:TRP:CG	3:D:531:LYS:HZ1	2.15	0.64
3:D:489:TRP:O	3:D:490:SER:HB3	1.97	0.64
3:A:704:HIS:HD2	3:A:767[A]:ASN:H	1.42	0.64
1:B:18:LEU:HA	1:B:36:SER:O	1.97	0.64
3:A:62:ARG:HH12	3:A:82:ILE:HG13	1.63	0.64
1:E:261:HIS:HD2	1:E:263:GLN:H	1.44	0.64
3:D:52:HIS:ND1	3:D:82:ILE:HD12	2.12	0.64
3:D:201:GLU:O	3:D:204:GLN:HG3	1.97	0.64
3:A:437:GLN:HG2	3:A:746:ARG:HG2	1.79	0.64
3:D:972:MET:HE2	3:D:972:MET:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HD11	3:D:521:ILE:HG13	1.78	0.64
3:A:678:ILE:HD12	3:A:679:LEU:N	2.12	0.64
1:B:123:VAL:HG21	1:B:250:PHE:CZ	2.33	0.64
3:D:210:GLN:O	3:D:214:GLU:HG2	1.97	0.64
3:A:146:TRP:CE3	3:A:149:PHE:HB2	2.33	0.63
3:D:887:ARG:HH21	3:D:891:ASP:HB3	1.63	0.63
1:B:278:ARG:HG2	1:B:281:MET:HE3	1.81	0.63
3:A:548:VAL:HG13	3:A:555:LEU:HD21	1.80	0.63
3:A:677:ASP:O	3:A:680:LYS:HB3	1.98	0.63
3:D:677:ASP:O	3:D:680:LYS:HB3	1.98	0.63
3:A:30:ASN:HD22	3:A:47:GLN:HE22	1.45	0.63
3:D:257:VAL:HG21	3:D:260:PHE:HD2	1.63	0.63
3:A:489:TRP:O	3:A:490:SER:HB3	1.98	0.63
3:A:257:VAL:HG21	3:A:260:PHE:HD2	1.64	0.63
3:A:678:ILE:HD12	3:A:679:LEU:H	1.64	0.63
3:A:926:ILE:HG21	3:A:946:LEU:HD11	1.80	0.63
3:A:788:TYR:CE1	3:A:796:ARG:HB3	2.34	0.63
3:D:704:HIS:HD2	3:D:767:ASN:H	1.45	0.63
3:D:146:TRP:CE3	3:D:149:PHE:HB2	2.34	0.63
3:D:276:VAL:HA	3:D:283:PHE:CE2	2.34	0.63
1:B:102:LEU:HB3	1:B:129:ARG:HH12	1.64	0.62
2:F:155:TYR:CD1	3:D:445:MET:HE3	2.33	0.62
3:D:150:ILE:HG21	3:D:201:GLU:CD	2.24	0.62
3:A:888:ASN:HD22	3:A:889:VAL:H	1.46	0.62
3:A:961:PRO:HD3	3:A:970:ASN:HD21	1.62	0.62
1:E:18:LEU:HA	1:E:36:SER:O	1.99	0.62
3:A:229:LEU:HD11	3:A:246:LEU:HD11	1.80	0.62
3:A:388:THR:HG23	3:A:401:ASP:HB3	1.81	0.62
3:D:45:MET:O	3:D:49:VAL:HG12	1.98	0.62
3:A:187:THR:HG22	3:A:190:LYS:HB2	1.81	0.62
2:C:42:THR:HG23	8:C:826:HOH:O	1.98	0.62
3:A:276:VAL:HA	3:A:283:PHE:CE2	2.35	0.62
3:A:583:MET:HG2	8:A:1255:HOH:O	1.98	0.62
3:A:681:ASP:OD2	3:A:684:THR:HG23	2.00	0.62
3:A:810:LYS:O	3:A:810:LYS:HD3	1.99	0.62
3:D:437:GLN:HG2	3:D:746:ARG:HG2	1.81	0.62
3:A:1046:GLN:O	3:A:1049:LYS:HB2	1.99	0.62
3:D:429:GLU:HG3	3:D:445:MET:HG3	1.82	0.62
1:E:278:ARG:CG	1:E:281:MET:HE3	2.30	0.62
3:D:90:ARG:O	3:D:94:LEU:HG	1.99	0.62
3:D:229:LEU:HD11	3:D:246:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-1:GLY:O	1:B:3:GLU:HG2	1.99	0.61
3:A:216:SER:O	3:A:217:GLN:HG2	1.98	0.61
1:B:160:ASN:CG	1:B:161:ARG:N	2.54	0.61
3:A:187:THR:HG22	3:A:190:LYS:HE3	1.81	0.61
3:D:32:VAL:HG22	3:D:71:GLN:HB2	1.82	0.61
1:B:285:VAL:HG12	1:B:286:LEU:CD1	2.29	0.61
3:A:210:GLN:O	3:A:214:GLU:HG2	1.99	0.61
3:A:33:ASN:CB	3:A:44:ARG:HG3	2.28	0.61
3:A:110:ILE:CD1	3:A:130:LEU:HB3	2.30	0.61
3:D:141:GLU:HG2	3:D:145[A]:HIS:HD2	1.63	0.61
2:C:50:LEU:HD12	2:C:63:VAL:HG21	1.82	0.61
3:A:1003:SER:HA	3:A:1046:GLN:NE2	2.15	0.61
1:B:261:HIS:CD2	1:B:263:GLN:H	2.19	0.61
3:A:30:ASN:HA	3:A:44:ARG:HD2	1.82	0.61
3:D:888:ASN:HD22	3:D:889:VAL:H	1.46	0.61
3:A:150:ILE:HG21	3:A:201:GLU:CD	2.26	0.61
3:D:28:LEU:CD1	3:D:66:ILE:HG23	2.29	0.61
1:E:52[A]:LYS:HE3	1:E:265:HIS:N	2.12	0.61
2:F:54:THR:HA	2:F:176:PHE:HA	1.83	0.61
3:A:62:ARG:NH1	3:A:82:ILE:HG13	2.15	0.60
3:D:402:ILE:HD13	3:D:407:GLN:NE2	2.16	0.60
3:D:1050:HIS:O	3:D:1054:MET:HG2	2.01	0.60
1:B:211:LYS:HD2	1:B:211:LYS:N	2.16	0.60
1:B:218:LEU:HG	1:B:229:PHE:HB2	1.83	0.60
3:A:131:ASN:HD21	3:A:166:ASN:ND2	1.91	0.60
1:E:173:ASP:CB	1:E:189:MET:HE1	2.31	0.60
3:D:218:ASN:HD22	3:D:220:PRO:HD2	1.67	0.60
3:A:45:MET:O	3:A:49:VAL:HG12	2.00	0.60
3:A:962:LEU:O	3:A:963:ASN:HB2	2.01	0.60
2:F:117:ILE:HB	2:F:144:LEU:HD22	1.84	0.60
3:D:399:HIS:C	3:D:401:ASP:H	2.09	0.60
3:A:33:ASN:HB2	3:A:44:ARG:CG	2.26	0.60
3:A:225:THR:O	3:A:228:THR:HG22	2.02	0.60
3:A:295:LYS:HG2	3:A:300:LEU:HD11	1.83	0.60
3:D:429:GLU:HB3	3:D:445:MET:HB2	1.84	0.60
1:E:52[B]:LYS:NZ	1:E:263:GLN:O	2.34	0.60
1:E:264:THR:HB	1:E:273:LEU:HD13	1.84	0.60
2:F:10:GLN:HG2	2:F:60:LYS:HD3	1.83	0.60
3:D:225:THR:O	3:D:228:THR:HG22	2.01	0.60
1:E:173:ASP:HB2	1:E:189:MET:HE1	1.84	0.59
2:F:54:THR:HG22	2:F:176:PHE:CB	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:22:LYS:HG2	3:D:58:ASP:OD1	2.02	0.59
3:D:300:LEU:HD12	3:D:300:LEU:H	1.66	0.59
1:E:261:HIS:CD2	1:E:263:GLN:H	2.20	0.59
3:A:32:VAL:HG22	3:A:71:GLN:CG	2.32	0.59
2:F:50:LEU:HD12	2:F:63:VAL:HG21	1.84	0.59
1:E:211:LYS:HD2	1:E:211:LYS:N	2.18	0.59
3:A:206:PHE:HE2	3:A:244:THR:HG21	1.66	0.59
3:A:216:SER:HB2	3:A:222:VAL:CG2	2.33	0.59
1:E:128:LYS:O	1:E:175:ILE:HA	2.03	0.59
3:D:476:MET:CE	3:D:516:PHE:HZ	2.13	0.59
3:A:33:ASN:ND2	3:A:44:ARG:HE	1.99	0.59
3:D:218:ASN:ND2	3:D:220:PRO:HD2	2.18	0.59
3:D:295:LYS:HG2	3:D:300:LEU:HD11	1.84	0.59
1:B:278:ARG:CG	1:B:281:MET:HE3	2.31	0.59
3:A:483:GLN:HE22	3:A:489:TRP:HA	1.68	0.59
1:B:52:LYS:HD3	1:B:265:HIS:CG	2.37	0.59
1:B:52:LYS:CE	1:B:265:HIS:H	2.15	0.59
3:A:728:ILE:HD13	3:A:749:ARG:HD2	1.85	0.59
1:B:201:THR:HG22	1:B:264:THR:O	2.03	0.58
3:A:429:GLU:HG3	3:A:445:MET:HG3	1.85	0.58
3:A:476:MET:CE	3:A:516:PHE:HZ	2.15	0.58
3:D:681:ASP:OD2	3:D:684:THR:HG23	2.03	0.58
3:A:218:ASN:HD22	3:A:220:PRO:HD2	1.68	0.58
3:A:300:LEU:H	3:A:300:LEU:HD12	1.67	0.58
3:A:838:PHE:HA	3:A:845:ARG:NH2	2.18	0.58
3:D:788:TYR:CE1	3:D:796:ARG:HB3	2.38	0.58
3:A:30:ASN:ND2	3:A:47:GLN:NE2	2.49	0.58
1:E:209:HIS:CE1	1:E:232:LEU:O	2.57	0.58
3:D:216:SER:HB2	3:D:222:VAL:CG2	2.34	0.58
1:E:188[B]:VAL:C	1:E:189:MET:HE3	2.28	0.58
3:D:293:GLN:O	3:D:297:MET:HG3	2.02	0.58
3:D:483:GLN:HE22	3:D:489:TRP:HA	1.69	0.58
3:D:926:ILE:HG21	3:D:946:LEU:CD1	2.34	0.58
3:A:265:LEU:HD21	3:A:322:LEU:HA	1.84	0.58
3:D:963:ASN:N	3:D:964:PRO:HD3	2.18	0.58
2:C:117:ILE:HB	2:C:144:LEU:HD22	1.86	0.58
3:A:745[A]:ILE:HD13	3:A:748:MET:CE	2.33	0.58
1:E:185:VAL:HG12	1:E:208:MET:SD	2.44	0.58
3:D:146:TRP:N	3:D:147:PRO:HD3	2.18	0.58
3:D:284:GLU:CD	3:D:343:LEU:HD11	2.29	0.58
2:F:52:PHE:HB2	2:F:59:ILE:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:ARG:O	3:D:66:ILE:HG13	2.04	0.58
3:D:340:ARG:HB3	3:D:343:LEU:HD12	1.85	0.57
3:D:545:MET:HG3	3:D:583:MET:SD	2.43	0.57
1:B:128:LYS:HE3	1:B:176:TYR:HD2	1.69	0.57
1:E:259:PHE:O	1:E:274:VAL:HA	2.03	0.57
3:D:150:ILE:HD11	3:D:205:ILE:HG23	1.85	0.57
3:D:360:VAL:HG11	3:D:365:ILE:HD12	1.85	0.57
1:B:12:PHE:HE2	3:A:545:MET:HE2	1.69	0.57
3:D:597:ARG:HE	3:D:601:GLN:NE2	2.02	0.57
3:A:218:ASN:ND2	3:A:220:PRO:HD2	2.20	0.57
3:D:92:LYS:HD2	3:D:1030:THR:HG21	1.86	0.57
2:C:52:PHE:HB2	2:C:59:ILE:HG22	1.86	0.57
3:A:146:TRP:N	3:A:147:PRO:HD3	2.18	0.57
3:A:399:HIS:CD2	3:A:401:ASP:HB2	2.40	0.57
3:A:705:PRO:O	3:A:708:ILE:HG22	2.04	0.57
3:A:799:GLU:HG2	8:A:1286:HOH:O	2.04	0.57
3:A:962:LEU:O	3:A:964:PRO:HD3	2.03	0.57
3:D:485:ASN:O	3:D:487:THR:N	2.38	0.57
3:D:1005:ASN:OD1	3:D:1049:LYS:HE3	2.05	0.57
3:A:303:ASN:HD21	3:A:305:ARG:NH2	2.03	0.57
3:D:728:ILE:HD13	3:D:749:ARG:HD2	1.87	0.57
1:B:259:PHE:O	1:B:274:VAL:HA	2.05	0.57
3:A:160:SER:HB3	3:A:163:LEU:HD12	1.87	0.57
3:A:341:LEU:HD23	3:A:341:LEU:O	2.05	0.57
3:D:107:VAL:O	3:D:111:ILE:HG12	2.05	0.57
3:A:284:GLU:CD	3:A:343:LEU:HD11	2.30	0.57
3:A:388:THR:HG23	3:A:401:ASP:CB	2.35	0.57
3:A:1053:GLN:O	3:A:1054:MET:HE2	2.05	0.57
1:E:26:PRO:HG2	1:E:109:ILE:HD11	1.87	0.57
3:D:21:GLN:HG2	3:D:22:LYS:N	2.20	0.57
3:D:265:LEU:HD21	3:D:322:LEU:HA	1.86	0.57
3:D:1038:ARG:HH21	3:D:1042:LEU:HD21	1.69	0.57
2:F:123:LYS:HE2	5:F:217:GTP:C4	2.40	0.56
3:D:810:LYS:O	3:D:810:LYS:HD3	2.05	0.56
3:A:441:VAL:HB	3:A:628:GLN:OE1	2.05	0.56
