



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:32 PM UTC

PDB ID : 3F3F / pdb_00003f3f
Title : Crystal structure of the nucleoporin pair Nup85-Seh1, space group P21
Authors : Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.
Deposited on : 2008-10-30
Resolution : 2.90 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:

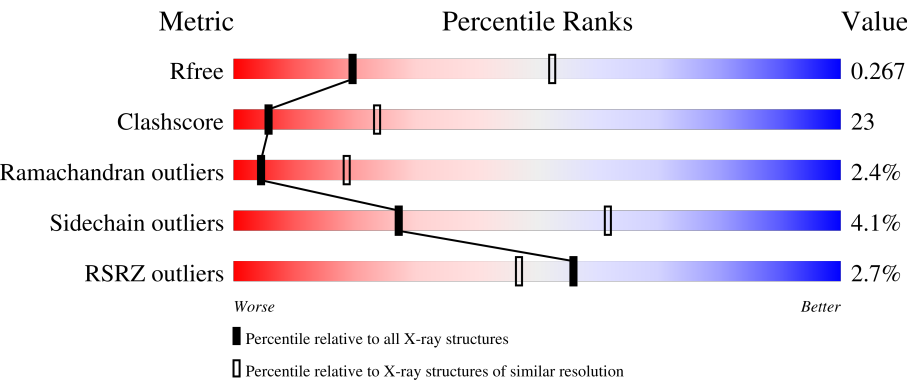
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	351	
1	B	351	
1	E	351	
1	F	351	
2	C	570	

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Mol	Chain	Length	Quality of chain
2	D	570	2% 51% 32% • 13%
2	G	570	2% 52% 27% • 16%
2	H	570	3% 52% 29% 5% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25239 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2448	1549	425	463	11			
1	B	307	Total	C	N	O	S	0	0	0
			2438	1543	423	461	11			
1	E	306	Total	C	N	O	S	0	0	0
			2432	1540	422	459	11			
1	F	306	Total	C	N	O	S	0	0	0
			2430	1538	422	459	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P53011
A	1A	HIS	-	expression tag	UNP P53011
B	1A	PRO	-	expression tag	UNP P53011
B	1B	HIS	-	expression tag	UNP P53011
E	1A	PRO	-	expression tag	UNP P53011
E	1B	HIS	-	expression tag	UNP P53011
F	0	PRO	-	expression tag	UNP P53011
F	1A	HIS	-	expression tag	UNP P53011

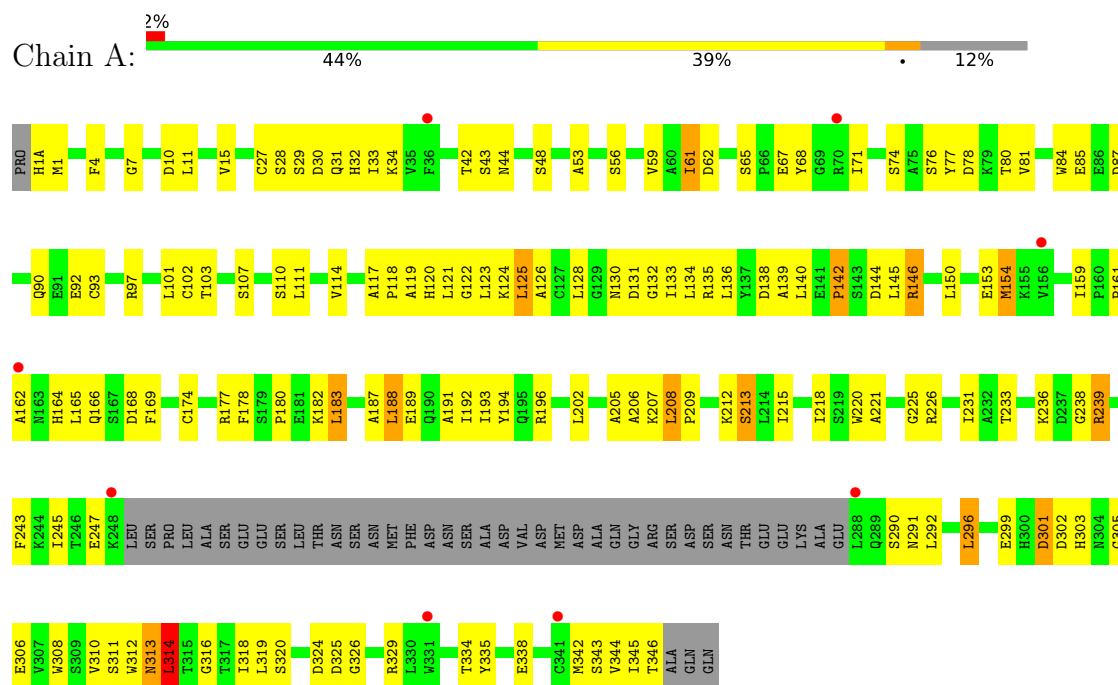
- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	475	Total	C	N	O	S	0	0	0
			3812	2451	608	732	21			
2	D	495	Total	C	N	O	S	0	0	0
			3959	2533	633	770	23			
2	G	476	Total	C	N	O	S	0	0	0
			3820	2447	613	738	22			
2	H	487	Total	C	N	O	S	0	0	0
			3900	2501	624	753	22			