3:A:681:ASP:O	3:A:685:VAL:HG13	2.05	0.56
2:F:9:VAL:O	2:F:9:VAL:HG22	2.04	0.56
3:D:91:TRP:HA	3:D:94:LEU:HD12	1.88	0.56
2:C:31:LEU:HD12	2:C:32:THR:CG2	2.36	0.56
2:C:177:VAL:O	2:C:178:ALA:HB3	2.04	0.56
3:A:344:ARG:NH1	3:A:408:LEU:HD21	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:961:PRO:HD3	3:A:970:ASN:ND2	2.21	0.56
3:D:851:LEU:O	3:D:855:VAL:HG23	2.06	0.56
3:A:481:GLN:OE1	3:A:481:GLN:HA	2.04	0.56
1:E:52[A]:LYS:HZ2	1:E:265:HIS:HB2	1.70	0.56
1:B:52:LYS:HE3	1:B:265:HIS:H	1.71	0.56
1:B:351:PRO:HB3	1:B:352:ASP:OD2	2.06	0.56
2:C:31:LEU:HD12	2:C:32:THR:HG23	1.88	0.56
3:A:150:ILE:HD11	3:A:205:ILE:HG22	1.86	0.56
3:A:926:ILE:HG21	3:A:946:LEU:CD1	2.36	0.56
3:D:142:TRP:HH2	3:D:198:MET:HA	1.71	0.56
1:B:209:HIS:CE1	1:B:232:LEU:O	2.58	0.56
3:A:360:VAL:HG11	3:A:365:ILE:HD12	1.86	0.56
3:D:84:GLU:O	3:D:88:LYS:HG3	2.05	0.56
3:D:426:LYS:HD2	3:D:426:LYS:N	2.08	0.56
3:D:431:LEU:HD22	3:D:445:MET:CE	2.36	0.56
3:D:709:GLN:O	3:D:712:ARG:HB3	2.06	0.56
3:D:888:ASN:HD22	3:D:888:ASN:N	2.01	0.56
3:A:256:ASN:HB3	3:A:293:GLN:NE2	2.07	0.56
3:A:340:ARG:HB2	3:A:343:LEU:HD12	1.86	0.56
3:A:962:LEU:HB2	3:A:973:PHE:HD2	1.68	0.56
3:D:21:GLN:HG2	3:D:22:LYS:H	1.71	0.56
3:A:142:TRP:HH2	3:A:198:MET:HA	1.71	0.56
3:A:841:TYR:O	3:A:845:ARG:HG3	2.05	0.56
1:B:212:LEU:HB2	1:B:213:PRO:HD3	1.88	0.56
3:A:485:ASN:O	3:A:487:THR:N	2.39	0.56
3:A:957:LYS:HZ1	3:A:961:PRO:HB3	1.71	0.56
1:E:19:ASN:HD21	1:E:38:LEU:H	1.53	0.56
3:D:93:ILE:HG22	3:D:1027:GLY:HA3	1.88	0.56
3:D:312:LYS:HG3	3:D:313:ASP:H	1.70	0.56
2:C:10:GLN:HG2	2:C:60:LYS:HE2	1.87	0.55
1:B:61:HIS:HE1	1:B:101:GLN:HE22	1.53	0.55
1:E:52[A]:LYS:HE3	1:E:264:THR:HA	1.88	0.55
3:D:66:ILE:HG22	3:D:72:ASN:HB3	1.87	0.55
3:D:187:THR:HG23	3:D:190:LYS:H	1.72	0.55
3:D:962:LEU:HB2	3:D:973:PHE:HD2	1.68	0.55
3:D:1003:SER:HA	3:D:1046:GLN:NE2	2.21	0.55
3:A:388:THR:HG22	3:A:389:SER:N	2.21	0.55
3:D:132:MET:O	3:D:136:GLN:HG2	2.06	0.55
1:B:137:GLY:O	1:B:160:ASN:HB2	2.07	0.55
3:A:23:LEU:HD12	3:A:23:LEU:H	1.71	0.55
3:A:218:ASN:HB3	3:A:221:LEU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:LYS:HG3	8:F:915:HOH:O	2.05	0.55
3:D:58:ASP:CG	3:D:62:ARG:HE	2.14	0.55
3:A:709:GLN:O	3:A:712:ARG:HB3	2.06	0.55
3:A:1016:ARG:HH11	3:A:1016:ARG:CG	2.13	0.55
3:A:293:GLN:O	3:A:297:MET:HG3	2.06	0.55
1:B:26:PRO:HG2	1:B:109:ILE:HD11	1.89	0.55
1:B:201:THR:HG22	1:B:204:ARG:NH1	2.21	0.55
3:D:681:ASP:O	3:D:685:VAL:HG13	2.06	0.55
3:D:957:LYS:HZ1	3:D:961:PRO:HB3	1.71	0.55
3:D:960:THR:HG23	3:D:968:VAL:CG1	2.28	0.55
1:B:34:LYS:N	8:B:363:HOH:O	2.39	0.55
1:B:360:ASN:HB2	8:B:494:HOH:O	2.06	0.55
1:E:349:HIS:CE1	3:D:708[A]:ILE:HD12	2.42	0.55
1:B:19:ASN:HD21	1:B:38:LEU:H	1.54	0.55
1:E:218:LEU:HG	1:E:229:PHE:HB2	1.89	0.55
3:D:66:ILE:HG21	3:D:75:THR:HB	1.89	0.55
1:B:264:THR:OG1	1:B:273:LEU:HD13	2.07	0.54
3:A:132:MET:O	3:A:136:GLN:HG2	2.06	0.54
3:A:888:ASN:ND2	3:A:889:VAL:N	2.55	0.54
3:A:239:GLY:HA2	3:A:243:GLU:HG3	1.88	0.54
3:D:402:ILE:HG21	3:D:407:GLN:HE21	1.72	0.54
1:B:215:GLU:O	1:B:216:GLU:C	2.50	0.54
3:A:793:PRO:HB3	3:A:833:MET:HE3	1.90	0.54
3:D:888:ASN:ND2	3:D:889:VAL:N	2.55	0.54
3:D:939:LEU:CD2	3:D:1016:ARG:HH11	2.20	0.54
3:A:483:GLN:NE2	3:A:489:TRP:HA	2.23	0.54
3:D:66:ILE:HD13	3:D:75:THR:HG22	1.90	0.54
3:D:327:CYS:HB2	3:D:354:MET:HE1	1.90	0.54
3:D:344:ARG:NH1	3:D:408:LEU:HD21	2.23	0.54
1:B:61:HIS:CE1	1:B:101:GLN:HE22	2.25	0.54
3:A:73:MET:HG3	3:A:126:TYR:HB2	1.88	0.54
3:D:284:GLU:HG3	3:D:343:LEU:HD21	1.89	0.54
3:D:435:ASN:CG	3:D:439:GLU:HB2	2.32	0.54
3:D:894:LEU:HD13	3:D:941:MET:HB2	1.90	0.54
3:A:251:ILE:HG21	3:A:289:LEU:HB3	1.89	0.54
3:D:218:ASN:HB3	3:D:221:LEU:HB3	1.89	0.54
1:B:171:ILE:O	1:B:189:MET:HG2	2.08	0.54
3:A:429:GLU:CG	3:A:445:MET:HG3	2.38	0.54
3:A:887:ARG:HD3	3:A:937:ALA:CB	2.37	0.54
3:A:888:ASN:HD22	3:A:888:ASN:N	2.04	0.54
3:D:73:MET:HG3	3:D:126:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:187:THR:HG23	3:A:190:LYS:H	1.73	0.54
3:A:274:VAL:HG12	3:A:275:SER:N	2.23	0.54
2:C:123:LYS:HE2	5:C:217:GTP:C4	2.43	0.54
3:A:864:LEU:HD11	3:A:907:GLU:OE1	2.08	0.54
1:E:70:TRP:CD2	1:E:96:LYS:O	2.61	0.54
3:A:437:GLN:HB3	8:A:1267:HOH:O	2.07	0.53
3:A:672:ALA:CA	3:A:678:ILE:HD11	2.38	0.53
3:D:22:LYS:HE2	3:D:58:ASP:HB2	1.88	0.53
3:D:274:VAL:HG12	3:D:275:SER:N	2.24	0.53
3:D:390:ALA:HB3	8:D:1367:HOH:O	2.09	0.53
3:D:511:GLU:HB2	8:D:1128:HOH:O	2.07	0.53
3:D:882:PHE:CD1	3:D:882:PHE:C	2.86	0.53
2:F:176:PHE:HD2	2:F:176:PHE:O	1.90	0.53
3:D:705:PRO:O	3:D:708[A]:ILE:HG22	2.08	0.53
3:A:87:ILE:O	3:A:91:TRP:HB2	2.08	0.53
3:D:153:ILE:HD11	3:D:171:LEU:HD21	1.89	0.53
3:D:160:SER:HB3	3:D:163:LEU:HD12	1.90	0.53
1:B:138:SER:HA	1:B:159:GLY:O	2.09	0.53
3:A:30:ASN:HA	3:A:33:ASN:HD22	1.73	0.53
3:A:393:LEU:HB3	3:A:399:HIS:ND1	2.23	0.53
3:A:514:LYS:NZ	8:A:1321:HOH:O	2.39	0.53
3:D:256:ASN:HB3	3:D:293:GLN:NE2	2.22	0.53
1:B:171:ILE:HG22	1:B:189:MET:HG3	1.90	0.53
1:B:352:ASP:HB3	3:A:711:GLY:O	2.08	0.53
3:A:882:PHE:C	3:A:882:PHE:CD1	2.86	0.53
2:F:28:LYS:HG2	8:F:745:HOH:O	2.08	0.53
3:D:716:ASP:O	3:D:720:VAL:HG13	2.09	0.53
3:A:187:THR:H	3:A:190:LYS:NZ	2.07	0.53
3:A:32:VAL:HG22	3:A:71:GLN:CB	2.38	0.53
3:A:299:PRO:HB2	3:A:302:THR:HG23	1.89	0.53
3:A:739:VAL:HG12	3:A:745[A]:ILE:HG13	1.89	0.53
3:D:299:PRO:HB2	3:D:302:THR:HG23	1.89	0.53
3:D:208:LEU:C	3:D:208:LEU:HD23	2.33	0.53
3:D:486:GLY:O	3:D:487:THR:C	2.51	0.53
3:A:153:ILE:HD11	3:A:171:LEU:HD21	1.90	0.53
3:A:435:ASN:C	3:A:437:GLN:H	2.16	0.53
3:D:87:ILE:O	3:D:91:TRP:HB2	2.08	0.53
3:D:1033:LEU:HB2	3:D:1035:LEU:HG	1.91	0.53
3:A:84:GLU:O	3:A:88:LYS:HG3	2.08	0.53
3:A:142:TRP:HB3	3:A:143:PRO:HD3	1.90	0.53
3:D:145[A]:HIS:C	3:D:147:PRO:HD3	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:912:GLN:O	3:D:916[B]:GLN:HG3	2.09	0.53
3:D:887:ARG:HD3	3:D:937:ALA:CB	2.39	0.52
3:D:393:LEU:HD21	3:D:397:SER:HB3	1.90	0.52
1:B:187:ASP:OD1	1:B:204:ARG:HD2	2.10	0.52
3:A:142:TRP:CZ3	3:A:197:SER:HB3	2.44	0.52
3:A:437:GLN:HG2	3:A:746:ARG:CG	2.39	0.52
3:A:962:LEU:HD13	3:A:973:PHE:CE2	2.43	0.52
3:A:990:GLN:HG2	3:A:993:GLN:HE21	1.74	0.52
1:E:104:LEU:O	1:E:270:SER:HA	2.09	0.52
3:D:1029:ASP:OD1	3:D:1029:ASP:N	2.42	0.52
3:A:142:TRP:O	3:A:146:TRP:HB3	2.09	0.52
3:A:285:THR:O	3:A:289:LEU:HD13	2.08	0.52
3:A:486:GLY:O	3:A:487:THR:C	2.52	0.52
3:A:724:LEU:HD12	3:A:751:VAL:HG11	1.90	0.52
3:A:960:THR:HG22	3:A:963:ASN:H	1.74	0.52
3:D:142:TRP:HB3	3:D:143:PRO:HD3	1.90	0.52
3:D:212:VAL:O	3:D:216:SER:HB3	2.09	0.52
3:D:672:ALA:CA	3:D:678:ILE:HD11	2.39	0.52
3:A:735:ASN:HB2	3:A:739:VAL:CG2	2.40	0.52
2:F:29:ARG:CB	2:F:157:PHE:HZ	2.14	0.52
3:D:142:TRP:CZ3	3:D:197:SER:HB3	2.44	0.52
3:D:735:ASN:HB2	3:D:739:VAL:CG2	2.40	0.52
1:E:352:ASP:HB2	3:D:711:GLY:O	2.09	0.52
3:D:290:THR:HG21	3:D:325:PHE:CE2	2.45	0.52
3:D:957:LYS:HZ3	3:D:961:PRO:HB3	1.74	0.52
1:E:358:MET:O	1:E:359:GLU:HB2	2.10	0.52
3:D:141:GLU:HG2	3:D:145[A]:HIS:CD2	2.43	0.52
1:E:172:LEU:HD22	1:E:188[B]:VAL:HG12	1.92	0.52
3:D:960:THR:HG22	3:D:963:ASN:H	1.75	0.52
3:D:990:GLN:HG2	3:D:993:GLN:HE21	1.74	0.52
3:D:105:TYR:O	3:D:109:LEU:HG	2.10	0.52
3:D:963:ASN:N	3:D:964:PRO:CD	2.73	0.51
3:A:566:VAL:HG11	3:A:610:PHE:HE2	1.74	0.51
3:D:127:ILE:HD12	3:D:127:ILE:N	2.25	0.51
3:D:821:GLN:OE1	3:D:821:GLN:HA	2.10	0.51
3:D:961:PRO:HD3	3:D:970:ASN:OD1	2.11	0.51
3:A:333:HIS:HB3	3:A:336:LEU:HD23	1.92	0.51
1:E:188[A]:VAL:C	1:E:189:MET:HE3	2.35	0.51
3:D:437:GLN:HG2	3:D:746:ARG:CG	2.39	0.51
1:B:128:LYS:O	1:B:175:ILE:HA	2.11	0.51
3:A:912:GLN:NE2	3:A:958:ILE:HG23	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:59:ILE:HD13	2:F:60:LYS:N	2.25	0.51
3:D:436:ASP:C	3:D:437:GLN:HG3	2.34	0.51
1:B:59:VAL:HA	1:B:195:PRO:HG2	1.91	0.51
3:D:131:ASN:HD21	3:D:166:ASN:ND2	1.90	0.51
3:A:187:THR:H	3:A:190:LYS:HZ2	1.58	0.51
3:A:212:VAL:O	3:A:216:SER:HB3	2.10	0.51
1:E:188[A]:VAL:HG13	1:E:188[A]:VAL:O	2.10	0.51
3:D:788:TYR:CD2	3:D:826:VAL:HG12	2.45	0.51
3:A:219:ALA:HB3	3:A:220:PRO:HD3	1.91	0.51
3:A:491:TRP:CH2	3:A:535:ASP:HB3	2.46	0.51
3:A:509[B]:HIS:HD2	3:A:511:GLU:HB3	1.71	0.51
3:A:721:TYR:C	3:A:721:TYR:CD2	2.88	0.51
1:E:44:ARG:NH2	1:E:272:PRO:HG3	2.26	0.51
3:D:305:ARG:HG3	8:D:1384:HOH:O	2.11	0.51
3:D:434:GLU:HA	3:D:439:GLU:O	2.10	0.51
3:D:436:ASP:O	3:D:437:GLN:HG3	2.11	0.51
3:D:518:VAL:O	3:D:522:LYS:HB2	2.10	0.51
3:D:912:GLN:NE2	3:D:958:ILE:HG23	2.25	0.51
3:A:110:ILE:HD13	3:A:130:LEU:HD13	1.93	0.51
3:A:664:VAL:CG1	3:A:691:ILE:HD11	2.40	0.51
1:B:29:SER:O	1:B:30:GLN:C	2.52	0.51
1:B:353:HIS:N	1:B:353:HIS:CD2	2.79	0.51
3:A:261:ARG:HD2	3:A:318:PHE:CG	2.46	0.51
3:A:755:THR:O	3:A:759:ILE:HG13	2.11	0.51
3:D:104:LYS:HA	3:D:107:VAL:HG22	1.92	0.51
3:D:429:GLU:HA	3:D:429:GLU:OE1	2.10	0.51
3:D:721:TYR:CD2	3:D:721:TYR:C	2.89	0.51
3:A:851:LEU:O	3:A:855:VAL:HG23	2.11	0.51
1:E:356:CYS:HB3	3:D:673:THR:OG1	2.11	0.51
2:F:89:MET:HE2	2:F:120:CYS:HB2	1.93	0.51
3:D:19:PHE:O	3:D:19:PHE:CD1	2.64	0.51
2:C:98:TYR:O	2:C:101:VAL:HG23	2.11	0.50
3:D:962:LEU:O	3:D:963:ASN:CB	2.59	0.50
1:B:57:ASP:OD1	1:B:59:VAL:HB	2.10	0.50
3:A:105:TYR:O	3:A:109:LEU:HG	2.11	0.50
3:A:129:LYS:O	3:A:133:ILE:HG13	2.11	0.50
3:A:887:ARG:NH2	3:A:891:ASP:HB3	2.25	0.50
3:A:1048:GLU:O	3:A:1052:LEU:N	2.45	0.50
1:E:189:MET:HE2	1:E:266:TYR:CE2	2.46	0.50
3:D:219:ALA:HB3	3:D:220:PRO:HD3	1.92	0.50
3:D:881:ALA:O	3:D:884:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:887:ARG:NH2	3:D:891:ASP:HB3	2.25	0.50
1:B:106[B]:GLU:O	1:B:275:GLY:HA2	2.12	0.50
2:C:32:THR:OG1	2:C:34:GLU:HG2	2.11	0.50
3:A:276:VAL:HB	3:A:333:HIS:ND1	2.25	0.50
3:A:284:GLU:HG3	3:A:343:LEU:HD21	1.93	0.50
2:F:176:PHE:O	2:F:176:PHE:CD2	2.64	0.50
2:C:129:ARG:NH1	3:A:447:ASP:O	2.45	0.50
1:E:59:VAL:HA	1:E:195:PRO:HG2	1.92	0.50
3:D:333:HIS:HB3	3:D:336:LEU:HD23	1.93	0.50
3:D:491:TRP:CH2	3:D:535:ASP:HB3	2.46	0.50
3:D:996:LEU:O	3:D:999:THR:HG22	2.11	0.50
1:E:225:ASN:N	1:E:226:PRO:HD3	2.27	0.50
1:E:360:ASN:O	1:E:360:ASN:CG	2.54	0.50
3:D:66:ILE:CD1	3:D:75:THR:HG22	2.42	0.50
3:D:566:VAL:HG11	3:D:610:PHE:HE2	1.75	0.50
3:D:1050:HIS:HA	3:D:1053:GLN:HG2	1.92	0.50
3:A:123:GLU:OE1	3:A:123:GLU:HA	2.11	0.50
2:F:38:LYS:HG2	3:D:842:PRO:HG3	1.94	0.50
3:D:168:MET:HE2	3:D:168:MET:HA	1.94	0.50
3:D:755:THR:O	3:D:759:ILE:HG13	2.12	0.50
1:B:202:ASP:HB3	1:B:262:LYS:HG2	1.94	0.50
3:A:1038:ARG:HH21	3:A:1042:LEU:HD21	1.76	0.50
3:D:1008:ILE:CG2	3:D:1009:PRO:HD3	2.30	0.50
2:C:29:ARG:CB	2:C:157:PHE:HZ	2.15	0.50
3:D:483:GLN:NE2	3:D:489:TRP:HA	2.26	0.50
2:C:52:PHE:HE1	2:C:61:PHE:HD2	1.60	0.50
3:A:476:MET:CE	3:A:516:PHE:CZ	2.94	0.50
3:D:729:SER:OG	3:D:792:VAL:HG22	2.12	0.50
2:C:59:ILE:HD13	2:C:60:LYS:N	2.26	0.49
3:A:181:PHE:O	3:A:185:GLN:HG2	2.12	0.49
3:A:559:TRP:CD2	3:A:603:GLN:HG3	2.46	0.49
3:A:968:VAL:HG12	3:A:973:PHE:HB2	1.93	0.49
3:D:399:HIS:C	3:D:401:ASP:N	2.68	0.49
3:A:393:LEU:HD22	3:A:398:GLN:CA	2.35	0.49
3:A:957:LYS:HZ3	3:A:961:PRO:HB3	1.75	0.49
3:D:326:LEU:O	3:D:330:LEU:HG	2.12	0.49
3:A:894:LEU:HD13	3:A:941:MET:HB2	1.95	0.49
1:E:25:HIS:HE1	1:E:27:ARG:HD3	1.78	0.49
1:E:57:ASP:OD1	1:E:59:VAL:HB	2.11	0.49
2:F:29:ARG:HG2	2:F:34:GLU:O	2.12	0.49
3:D:175[B]:SER:OG	3:D:232:PHE:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:788:TYR:O	3:D:796:ARG:HG2	2.12	0.49
1:B:8:LEU:HD22	3:A:564:THR:HG22	1.93	0.49
1:E:358:MET:O	1:E:359:GLU:CB	2.60	0.49
3:D:129:LYS:O	3:D:133:ILE:HG13	2.12	0.49
3:D:261:ARG:HD2	3:D:318:PHE:CG	2.48	0.49
1:B:70:TRP:CD1	1:B:97:HIS:CE1	3.00	0.49
1:B:222:THR:HG22	1:B:225:ASN:N	2.26	0.49
3:A:875:LEU:O	3:A:879:ILE:HG12	2.13	0.49
3:D:30:ASN:HB3	3:D:44:ARG:HD2	1.94	0.49
3:D:103:LYS:HE3	3:D:146:TRP:CD1	2.47	0.49
3:D:344:ARG:O	3:D:348:MET:HG2	2.12	0.49
3:A:26:ASN:HB3	8:A:1204:HOH:O	2.12	0.49
3:A:996:LEU:O	3:A:999:THR:HG22	2.12	0.49
3:A:1050:HIS:HD2	3:A:1054:MET:HE3	1.77	0.49
3:D:56:HIS:O	3:D:56:HIS:CD2	2.66	0.49
3:D:797:GLU:OE2	3:D:798:PRO:HD2	2.13	0.49
3:D:875:LEU:O	3:D:879:ILE:HG12	2.13	0.49
3:A:76:LYS:HB3	3:A:126:TYR:CE1	2.47	0.49
3:A:187:THR:CG2	3:A:190:LYS:HB2	2.43	0.49
3:A:967:PRO:HG2	3:A:968:VAL:HG23	1.95	0.49
1:E:180:ASN:O	1:E:181:GLN:C	2.53	0.49
2:F:86:ALA:HB3	2:F:108:LEU:HD21	1.94	0.49
3:D:142:TRP:O	3:D:146:TRP:HB3	2.12	0.49
2:C:86:ALA:HB3	2:C:108:LEU:HD21	1.93	0.49
3:A:990:GLN:H	3:A:993:GLN:NE2	2.04	0.49
1:E:240:GLU:CD	1:E:240:GLU:H	2.20	0.49
1:B:12:PHE:CE2	3:A:545:MET:HE2	2.47	0.49
2:C:47:VAL:HG13	2:C:47:VAL:O	2.12	0.49
1:E:114:ASP:HB3	8:E:876:HOH:O	2.13	0.49
3:D:28:LEU:HD12	3:D:75:THR:OG1	2.13	0.49
3:D:54:LYS:O	3:D:55:GLU:HG2	2.13	0.49
3:D:276:VAL:HB	3:D:333:HIS:ND1	2.27	0.49
3:A:437:GLN:C	3:A:439:GLU:H	2.21	0.49
1:E:219:GLY:O	1:E:228:LYS:HD2	2.13	0.49
3:D:1033:LEU:CD1	3:D:1035:LEU:HD21	2.43	0.49
3:A:429:GLU:OE1	3:A:429:GLU:HA	2.12	0.48
1:E:350:SER:CB	1:E:351:PRO:HD2	2.17	0.48
3:D:988:HIS:CD2	3:D:988:HIS:H	2.31	0.48
3:A:545:MET:SD	3:A:569:LEU:HD11	2.52	0.48
3:D:406:ARG:HD3	8:D:1182:HOH:O	2.13	0.48
2:C:91:ASP:CG	2:C:123:LYS:HD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:LEU:H	3:A:23:LEU:CD1	2.26	0.48
3:A:56:HIS:O	3:A:56:HIS:CD2	2.66	0.48
3:A:290:THR:HG21	3:A:325:PHE:CE2	2.48	0.48
3:D:1054:MET:HA	3:D:1054:MET:HE2	1.94	0.48
3:D:357:VAL:HG13	3:D:369:CYS:SG	2.53	0.48
3:D:429:GLU:CG	3:D:445:MET:HG3	2.42	0.48
3:D:841:TYR:O	3:D:845:ARG:HG3	2.13	0.48
2:C:29:ARG:HG2	2:C:34:GLU:O	2.14	0.48
3:A:19:PHE:C	3:A:21:GLN:H	2.20	0.48
3:D:435:ASN:C	3:D:437:GLN:H	2.21	0.48
3:D:517:LEU:HD11	3:D:551:TYR:CD1	2.47	0.48
1:B:44:ARG:NH2	1:B:272:PRO:HG3	2.29	0.48
3:A:27:LEU:O	3:A:31:VAL:HG23	2.14	0.48
3:A:344:ARG:O	3:A:348:MET:HG2	2.13	0.48
3:A:707:VAL:HG21	3:A:771:MET:HE1	1.96	0.48
3:A:738:MET:C	3:A:740:THR:H	2.21	0.48
3:A:962:LEU:CD2	3:A:968:VAL:HG11	2.40	0.48
1:E:283:SER:O	1:E:288:VAL:HG13	2.14	0.48
2:F:52:PHE:HE1	2:F:61:PHE:HD2	1.61	0.48
2:F:81:ILE:O	2:F:82:GLN:HB2	2.13	0.48
2:C:125:ASP:O	2:C:127:LYS:HE3	2.13	0.48
3:A:518:VAL:O	3:A:522:LYS:HB2	2.12	0.48
3:A:881:ALA:O	3:A:884:HIS:HB2	2.13	0.48
1:E:289:ALA:O	1:E:290:VAL:HB	2.13	0.48
3:D:268:LEU:HD22	3:D:286:LEU:HD11	1.95	0.48
1:B:104:LEU:O	1:B:270:SER:HA	2.13	0.48
2:C:178:ALA:O	2:C:179:MET:HB2	2.14	0.48
3:A:76:LYS:HB3	3:A:126:TYR:HE1	1.78	0.48
3:A:218:ASN:HD22	3:A:218:ASN:C	2.22	0.48
3:A:953:VAL:CG2	3:A:974:ILE:HD12	2.43	0.48
1:E:215:GLU:O	1:E:216:GLU:C	2.57	0.48
3:D:354:MET:HB3	3:D:373:TRP:CZ2	2.49	0.48
3:D:838:PHE:HA	3:D:845:ARG:NH2	2.29	0.48
1:B:60:ASN:O	1:B:64:ARG:HG3	2.14	0.48
2:C:89:MET:HE2	2:C:120:CYS:HB2	1.95	0.48
3:A:23:LEU:HD13	3:A:26:ASN:HB2	1.96	0.48
3:A:62:ARG:HH11	3:A:79:GLY:CA	2.17	0.48
3:A:993:GLN:HG2	3:A:1033:LEU:HD22	1.96	0.48
3:D:27:LEU:O	3:D:31:VAL:HG23	2.14	0.48
3:D:52:HIS:CE1	3:D:82:ILE:HD12	2.49	0.48
3:D:120:VAL:HG23	3:D:121:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:GLN:HG3	3:D:186:ILE:HG13	1.95	0.48
3:A:104:LYS:HA	3:A:107:VAL:HG22	1.95	0.48
3:A:136:GLN:OE1	3:A:136:GLN:HA	2.14	0.48