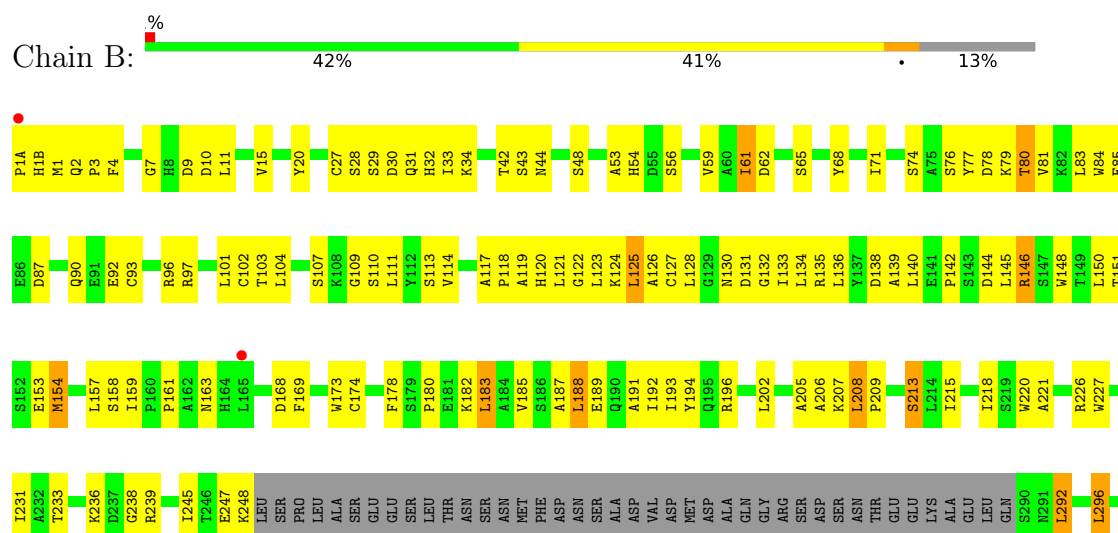
3 Residue-property plots

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: Nucleoporin SEH1

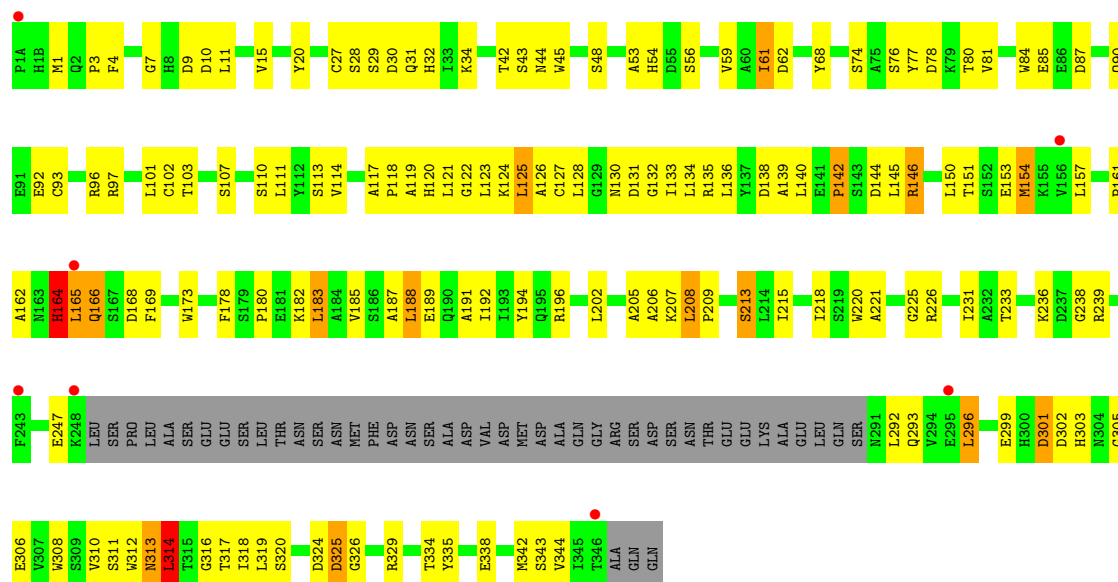
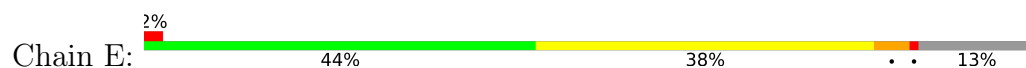