3:D:175[B]:SER:OG	3:D:232:PHE:CE1	2.66	0.48
3:D:181:PHE:O	3:D:185:GLN:HG2	2.13	0.48
2:C:31:LEU:CD1	2:C:32:THR:HG23	2.44	0.47
3:A:578:ASP:HA	8:A:1148:HOH:O	2.13	0.47
3:A:1030:THR:HG23	3:A:1032:ASP:OD1	2.14	0.47
1:B:2:GLU:C	1:B:2:GLU:OE2	2.56	0.47
1:B:245:VAL:HA	1:B:248:MET:SD	2.54	0.47
2:C:86:ALA:CB	2:C:108:LEU:HD21	2.44	0.47
1:E:204:ARG:HA	8:E:492:HOH:O	2.13	0.47
1:E:358:MET:HB3	1:E:359:GLU:H	1.39	0.47
3:D:739:VAL:HG12	3:D:745:ILE:HG13	1.95	0.47
2:C:80:TYR:O	2:C:81:ILE:C	2.57	0.47
3:D:575:GLU:HG2	3:D:580:VAL:HG11	1.97	0.47
2:C:15:LEU:HD22	2:C:23:LYS:HD2	1.96	0.47
1:E:43:ARG:HE	1:E:43:ARG:HB3	1.41	0.47
3:D:476:MET:CE	3:D:516:PHE:CZ	2.93	0.47
3:D:511:GLU:HG2	3:D:515:ARG:NH1	2.29	0.47
3:D:607:VAL:HG23	3:D:608:MET:HG2	1.96	0.47
2:C:52:PHE:CE1	2:C:61:PHE:HD2	2.32	0.47
3:A:28:LEU:HD12	3:A:75:THR:OG1	2.14	0.47
3:A:716:ASP:O	3:A:720:VAL:HG13	2.15	0.47
3:A:960:THR:HA	3:A:961:PRO:HD3	1.74	0.47
1:B:171:ILE:HG22	1:B:189:MET:CG	2.45	0.47
1:B:359:GLU:O	1:B:360:ASN:C	2.58	0.47
3:A:122:LYS:O	3:A:123:GLU:O	2.33	0.47
3:A:409:TYR:O	3:A:410:LEU:C	2.57	0.47
3:A:424:MET:HA	3:A:457:MET:CE	2.44	0.47
3:A:688:LEU:O	3:A:692:LEU:HG	2.14	0.47
3:A:953:VAL:HG21	3:A:974:ILE:HD12	1.97	0.47
3:A:962:LEU:O	3:A:963:ASN:CB	2.61	0.47
2:F:101:VAL:HB	2:F:102:PRO:HD3	1.96	0.47
3:D:257:VAL:HG21	3:D:260:PHE:CD2	2.48	0.47
3:D:344:ARG:CZ	3:D:408:LEU:HD11	2.44	0.47
3:D:664:VAL:CG1	3:D:691:ILE:HD11	2.45	0.47
1:B:42:GLU:HB3	8:B:948:HOH:O	2.14	0.47
1:B:128:LYS:HG3	1:B:176:TYR:HB3	1.96	0.47
3:A:257:VAL:HG21	3:A:260:PHE:CD2	2.49	0.47
3:A:326:LEU:O	3:A:330:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:VAL:HG13	1:E:253:GLU:HB2	1.95	0.47
2:F:88:ILE:HG21	2:F:101:VAL:HG13	1.96	0.47
3:D:485:ASN:C	3:D:487:THR:N	2.68	0.47
3:D:996:LEU:HD22	3:D:1035:LEU:HD23	1.97	0.47
3:A:185:GLN:HG3	3:A:186:ILE:HG13	1.96	0.47
3:D:135:VAL:HG12	3:D:139:LYS:HE2	1.96	0.47
3:D:688:LEU:O	3:D:692:LEU:HG	2.14	0.47
1:B:219:GLY:O	1:B:228:LYS:HD2	2.15	0.47
3:A:988:HIS:H	3:A:988:HIS:CD2	2.32	0.47
3:D:136:GLN:HA	3:D:136:GLN:OE1	2.15	0.47
3:D:218:ASN:HD22	3:D:218:ASN:C	2.23	0.47
3:D:453:LEU:O	3:D:457:MET:HG3	2.15	0.47
2:C:88:ILE:HG21	2:C:101:VAL:HG13	1.96	0.46
3:A:73:MET:CG	3:A:126:TYR:HB2	2.45	0.46
3:A:179:PHE:HE2	3:A:198:MET:HE3	1.80	0.46
3:A:453:LEU:O	3:A:457:MET:HG3	2.15	0.46
3:A:837:ASP:O	3:A:845:ARG:NH2	2.46	0.46
3:D:424:MET:HA	3:D:457:MET:CE	2.45	0.46
3:D:953:VAL:CG2	3:D:974:ILE:HD12	2.45	0.46
3:A:788:TYR:O	3:A:796:ARG:HG2	2.15	0.46
1:E:25:HIS:CE1	1:E:27:ARG:HD3	2.50	0.46
3:D:35:LEU:HD12	3:D:71:GLN:OE1	2.14	0.46
3:D:327:CYS:HB2	3:D:354:MET:CE	2.45	0.46
3:D:738:MET:C	3:D:740:THR:H	2.22	0.46
2:C:91:ASP:OD1	2:C:123:LYS:HD2	2.15	0.46
3:A:139:LYS:HD3	3:A:186:ILE:HD11	1.97	0.46
3:A:146:TRP:CD2	3:A:149:PHE:HB2	2.50	0.46
3:A:962:LEU:HB2	3:A:973:PHE:CE2	2.50	0.46
1:E:176:TYR:HB2	1:E:183:TYR:CD1	2.50	0.46
2:F:156:ASN:ND2	2:F:159:LYS:HZ1	2.13	0.46
3:D:73:MET:CG	3:D:126:TYR:HB2	2.45	0.46
3:D:202:PHE:CZ	3:D:236:ILE:HG21	2.51	0.46
3:D:760:SER:HB3	3:D:803:THR:HG23	1.98	0.46
1:B:106[A]:GLU:HG3	1:B:271:THR:O	2.15	0.46
2:C:81:ILE:O	2:C:82:GLN:HB2	2.15	0.46
3:A:114:SER:C	3:A:116:ASP:H	2.23	0.46
3:A:96:ARG:NH2	3:A:145:HIS:CG	2.83	0.46
3:A:517:LEU:HD11	3:A:551:TYR:CD1	2.50	0.46
3:A:788:TYR:CD2	3:A:826:VAL:HG12	2.50	0.46
1:E:265:HIS:CE1	8:E:497:HOH:O	2.68	0.46
3:D:435:ASN:HD21	3:D:439:GLU:HB2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:239:GLY:O	3:A:243:GLU:HB2	2.15	0.46
3:A:525:LEU:CD1	3:A:544:ILE:HD13	2.46	0.46
3:A:574:HIS:HD2	3:A:624:ASP:CG	2.24	0.46
1:E:52[A]:LYS:HD3	1:E:265:HIS:CG	2.50	0.46
2:F:36:GLU:OE2	2:F:38:LYS:HE3	2.16	0.46
3:D:24:ASP:OD2	3:D:62:ARG:HA	2.16	0.46
3:D:716:ASP:O	3:D:720:VAL:CG1	2.64	0.46
3:D:739:VAL:O	3:D:742:GLN:HG2	2.16	0.46
1:B:285:VAL:O	1:B:286:LEU:HD12	2.16	0.46
3:A:124:LYS:H	3:A:124:LYS:HD2	1.81	0.46
3:A:668:ILE:HG12	8:A:1279:HOH:O	2.15	0.46
3:A:797:GLU:OE2	3:A:798:PRO:HD2	2.16	0.46
2:F:122:ASN:O	2:F:123:LYS:HB2	2.15	0.46
2:C:178:ALA:O	2:C:179:MET:CB	2.63	0.46
3:A:509[B]:HIS:HD2	3:A:511:GLU:N	2.09	0.46
3:A:575:GLU:HG2	3:A:580:VAL:HG11	1.98	0.46
1:E:349:HIS:NE2	3:D:708[A]:ILE:HD12	2.31	0.46
2:F:53:HIS:O	2:F:176:PHE:HB2	2.15	0.46
2:C:159:LYS:HB2	2:C:160:PRO:HD3	1.97	0.46
3:A:24:ASP:OD1	3:A:24:ASP:C	2.59	0.46
3:A:106:VAL:O	3:A:110:ILE:HG12	2.15	0.46
3:A:168:MET:HA	3:A:168:MET:HE2	1.98	0.46
3:A:268:LEU:HD22	3:A:286:LEU:HD11	1.97	0.46
3:A:307:ALA:O	3:A:315:GLU:OE2	2.34	0.46
3:A:393:LEU:CD2	3:A:398:GLN:HA	2.39	0.46
3:A:485:ASN:C	3:A:487:THR:N	2.69	0.46
1:E:212:LEU:N	1:E:213:PRO:CD	2.79	0.46
3:D:119:CYS:SG	3:D:127:ILE:HG12	2.56	0.46
3:D:217:GLN:HE21	3:D:217:GLN:HB2	1.54	0.46
3:D:815:ILE:HA	3:D:818:GLU:OE1	2.16	0.46
3:D:124:LYS:H	3:D:124:LYS:HD2	1.81	0.46
3:D:179:PHE:HE2	3:D:198:MET:HE3	1.81	0.46
3:D:982:LEU:HD13	3:D:1018:PHE:CZ	2.51	0.46
1:B:52:LYS:HD3	1:B:265:HIS:ND1	2.30	0.45
1:B:208:MET:HG2	1:B:212:LEU:CD1	2.46	0.45
1:B:209:HIS:O	1:B:213:PRO:HG2	2.16	0.45
3:A:969:ASN:O	3:A:970:ASN:C	2.60	0.45
1:E:359:GLU:HB3	3:D:722:LYS:HD3	1.98	0.45
2:F:52:PHE:CE1	2:F:61:PHE:HD2	2.33	0.45
2:F:80:TYR:O	2:F:81:ILE:C	2.59	0.45
3:D:829:CYS:O	3:D:833:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:440:VAL:O	3:A:440:VAL:HG23	2.16	0.45
3:A:815:ILE:HA	3:A:818:GLU:OE1	2.16	0.45
1:E:189:MET:O	1:E:196:PHE:N	2.43	0.45
2:F:159:LYS:HB2	2:F:160:PRO:HD3	1.97	0.45
3:D:600:VAL:HG13	3:D:644:GLN:NE2	2.30	0.45
3:D:953:VAL:HG21	3:D:974:ILE:HD12	1.98	0.45
1:B:1:MET:HE2	3:A:558:HIS:CG	2.52	0.45
3:A:611:ILE:HG13	3:A:615[B]:LEU:HD22	1.99	0.45
3:A:1034:PHE:C	3:A:1036:GLU:H	2.24	0.45
3:D:16:LEU:HD12	3:D:16:LEU:C	2.41	0.45
3:D:402:ILE:HG21	3:D:407:GLN:NE2	2.31	0.45
3:D:497:LEU:HD12	3:D:497:LEU:O	2.16	0.45
3:D:654:ILE:HB	3:D:708[B]:ILE:HD11	1.99	0.45
3:A:186:ILE:HG22	3:A:187:THR:O	2.17	0.45
3:A:829:CYS:O	3:A:833:MET:HG3	2.17	0.45
2:F:81:ILE:HD11	3:D:77:TYR:CD2	2.51	0.45
3:D:290:THR:HG21	3:D:325:PHE:CZ	2.51	0.45
3:D:409:TYR:O	3:D:410:LEU:C	2.58	0.45
1:B:225:ASN:N	1:B:226:PRO:HD3	2.32	0.45
3:A:223:HIS:CE1	3:A:263:VAL:HG21	2.51	0.45
3:A:739:VAL:O	3:A:742:GLN:HG2	2.17	0.45
2:F:98:TYR:O	2:F:101:VAL:HG23	2.17	0.45
3:D:593:GLN:HB3	8:D:1328:HOH:O	2.16	0.45
3:D:665:TRP:CZ3	3:D:692:LEU:HD21	2.50	0.45
1:B:160:ASN:O	1:B:161:ARG:HB2	2.17	0.45
3:A:70:SER:O	3:A:71:GLN:HB2	2.16	0.45
3:A:738:MET:C	3:A:740:THR:N	2.74	0.45
1:E:129:ARG:HG2	1:E:144:LYS:HE3	1.98	0.45
1:E:173:ASP:HB2	1:E:189:MET:CE	2.46	0.45
2:C:123:LYS:HG2	5:C:217:GTP:C6	2.51	0.45
3:A:261:ARG:HG3	3:A:297:MET:HE1	1.97	0.45
1:E:209:HIS:HE1	1:E:232:LEU:O	1.99	0.45
3:D:146:TRP:CD2	3:D:149:PHE:HB2	2.52	0.45
1:B:209:HIS:NE2	1:B:232:LEU:O	2.50	0.45
1:B:212:LEU:N	1:B:213:PRO:CD	2.79	0.45
3:A:19:PHE:CG	3:A:19:PHE:O	2.70	0.45
3:A:940:THR:O	3:A:944:SER:HB2	2.17	0.45
3:D:480:LEU:O	3:D:483:GLN:HB2	2.16	0.45
3:D:837:ASP:O	3:D:845:ARG:NH2	2.47	0.45
1:B:264:THR:OG1	1:B:273:LEU:HB3	2.17	0.45
2:C:95:ARG:NH1	2:C:130:LYS:HE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:534:LYS:HE2	3:A:577:HIS:HB2	1.99	0.45
1:E:41:SER:HB2	1:E:110:ASP:HB3	1.97	0.45
3:D:989:LEU:HD11	3:D:1022:ILE:HG22	1.99	0.45
1:B:7:ALA:HA	8:B:410:HOH:O	2.16	0.45
3:A:95:PRO:HG2	3:A:98:GLN:HB2	1.99	0.45
3:A:110:ILE:HD11	3:A:130:LEU:HB3	1.96	0.45
3:A:458:ARG:HG3	3:A:503:SER:HB2	1.99	0.45
3:A:989:LEU:HD11	3:A:1022:ILE:HG22	1.99	0.45
2:F:86:ALA:CB	2:F:108:LEU:HD21	2.47	0.45
2:F:91:ASP:CG	2:F:123:LYS:HD2	2.41	0.45
3:D:127:ILE:N	3:D:127:ILE:CD1	2.80	0.45
3:D:772:VAL:HG12	3:D:811:LEU:HD11	1.98	0.45
3:D:962:LEU:O	3:D:963:ASN:HB2	2.17	0.45
1:B:57:ASP:HB3	8:B:903:HOH:O	2.16	0.44
1:B:285:VAL:O	1:B:286:LEU:HB2	2.17	0.44
3:A:274:VAL:HG12	3:A:275:SER:H	1.82	0.44
1:E:8:LEU:HD22	3:D:564:THR:HG22	1.99	0.44
3:D:707:VAL:HG21	3:D:771:MET:HE1	1.99	0.44
3:D:1034:PHE:C	3:D:1036:GLU:H	2.25	0.44
1:B:208:MET:HG2	1:B:212:LEU:HD11	1.98	0.44
2:C:101:VAL:HB	2:C:102:PRO:HD3	1.98	0.44
3:A:55:GLU:HG2	3:A:56:HIS:N	2.28	0.44
3:A:276:VAL:O	3:A:277:SER:C	2.60	0.44
3:A:534:LYS:HB3	3:A:577:HIS:CD2	2.51	0.44
1:E:187:ASP:OD1	1:E:204:ARG:HD2	2.17	0.44
3:A:287:PHE:HB2	3:A:329:PHE:CZ	2.51	0.44
2:F:38:LYS:HE3	2:F:38:LYS:HB2	1.77	0.44
3:D:148:THR:O	3:D:149:PHE:C	2.60	0.44
3:D:216:SER:HB2	3:D:222:VAL:HG22	1.99	0.44
3:D:693:LYS:O	3:D:697:ARG:HG2	2.17	0.44
3:A:30:ASN:CA	3:A:44:ARG:HD2	2.48	0.44
3:A:594:LYS:HE2	3:A:594:LYS:HA	2.00	0.44
3:A:962:LEU:C	3:A:964:PRO:CD	2.89	0.44
1:E:97[A]:HIS:CD2	1:E:98:TYR:N	2.85	0.44
3:D:53:LEU:CD1	3:D:54:LYS:H	2.19	0.44
3:D:939:LEU:HD21	3:D:1016:ARG:HH11	1.82	0.44
3:D:966:ASN:N	3:D:967:PRO:HD2	2.33	0.44
1:B:250:PHE:C	1:B:252:PHE:H	2.25	0.44
3:D:218:ASN:O	3:D:222:VAL:HG23	2.18	0.44
3:D:716:ASP:HA	8:D:1253:HOH:O	2.16	0.44
3:A:600:VAL:HG13	3:A:644:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:693:LYS:O	3:A:697:ARG:HG2	2.18	0.44
3:A:1046:GLN:OE1	3:A:1049:LYS:HD3	2.17	0.44
3:A:1054:MET:HE2	3:A:1054:MET:HA	2.00	0.44
2:F:47:VAL:O	2:F:47:VAL:HG23	2.18	0.44
3:D:257:VAL:HG22	3:D:260:PHE:HB2	2.00	0.44
3:D:289:LEU:HA	3:D:292:MET:HE2	1.99	0.44
3:D:402:ILE:O	3:D:402:ILE:HG23	2.17	0.44
3:D:458:ARG:HG3	3:D:503:SER:HB2	2.00	0.44
1:B:58:TYR:HB3	1:B:197:TYR:HD1	1.83	0.44
3:A:607:VAL:HG23	3:A:608:MET:HG2	1.99	0.44
1:E:278:ARG:HB2	1:E:281:MET:HE3	2.00	0.44
2:F:77:ASP:OD1	2:F:77:ASP:N	2.50	0.44
3:D:685:VAL:HA	3:D:688:LEU:HD12	2.00	0.44
3:D:849:PHE:CZ	3:D:881:ALA:HB2	2.52	0.44
1:B:176:TYR:HB2	1:B:183:TYR:CD1	2.52	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG22	2.00	0.44
3:A:277:SER:HB3	3:A:278:GLN:OE1	2.18	0.44
3:A:388:THR:HG22	3:A:389:SER:H	1.81	0.44
3:A:414:SER:OG	3:A:471:ASP:OD2	2.32	0.44
1:E:-1:GLY:O	1:E:3[A]:GLU:HG2	2.17	0.44
2:F:123:LYS:HG2	5:F:217:GTP:C6	2.53	0.44
3:D:17:LEU:HA	3:D:17:LEU:HD12	1.76	0.44
3:D:123:GLU:C	3:D:125:VAL:N	2.76	0.44
3:D:887:ARG:HD2	3:D:887:ARG:HA	1.58	0.44
3:D:1038:ARG:O	3:D:1042:LEU:HG	2.18	0.44
3:A:186:ILE:HG23	3:A:190:LYS:HD2	1.99	0.44
3:A:216:SER:HB2	3:A:222:VAL:HG21	2.00	0.44
3:A:286:LEU:HD12	3:A:286:LEU:O	2.18	0.44
1:E:208:MET:HG2	1:E:212:LEU:CD1	2.48	0.44
2:F:13:LEU:C	2:F:13:LEU:HD12	2.43	0.44
3:D:223:HIS:CE1	3:D:263:VAL:HG21	2.52	0.44
3:D:276:VAL:O	3:D:277:SER:C	2.61	0.44
3:D:731:ALA:HB1	3:D:739:VAL:HG11	1.99	0.44
1:E:102:LEU:CD1	1:E:129:ARG:HG3	2.48	0.43
2:F:40:VAL:HG13	3:D:839:GLU:OE1	2.18	0.43
2:F:91:ASP:OD1	2:F:123:LYS:HD2	2.18	0.43
3:D:22:LYS:HB2	3:D:61:THR:HG21	1.98	0.43
3:D:62:ARG:O	3:D:63:VAL:C	2.61	0.43
3:D:66:ILE:HD13	3:D:75:THR:CG2	2.48	0.43
3:D:236:ILE:O	3:D:237:PRO:C	2.61	0.43
1:B:253:GLU:H	1:B:253:GLU:HG3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89:MET:HE3	2:C:89:MET:HB2	1.93	0.43
3:A:94:LEU:HD22	3:A:98:GLN:HG2	1.99	0.43
3:A:223:HIS:CE1	3:A:263:VAL:CG2	3.01	0.43
3:D:274:VAL:HG12	3:D:275:SER:H	1.83	0.43
3:D:393:LEU:HD12	3:D:395:SER:N	2.23	0.43
3:D:397:SER:O	3:D:398:GLN:HB2	2.18	0.43
3:D:678:ILE:C	3:D:680:LYS:N	2.69	0.43
3:D:882:PHE:C	3:D:882:PHE:HD1	2.24	0.43
3:A:294:LEU:HD21	3:A:322:LEU:HD11	1.99	0.43
3:A:993:GLN:HG2	3:A:1033:LEU:CD2	2.48	0.43
1:E:351:PRO:O	1:E:352:ASP:OD1	2.37	0.43
3:D:186:ILE:HG22	3:D:187:THR:O	2.18	0.43
2:C:81:ILE:HD11	3:A:77:TYR:CD2	2.53	0.43
3:A:259:MET:HE3	3:A:259:MET:HB2	1.90	0.43
3:A:344:ARG:CZ	3:A:408:LEU:HD11	2.48	0.43
3:A:545:MET:SD	3:A:569:LEU:CD1	3.06	0.43
1:E:212:LEU:HB2	1:E:213:PRO:HD3	2.01	0.43
3:A:24:ASP:O	3:A:28:LEU:HB2	2.17	0.43
3:A:423:ARG:O	3:A:424:MET:C	2.61	0.43
3:A:778:PRO:HB2	3:A:779:PRO:HD3	2.01	0.43
1:E:209:HIS:O	1:E:213:PRO:HG2	2.19	0.43
2:C:45:VAL:HG22	2:C:46:GLU:N	2.33	0.43
3:A:236:ILE:O	3:A:237:PRO:C	2.61	0.43
1:E:212:LEU:C	1:E:214:GLU:H	2.25	0.43
3:D:259:MET:HE3	3:D:259:MET:HB2	1.91	0.43
3:D:303:ASN:HD21	3:D:305:ARG:NH2	2.15	0.43
3:D:476:MET:HE3	3:D:501:ILE:HA	2.00	0.43
3:D:534:LYS:HE2	3:D:577:HIS:HB2	2.00	0.43
3:D:622:ILE:O	3:D:623:CYS:C	2.61	0.43
3:D:666:ASP:O	3:D:670:GLN:HG3	2.19	0.43
3:A:58:ASP:O	3:A:59:ALA:C	2.61	0.43
3:A:218:ASN:O	3:A:222:VAL:HG23	2.19	0.43
3:A:223:HIS:NE2	3:A:263:VAL:HG21	2.34	0.43
3:A:689:GLY:O	3:A:693:LYS:HG3	2.18	0.43
3:A:820:PRO:HB2	8:A:1212:HOH:O	2.18	0.43
3:A:898:PHE:CE1	3:A:902:GLN:NE2	2.87	0.43
3:A:907:GLU:OE2	3:A:907:GLU:N	2.52	0.43
3:D:294:LEU:HD21	3:D:322:LEU:HD11	1.99	0.43
3:D:753:ARG:NH1	8:D:1310:HOH:O	2.51	0.43
3:D:778:PRO:HB2	3:D:779:PRO:HD3	2.01	0.43
3:D:961:PRO:HD2	3:D:962:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:HIS:ND1	1:B:26:PRO:HD2	2.34	0.43
2:C:169:ILE:HG22	2:C:170:GLY:N	2.31	0.43
3:A:206:PHE:CE2	3:A:244:THR:HG21	2.50	0.43
3:A:388:THR:CG2	3:A:399:HIS:HE2	2.29	0.43
1:E:188[B]:VAL:CA	1:E:189:MET:HE3	2.48	0.43
1:E:250:PHE:C	1:E:252:PHE:H	2.26	0.43
2:F:142:LYS:HB2	2:F:144:LEU:HG	2.01	0.43
3:D:54:LYS:O	3:D:55:GLU:CG	2.66	0.43
1:B:192:ARG:O	1:B:194:HIS:CD2	2.72	0.43
2:C:142:LYS:HB2	2:C:144:LEU:HG	2.01	0.43
3:A:617:ASN:O	3:A:618:ILE:C	2.61	0.43
3:A:678:ILE:C	3:A:680:LYS:N	2.69	0.43
1:E:12:PHE:HE2	3:D:545:MET:HE3	1.84	0.43
3:D:363:THR:O	3:D:367:LYS:HG3	2.19	0.43
1:B:356:CYS:O	3:A:719:ASN:ND2	2.52	0.43
3:A:716:ASP:O	3:A:720:VAL:CG1	2.67	0.43
3:A:720:VAL:HG22	8:A:1183:HOH:O	2.18	0.43
3:A:888:ASN:HD22	3:A:889:VAL:N	2.15	0.43
3:A:1038:ARG:O	3:A:1042:LEU:HG	2.19	0.43
3:D:92:LYS:HD2	3:D:1030:THR:CG2	2.49	0.43
3:D:223:HIS:NE2	3:D:263:VAL:HG21	2.34	0.43
3:D:287:PHE:HB2	3:D:329:PHE:CZ	2.53	0.43
3:D:426:LYS:CD	3:D:426:LYS:N	2.72	0.43
3:D:689:GLY:O	3:D:693:LYS:HG3	2.18	0.43
3:A:895:GLN:O	3:A:896:ILE:C	2.61	0.42
3:A:978:VAL:O	3:A:981:LEU:HB3	2.19	0.42
3:D:294:LEU:HD21	3:D:322:LEU:CD1	2.49	0.42
3:D:777:VAL:O	3:D:780:LEU:HB2	2.19	0.42
1:B:128:LYS:HE3	1:B:176:TYR:CD2	2.51	0.42
1:B:194:HIS:HA	1:B:195:PRO:HD3	1.92	0.42
2:C:9:VAL:HG13	2:C:9:VAL:O	2.19	0.42
3:A:511:GLU:HG2	3:A:515:ARG:NH1	2.34	0.42
3:A:840:GLU:O	3:A:845:ARG:HD2	2.18	0.42
3:A:1036:GLU:OE1	3:A:1037:GLU:HG3	2.18	0.42
1:E:70:TRP:CZ2	1:E:97[A]:HIS:HA	2.54	0.42
2:F:13:LEU:HB2	2:F:85:CYS:SG	2.59	0.42
3:D:202:PHE:HD1	3:D:205:ILE:HD11	1.83	0.42
3:A:123:GLU:C	3:A:125:VAL:N	2.73	0.42
3:A:148:THR:O	3:A:149:PHE:C	2.62	0.42
3:A:290:THR:O	3:A:294:LEU:HB2	2.19	0.42
3:A:704:HIS:HB3	3:A:705:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:793:PRO:C	3:A:795:ALA:H	2.26	0.42
3:D:87:ILE:HD13	3:D:137:ILE:HG13	2.00	0.42
3:D:737[B]:GLU:H	3:D:737[B]:GLU:CD	2.26	0.42
3:D:888:ASN:HD22	3:D:889:VAL:N	2.16	0.42
3:D:978:VAL:O	3:D:981:LEU:HB3	2.19	0.42
1:B:353:HIS:HA	1:B:354:PRO:HD3	1.63	0.42
2:C:36:GLU:HA	8:C:673:HOH:O	2.19	0.42
3:A:202:PHE:CZ	3:A:236:ILE:HG21	2.55	0.42
3:A:257:VAL:HG22	3:A:260:PHE:HB2	2.02	0.42
3:A:497:LEU:O	3:A:497:LEU:HD12	2.19	0.42
3:A:607:VAL:HA	8:A:1224:HOH:O	2.18	0.42
3:A:961:PRO:HD2	3:A:962:LEU:H	1.85	0.42
1:E:251:PRO:HG2	1:E:252:PHE:CD1	2.54	0.42