• Molecule 1: Nucleoporin SEH1

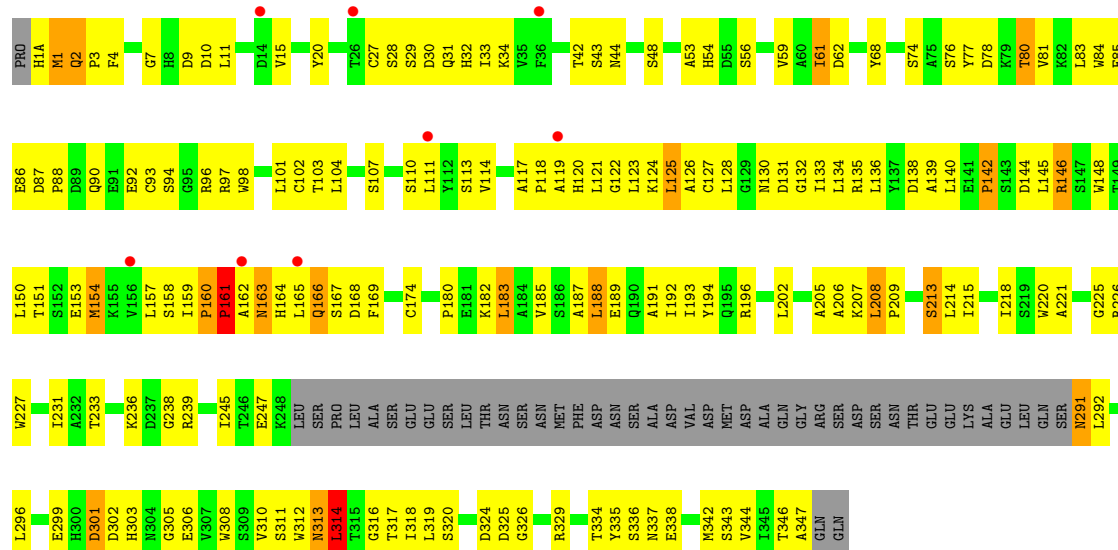




• Molecule 1: Nucleoporin SEH1

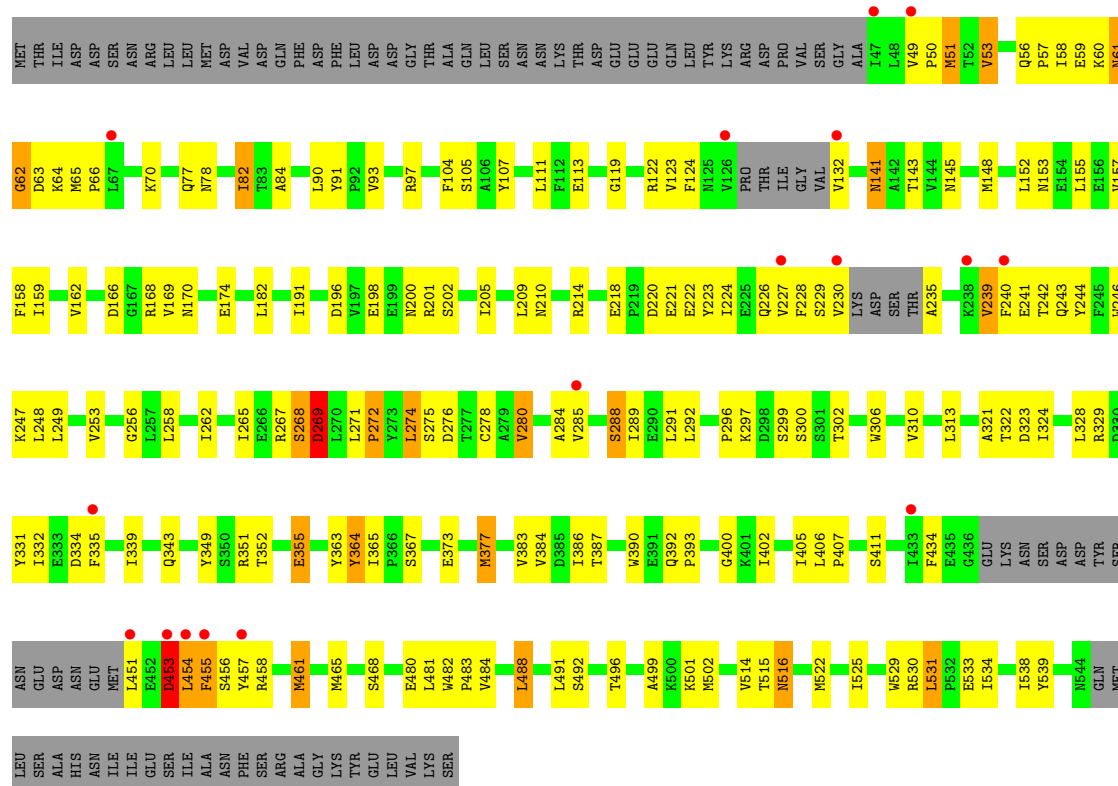