3:D:960:THR:CG2	3:D:968:VAL:HG11	2.29	0.42
2:C:106:ARG:NH1	2:C:107:ASP:OD1	2.52	0.42
3:A:281:GLU:OE2	3:A:281:GLU:HA	2.20	0.42
3:A:731:ALA:HB1	3:A:739:VAL:HG11	2.00	0.42
3:A:882:PHE:C	3:A:882:PHE:HD1	2.25	0.42
3:A:971:GLN:NE2	8:A:1078:HOH:O	2.51	0.42
3:A:978:VAL:HG12	3:A:998:VAL:HG22	2.02	0.42
2:F:15:LEU:HD22	2:F:23:LYS:HD2	2.01	0.42
3:D:261:ARG:HG3	3:D:297:MET:HE1	2.00	0.42
3:D:330:LEU:HB3	3:D:372:TYR:CE1	2.54	0.42
3:D:393:LEU:O	3:D:395:SER:N	2.52	0.42
3:D:738:MET:C	3:D:740:THR:N	2.77	0.42
3:A:436:ASP:C	3:A:437:GLN:HG3	2.44	0.42
3:A:665:TRP:CZ3	3:A:692:LEU:HD21	2.53	0.42
3:A:1036:GLU:HG2	3:A:1037:GLU:N	2.35	0.42
1:E:58:TYR:HB3	1:E:197:TYR:HD1	1.85	0.42
1:E:191:TRP:O	1:E:192:ARG:C	2.62	0.42
1:E:355:GLY:H	3:D:716:ASP:CG	2.28	0.42
3:D:55:GLU:HB3	3:D:56:HIS:H	1.69	0.42
3:D:58:ASP:O	3:D:59:ALA:C	2.62	0.42
3:D:437:GLN:O	3:D:439:GLU:N	2.53	0.42
3:D:724:LEU:CD2	3:D:751:VAL:HG11	2.49	0.42
3:A:294:LEU:HD21	3:A:322:LEU:CD1	2.50	0.42
3:A:930:VAL:HG12	3:A:931:THR:N	2.33	0.42
3:A:982:LEU:HD13	3:A:1018:PHE:CZ	2.55	0.42
1:E:95:PRO:HB2	1:E:101:GLN:HE22	1.85	0.42
3:D:544:ILE:HG22	3:D:545:MET:CE	2.46	0.42
3:D:916[A]:GLN:HA	3:D:916[A]:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ARG:NH1	8:B:384:HOH:O	2.52	0.42
3:A:87:ILE:HD13	3:A:137:ILE:HG13	2.01	0.42
3:A:327:CYS:O	3:A:331:LYS:HB2	2.20	0.42
3:A:487:THR:C	3:A:489:TRP:H	2.26	0.42
3:A:833:MET:HE2	3:A:833:MET:HB3	1.89	0.42
3:D:106:VAL:O	3:D:110:ILE:HG13	2.20	0.42
3:D:481:GLN:OE1	3:D:485:ASN:ND2	2.53	0.42
3:D:482:ASN:HA	3:D:486:GLY:HA3	2.01	0.42
3:D:569:LEU:HD11	3:D:591:ILE:HD12	2.02	0.42
1:B:191:TRP:O	1:B:192:ARG:C	2.63	0.42
3:A:482:ASN:HA	3:A:486:GLY:HA3	2.01	0.42
3:A:882:PHE:HA	3:A:890:ALA:HA	2.01	0.42
1:E:52[B]:LYS:HD2	1:E:265:HIS:CG	2.55	0.42
2:F:106:ARG:NH1	2:F:107:ASP:OD1	2.52	0.42
3:D:946:LEU:O	3:D:947:ALA:C	2.62	0.42
1:B:104:LEU:HB2	1:B:270:SER:HA	2.01	0.42
1:B:123:VAL:HG22	1:B:257:LEU:CD2	2.50	0.42
3:A:231:ARG:HA	3:A:231:ARG:HD3	1.90	0.42
3:A:920:CYS:O	3:A:923:LEU:HB2	2.20	0.42
1:E:128:LYS:CE	3:D:623:CYS:O	2.68	0.42
1:E:224:LEU:HA	8:E:767:HOH:O	2.19	0.42
2:F:89:MET:HE3	2:F:89:MET:HB2	1.94	0.42
3:D:19:PHE:O	3:D:19:PHE:CG	2.72	0.42
3:D:286:LEU:HD12	3:D:286:LEU:O	2.19	0.42
3:D:487:THR:C	3:D:489:TRP:H	2.26	0.42
3:A:685:VAL:HA	3:A:688:LEU:HD12	2.02	0.41
1:E:208:MET:HG2	1:E:212:LEU:HD11	2.01	0.41
1:E:278:ARG:HB2	1:E:281:MET:HG3	2.01	0.41
2:F:88:ILE:HB	2:F:119:LEU:HD23	2.02	0.41
3:D:104:LYS:HA	3:D:104:LYS:HD2	1.76	0.41
3:D:216:SER:HB2	3:D:222:VAL:HG21	2.02	0.41
1:B:153:SER:O	1:B:226:PRO:HD2	2.20	0.41
3:A:23:LEU:HD12	3:A:23:LEU:N	2.35	0.41
3:A:23:LEU:HD13	3:A:26:ASN:CB	2.50	0.41
3:A:246:LEU:O	3:A:250:LEU:HG	2.20	0.41
3:A:1054:MET:HA	8:A:1213:HOH:O	2.19	0.41
1:E:121:VAL:CG2	1:E:257:LEU:HB3	2.50	0.41
3:D:95:PRO:HG2	3:D:98:GLN:HB2	2.02	0.41
3:D:403:PRO:HA	3:D:404:PRO:HD3	1.83	0.41
3:A:251:ILE:HD13	3:A:289:LEU:HB2	2.02	0.41
3:A:849:PHE:CZ	3:A:881:ALA:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1005:ASN:OD1	3:A:1005:ASN:C	2.63	0.41
3:D:57:PRO:HA	3:D:60:TRP:CZ3	2.55	0.41
3:D:338:GLU:OE2	3:D:409:TYR:HE2	2.03	0.41
3:D:423:ARG:O	3:D:424:MET:C	2.63	0.41
2:C:9:VAL:O	2:C:9:VAL:HG22	2.20	0.41
2:C:39:TYR:HA	8:C:555:HOH:O	2.20	0.41
3:D:920:CYS:O	3:D:923:LEU:HB2	2.21	0.41
3:A:142:TRP:CD1	3:A:142:TRP:C	2.98	0.41
3:A:308:TYR:CE1	3:A:365:ILE:HD11	2.55	0.41
3:A:403:PRO:HA	3:A:404:PRO:HD3	1.84	0.41
3:A:1003:SER:HA	3:A:1046:GLN:HE21	1.86	0.41
1:E:43:ARG:CG	1:E:46:ARG:HH12	2.33	0.41
1:E:188[A]:VAL:CA	1:E:189:MET:HE3	2.50	0.41
3:D:268:LEU:HD22	3:D:286:LEU:CD1	2.50	0.41
3:D:918:TYR:O	3:D:921:ASP:HB2	2.20	0.41
3:D:1005:ASN:OD1	3:D:1005:ASN:C	2.63	0.41
1:B:121:VAL:CG2	1:B:257:LEU:HB3	2.50	0.41
1:E:25:HIS:ND1	1:E:26:PRO:HD2	2.35	0.41
3:D:930:VAL:HG12	3:D:931:THR:N	2.34	0.41
1:B:118:GLU:OE1	1:B:118:GLU:HA	2.21	0.41
3:A:153:ILE:HG13	3:A:154:VAL:N	2.36	0.41
3:A:338:GLU:OE2	3:A:409:TYR:HE2	2.03	0.41
3:A:887:ARG:HD2	3:A:887:ARG:HA	1.59	0.41
1:E:124:CYS:HA	1:E:125:PRO:HD3	1.68	0.41
1:E:235:PHE:CE2	1:E:248:MET:HE1	2.56	0.41
3:D:398:GLN:O	3:D:399:HIS:O	2.38	0.41
3:D:888:ASN:ND2	3:D:888:ASN:N	2.68	0.41
3:A:424:MET:HA	3:A:457:MET:HE2	2.03	0.41
2:F:118:VAL:HG23	2:F:164:LEU:HD21	2.03	0.41
3:D:142:TRP:CD1	3:D:142:TRP:C	2.98	0.41
3:D:146:TRP:N	3:D:147:PRO:CD	2.84	0.41
3:D:287:PHE:CE2	3:D:337:LEU:HD13	2.55	0.41
3:D:940:THR:O	3:D:944:SER:HB2	2.21	0.41
2:C:122:ASN:O	2:C:123:LYS:HB2	2.20	0.41
3:A:33:ASN:HD22	3:A:44:ARG:HE	1.69	0.41
3:A:290:THR:HG21	3:A:325:PHE:CZ	2.55	0.41
3:A:417:ARG:NH2	3:A:464:LEU:O	2.47	0.41
3:A:1009:PRO:O	3:A:1013:GLU:HG2	2.20	0.41
1:E:187:ASP:HB3	1:E:189:MET:CE	2.51	0.41
2:F:77:ASP:HA	2:F:80:TYR:CD2	2.56	0.41
3:D:97:ASN:H	3:D:97:ASN:HD22	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:223:HIS:CE1	3:D:263:VAL:CG2	3.04	0.41
3:D:517:LEU:O	3:D:521:ILE:HG12	2.21	0.41
3:D:574:HIS:HD2	3:D:624:ASP:CG	2.29	0.41
3:D:993:GLN:HG2	3:D:1033:LEU:HD13	2.03	0.41
3:D:1012:LYS:HE2	3:D:1012:LYS:HB3	1.85	0.41
1:B:58:TYR:HB3	1:B:197:TYR:CD1	2.56	0.41
2:C:42:THR:OG1	5:C:217:GTP:O1G	2.36	0.41
2:C:54:THR:HG22	2:C:176:PHE:HD1	1.86	0.41
3:A:63:VAL:HA	3:A:76:LYS:CG	2.48	0.41
3:A:190:LYS:HB2	3:A:190:LYS:HE3	1.78	0.41
1:E:242:LEU:O	1:E:246:LEU:HB2	2.21	0.41
3:D:24:ASP:O	3:D:28:LEU:HB2	2.20	0.41
3:D:202:PHE:CE2	3:D:206:PHE:HD1	2.38	0.41
3:D:242:PHE:HB3	3:D:282:GLN:HG2	2.03	0.41
1:B:15:SER:HB2	8:B:546:HOH:O	2.20	0.40
3:A:467:LEU:HD23	3:A:467:LEU:N	2.36	0.40
3:A:962:LEU:O	3:A:962:LEU:HG	2.20	0.40
2:F:106:ARG:HD3	3:D:181:PHE:CD2	2.54	0.40
3:D:1009:PRO:O	3:D:1013:GLU:HG2	2.21	0.40
1:B:201:THR:HG22	1:B:204:ARG:HH12	1.85	0.40
1:E:245:VAL:HA	1:E:248:MET:HG3	2.03	0.40
3:D:231:ARG:HA	3:D:231:ARG:HD3	1.92	0.40
3:D:393:LEU:C	3:D:395:SER:N	2.78	0.40
3:D:525:LEU:CD1	3:D:544:ILE:HD13	2.52	0.40
3:D:659:LEU:O	3:D:663:GLN:HG3	2.22	0.40
3:D:772:VAL:CG1	3:D:811:LEU:HD11	2.51	0.40
3:D:962:LEU:CB	3:D:964:PRO:HD3	2.51	0.40
3:D:975:GLN:HG2	3:D:998:VAL:HG12	2.02	0.40
1:B:35:TYR:CD2	1:B:35:TYR:O	2.75	0.40
1:B:41:SER:HB2	1:B:110:ASP:HB3	2.02	0.40
1:B:61:HIS:CG	1:B:94:LEU:HD13	2.55	0.40
1:B:124:CYS:HA	1:B:125:PRO:HD3	1.67	0.40
1:B:187:ASP:OD2	1:B:204:ARG:NH2	2.54	0.40
3:A:419:LEU:HD23	3:A:420:MET:CE	2.52	0.40
3:A:422:SER:OG	3:A:479:LYS:HE3	2.21	0.40
3:A:549:GLY:HA3	8:A:1115:HOH:O	2.21	0.40
1:E:245:VAL:HA	1:E:248:MET:SD	2.61	0.40
3:D:898:PHE:CE1	3:D:902:GLN:NE2	2.89	0.40
2:C:146:TYR:OH	2:C:148:ASP:OD1	2.30	0.40
3:A:146:TRP:N	3:A:147:PRO:CD	2.84	0.40
3:A:435:ASN:C	3:A:437:GLN:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:222:VAL:O	3:D:226:LEU:HB2	2.21	0.40
3:D:238:LEU:HD22	3:D:242:PHE:HE2	1.86	0.40
3:A:289:LEU:HD12	3:A:289:LEU:N	2.36	0.40
3:A:465:THR:O	3:A:469:TYR:HB3	2.21	0.40
3:A:575:GLU:OE2	3:A:577:HIS:HB2	2.21	0.40
3:D:53:LEU:O	3:D:54:LYS:C	2.65	0.40
3:D:76:LYS:HE2	3:D:126:TYR:CZ	2.56	0.40
3:D:441:VAL:HG12	3:D:628:GLN:CD	2.46	0.40
3:D:793:PRO:C	3:D:795:ALA:H	2.29	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	B	266/365 (73%)	241 (91%)	20 (8%)	5 (2%)	6	11
1	E	277/365 (76%)	253 (91%)	16 (6%)	8 (3%)	3	5
2	C	170/216 (79%)	157 (92%)	11 (6%)	2 (1%)	10	20
2	F	169/216 (78%)	157 (93%)	9 (5%)	3 (2%)	6	12
3	A	1042/1073 (97%)	945 (91%)	79 (8%)	18 (2%)	7	13
3	D	1045/1073 (97%)	952 (91%)	71 (7%)	22 (2%)	5	9
All	All	2969/3308 (90%)	2705 (91%)	206 (7%)	58 (2%)	6	10

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	216	GLU
1	B	351	PRO

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Mol	Chain	Res	Type
2	C	169	ILE
3	A	123	GLU
3	A	390	ALA
3	A	963	ASN
1	E	94	LEU
1	E	351	PRO
1	E	359	GLU
3	D	399	HIS
3	D	963	ASN
1	B	286	LEU
3	A	54	LYS
3	A	486	GLY
3	A	964	PRO
1	E	286	LEU
2	F	55	ASN
3	D	54	LYS
3	D	216	SER
3	D	486	GLY
3	D	490	SER
3	D	623	CYS
3	A	216	SER
3	A	217	GLN
3	A	490	SER
3	A	623	CYS
3	A	961	PRO
2	F	178	ALA
3	D	217	GLN
3	D	438	GLY
3	D	961	PRO
1	B	97	HIS
2	C	178	ALA
3	A	277	SER
3	A	281	GLU
3	A	743	PRO
1	E	358	MET
3	D	53	LEU
3	D	277	SER
3	D	487	THR
3	D	737[A]	GLU
3	D	737[B]	GLU
3	D	743	PRO
3	A	143	PRO

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Mol	Chain	Res	Type
3	A	487	THR
3	D	143	PRO
3	D	281	GLU
3	D	679	LEU
3	A	55	GLU
3	A	955	GLU
1	E	52[A]	LYS
1	E	52[B]	LYS
1	E	285	VAL
3	D	764	SER
3	D	955	GLU
3	D	111	ILE
2	F	81	ILE

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	B	249/327 (76%)	230 (92%)	19 (8%)	12	26
1	E	257/327 (79%)	242 (94%)	15 (6%)	18	38
2	C	151/185 (82%)	137 (91%)	14 (9%)	8	18
2	F	150/185 (81%)	137 (91%)	13 (9%)	9	21
3	A	950/973 (98%)	879 (92%)	71 (8%)	12	26
3	D	953/973 (98%)	882 (92%)	71 (8%)	12	26
All	All	2710/2970 (91%)	2507 (92%)	203 (8%)	12	26

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	TYR
1	B	111	VAL
1	B	120	ILE
1	B	129	ARG
1	B	156	LEU

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Mol	Chain	Res	Type
1	B	185	VAL
1	B	189	MET
1	B	201	THR
1	B	222	THR
1	B	245	VAL
1	B	271	THR
1	B	274	VAL
1	B	277	LEU
1	B	284	ASP
1	B	285	VAL
1	B	351	PRO
1	B	352	ASP
1	B	353	HIS
1	B	360	ASN
2	C	13	LEU
2	C	15	LEU
2	C	21	THR
2	C	28	LYS
2	C	40	VAL
2	C	59	ILE
2	C	60	LYS
2	C	77	ASP
2	C	95	ARG
2	C	127	LYS
2	C	134	LYS
2	C	140	ARG
2	C	154	ASN
2	C	173	ASN
3	A	18	ASP
3	A	23	LEU
3	A	24	ASP
3	A	25	ILE
3	A	50	LEU
3	A	60	TRP
3	A	62	ARG
3	A	71	GLN
3	A	80	LEU
3	A	81	GLN
3	A	97	ASN
3	A	103	LYS
3	A	119	CYS
3	A	146	TRP

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Mol	Chain	Res	Type
3	A	150	ILE
3	A	159	THR
3	A	168	MET
3	A	169	VAL
3	A	189	VAL
3	A	190	LYS
3	A	192	LYS
3	A	194	LEU
3	A	198	MET
3	A	205	ILE
3	A	208	LEU
3	A	218	ASN
3	A	226	LEU
3	A	229	LEU
3	A	257	VAL
3	A	263	VAL
3	A	294	LEU
3	A	301	ASN
3	A	331	LYS
3	A	393	LEU
3	A	394	LEU
3	A	401	ASP
3	A	426	LYS
3	A	443	GLU
3	A	445	MET
3	A	521	ILE
3	A	525	LEU
3	A	530	GLN
3	A	569	LEU
3	A	578	ASP
3	A	618	ILE
3	A	620	THR
3	A	646	ASP
3	A	653	LEU
3	A	656	LYS
3	A	678	ILE
3	A	685	VAL
3	A	710	LEU
3	A	720	VAL
3	A	727	ASN
3	A	740	THR
3	A	746	ARG

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Mol	Chain	Res	Type
3	A	781	LEU
3	A	807	ILE
3	A	815	ILE
3	A	818	GLU
3	A	875	LEU
3	A	882	PHE
3	A	888	ASN
3	A	900	LEU
3	A	907	GLU
3	A	930	VAL
3	A	958	ILE
3	A	968	VAL
3	A	999	THR
3	A	1008	ILE
3	A	1016	ARG
1	E	-2	LEU
1	E	35	TYR
1	E	43	ARG
1	E	47	LEU
1	E	56	LEU
1	E	120	ILE
1	E	126	VAL
1	E	149	VAL
1	E	189	MET
1	E	245	VAL
1	E	271	THR
1	E	282	VAL
1	E	283	SER
1	E	286	LEU
1	E	353	HIS
2	F	9	VAL
2	F	13	LEU
2	F	15	LEU
2	F	34	GLU
2	F	55	ASN
2	F	59	ILE
2	F	69	LEU
2	F	89	MET
2	F	119	LEU
2	F	134	LYS
2	F	140	ARG
2	F	154	ASN

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Mol	Chain	Res	Type
2	F	177	VAL
3	D	17	LEU
3	D	18	ASP
3	D	25	ILE
3	D	37	HIS
3	D	80	LEU
3	D	81	GLN
3	D	96	ARG
3	D	97	ASN
3	D	122	LYS
3	D	146	TRP
3	D	150	ILE
3	D	168	MET
3	D	169	VAL
3	D	189	VAL
3	D	192	LYS
3	D	194	LEU
3	D	198	MET
3	D	204	GLN
3	D	205	ILE
3	D	217	GLN
3	D	218	ASN
3	D	226	LEU
3	D	229	LEU
3	D	257	VAL
3	D	263	VAL
3	D	294	LEU
3	D	301	ASN
3	D	312	LYS
3	D	331	LYS
3	D	341	LEU
3	D	399	HIS
3	D	401	ASP
3	D	426	LYS
3	D	436	ASP
3	D	447	ASP
3	D	521	ILE
3	D	525	LEU
3	D	578	ASP
3	D	618	ILE
3	D	653	LEU
3	D	655	GLU

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Mol	Chain	Res	Type
3	D	656	LYS
3	D	678	ILE
3	D	685	VAL
3	D	708[A]	ILE
3	D	708[B]	ILE
3	D	710	LEU
3	D	720	VAL
3	D	724	LEU
3	D	727	ASN
3	D	740	THR
3	D	746	ARG
3	D	767	ASN
3	D	781	LEU
3	D	815	ILE
3	D	818	GLU
3	D	821	GLN
3	D	875	LEU
3	D	882	PHE
3	D	888	ASN
3	D	900	LEU
3	D	930	VAL
3	D	958	ILE
3	D	999	THR
3	D	1008	ILE
3	D	1016	ARG
3	D	1029	ASP
3	D	1030	THR
3	D	1031	SER
3	D	1032	ASP
3	D	1035	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	B	51	GLN
1	B	61	HIS
1	B	101	GLN
1	B	209	HIS
1	B	261	HIS
1	B	263	GLN
1	B	353	HIS

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Mol	Chain	Res	Type
2	C	30	HIS
2	C	62	ASN
2	C	103	ASN
2	C	105	HIS
2	C	145	GLN
2	C	156	ASN
3	A	30	ASN
3	A	33	ASN
3	A	37	HIS
3	A	56	HIS
3	A	97	ASN
3	A	166	ASN
3	A	200	ASN
3	A	204	GLN
3	A	210	GLN
3	A	215	ASN
3	A	218	ASN
3	A	293	GLN
3	A	296	GLN
3	A	321	ASN
3	A	352	HIS
3	A	437	GLN
3	A	456	ASN
3	A	466	HIS
3	A	483	GLN
3	A	577	HIS
3	A	626	GLN
3	A	663	GLN
3	A	704	HIS
3	A	775	ASN
3	A	809	ASN
3	A	858	HIS
3	A	888	ASN
3	A	924	GLN
3	A	963	ASN
3	A	969	ASN
3	A	970	ASN
3	A	988	HIS
3	A	990	GLN
3	A	993	GLN
3	A	1006	GLN
3	A	1021	GLN

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Mol	Chain	Res	Type
3	A	1046	GLN
3	A	1050	HIS
1	E	19	ASN
1	E	51	GLN
1	E	61	HIS
1	E	200	GLN
1	E	209	HIS
1	E	261	HIS
1	E	263	GLN
1	E	353	HIS
1	E	360	ASN
2	F	30	HIS
2	F	103	ASN
2	F	105	HIS
2	F	145	GLN
2	F	156	ASN
3	D	43	GLN
3	D	56	HIS
3	D	97	ASN
3	D	166	ASN
3	D	185	GLN
3	D	200	ASN
3	D	204	GLN
3	D	210	GLN
3	D	215	ASN
3	D	217	GLN
3	D	218	ASN
3	D	293	GLN
3	D	296	GLN
3	D	321	ASN
3	D	352	HIS
3	D	407	GLN
3	D	456	ASN
3	D	483	GLN
3	D	530	GLN
3	D	601	GLN
3	D	619	ASN
3	D	704	HIS
3	D	742	GLN
3	D	775	ASN
3	D	809	ASN
3	D	814	HIS

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Mol	Chain	Res	Type
3	D	856	ASN
3	D	858	HIS
3	D	888	ASN
3	D	924	GLN
3	D	963	ASN
3	D	988	HIS
3	D	993	GLN
3	D	1021	GLN
3	D	1044	GLN
3	D	1046	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	GTP	C	217	-	33,34,34	0.84	0	50,54,54	1.55	9 (18%)
5	GTP	F	217	-	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)

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	GTP	C	217	-	-	2/22/38/38	0/3/3/3
5	GTP	F	217	-	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	217	GTP	PB-O3B	2.01	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	217	GTP	C5-C4-N3	-4.64	121.01	128.39
5	C	217	GTP	C5-C4-N3	-4.60	121.07	128.39
5	C	217	GTP	C2-N3-C4	4.42	119.91	112.30
5	F	217	GTP	C2-N3-C4	4.26	119.63	112.30
5	F	217	GTP	N9-C8-N7	-3.03	107.79	113.40
5	F	217	GTP	C8-N7-C5	2.90	109.42	104.26
5	C	217	GTP	N9-C8-N7	-2.84	108.13	113.40
5	C	217	GTP	C2-N1-C6	-2.80	120.03	125.11
5	C	217	GTP	N9-C4-N3	2.68	131.32	125.95
5	F	217	GTP	N9-C4-N3	2.67	131.29	125.95
5	F	217	GTP	C2-N1-C6	-2.59	120.42	125.11
5	C	217	GTP	C8-N7-C5	2.53	108.78	104.26
5	C	217	GTP	C5-C6-N1	2.33	119.17	113.25
5	F	217	GTP	C5-C6-N1	2.25	118.98	113.25
5	F	217	GTP	C4-C5-N7	-2.23	107.14	110.67
5	C	217	GTP	O3G-PG-O3B	2.04	111.47	104.64
5	C	217	GTP	C4-C5-N7	-2.02	107.47	110.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

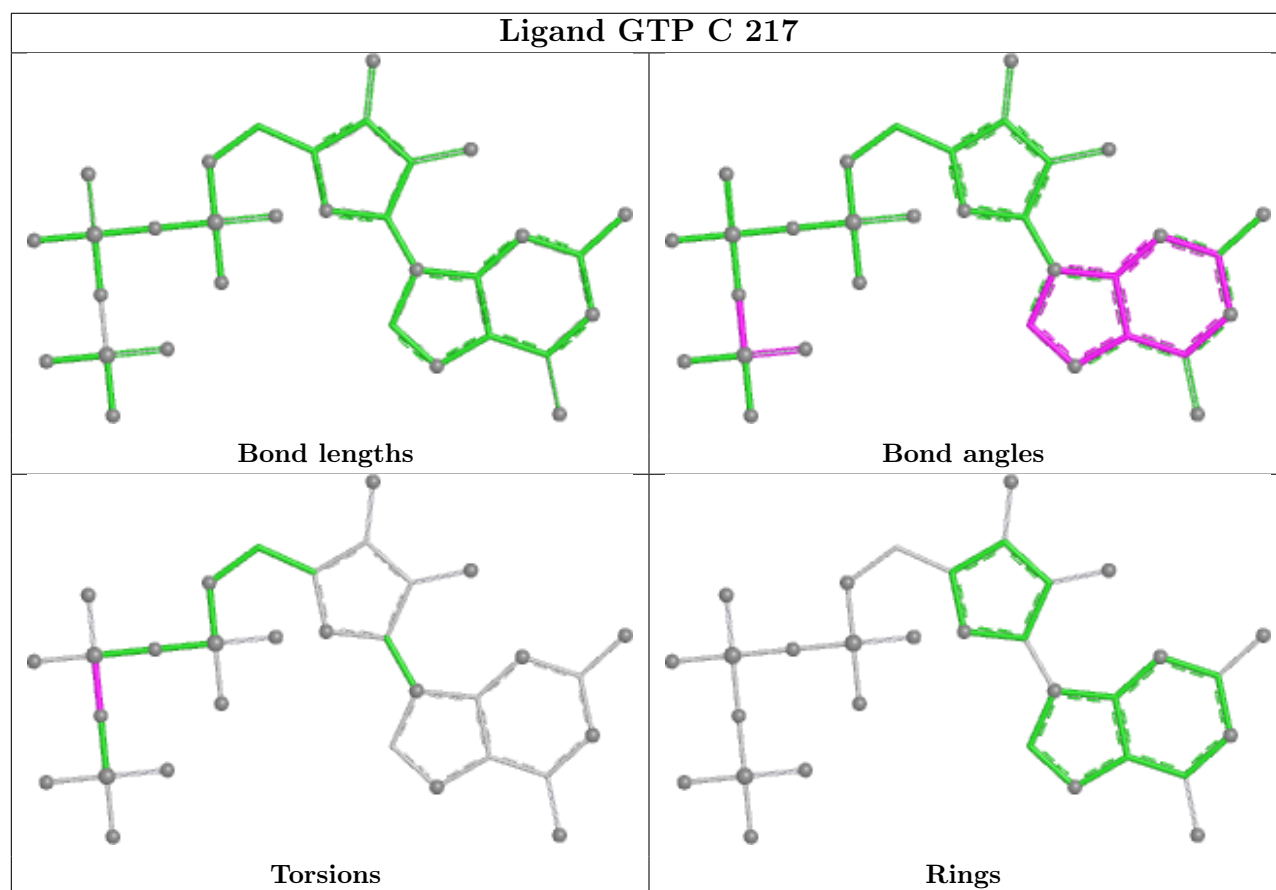
Mol	Chain	Res	Type	Atoms
5	F	217	GTP	PG-O3B-PB-O1B
5	C	217	GTP	PG-O3B-PB-O1B
5	C	217	GTP	PG-O3B-PB-O2B
5	F	217	GTP	PG-O3B-PB-O2B

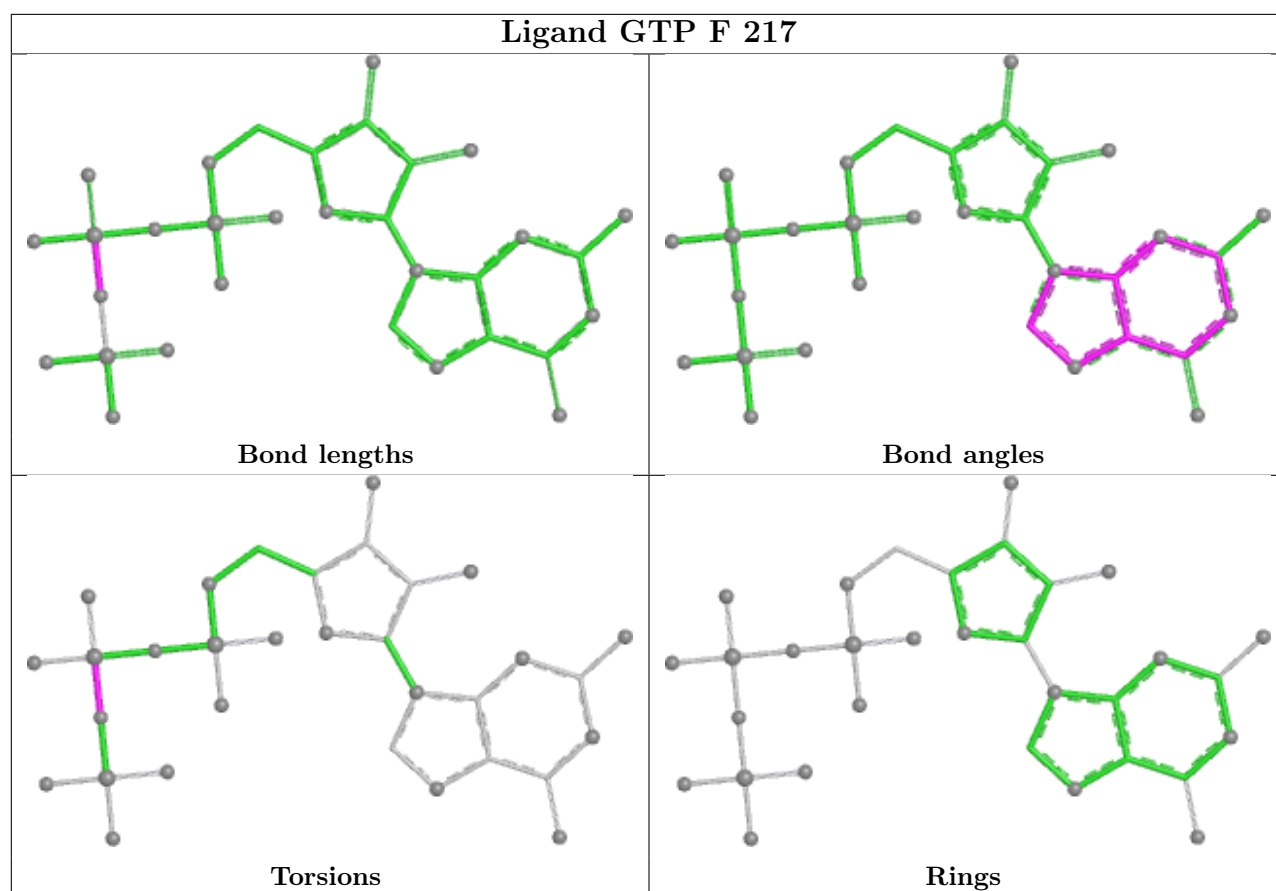
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	217	GTP	3	0
5	F	217	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	B	274/365 (75%)	-0.74	0	100	100	12, 36, 78, 112	4 (1%)
1	E	279/365 (76%)	-0.64	0	100	100	12, 36, 85, 126	8 (2%)
2	C	171/216 (79%)	-0.90	0	100	100	20, 43, 73, 99	1 (0%)
2	F	171/216 (79%)	-0.95	0	100	100	20, 42, 77, 99	0
3	A	1041/1073 (97%)	-0.73	1 (0%)	92	90	11, 46, 100, 152	6 (0%)
3	D	1041/1073 (97%)	-0.70	6 (0%)	85	83	12, 46, 107, 156	13 (1%)
All	All	2977/3308 (89%)	-0.73	7 (0%)	91	89	11, 43, 96, 156	32 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1053	GLN	2.7
3	D	70	SER	2.6
3	D	966	ASN	2.5
3	D	276	VAL	2.4
3	A	70	SER	2.1
3	D	395	SER	2.1
3	D	967	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

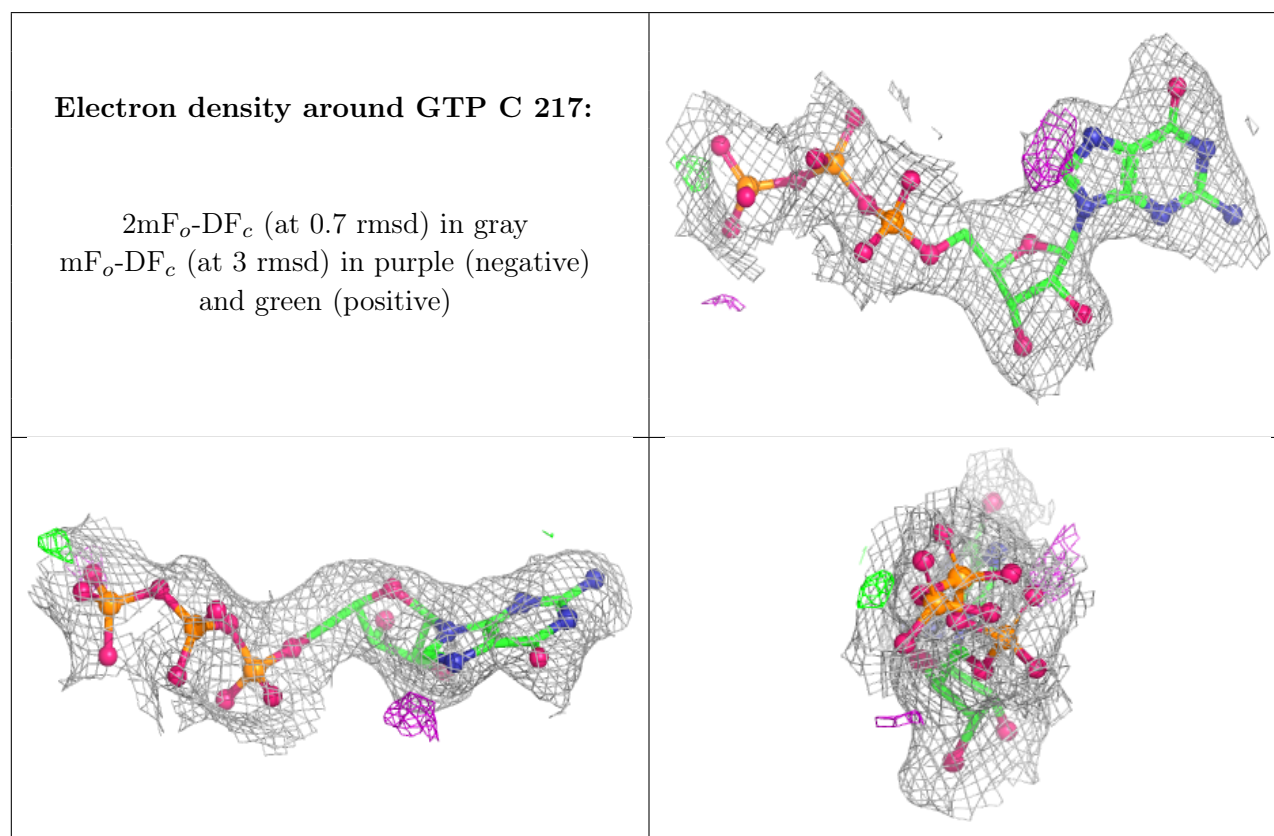
There are no oligosaccharides in this entry.

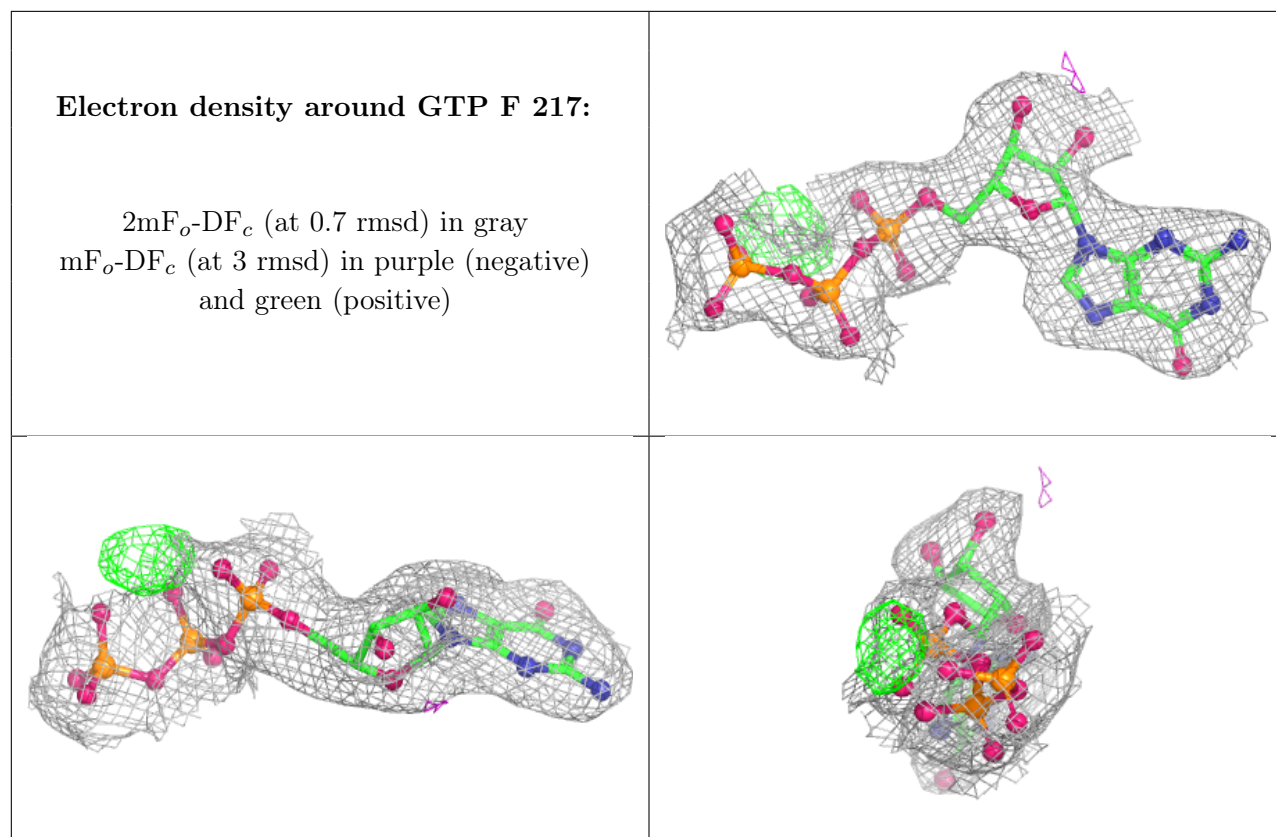
6.4 Ligands ⓘ

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, 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	B-factors(Å ²)	Q<0.9
6	MG	F	218	1/1	0.98	0.04	33,33,33,33	0
4	NA	E	361	1/1	0.99	0.09	64,64,64,64	0
5	GTP	C	217	32/32	0.99	0.03	13,27,39,52	0
5	GTP	F	217	32/32	0.99	0.03	14,27,40,50	0
4	NA	B	361	1/1	0.99	0.06	34,34,34,34	0
7	CL	E	362	1/1	0.99	0.04	49,49,49,49	0
6	MG	C	218	1/1	1.00	0.02	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.