• Molecule 1: Nucleoporin SEH1

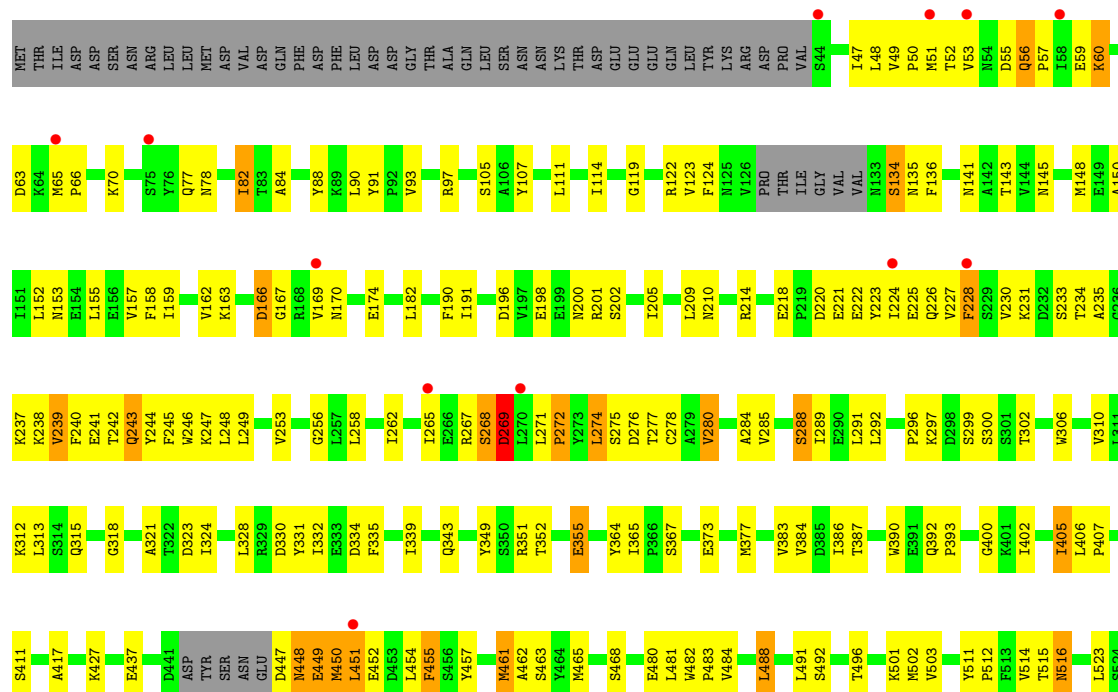


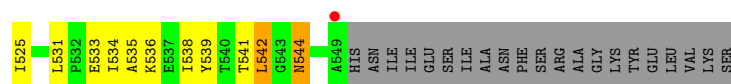
• Molecule 2: Nucleoporin NUP85



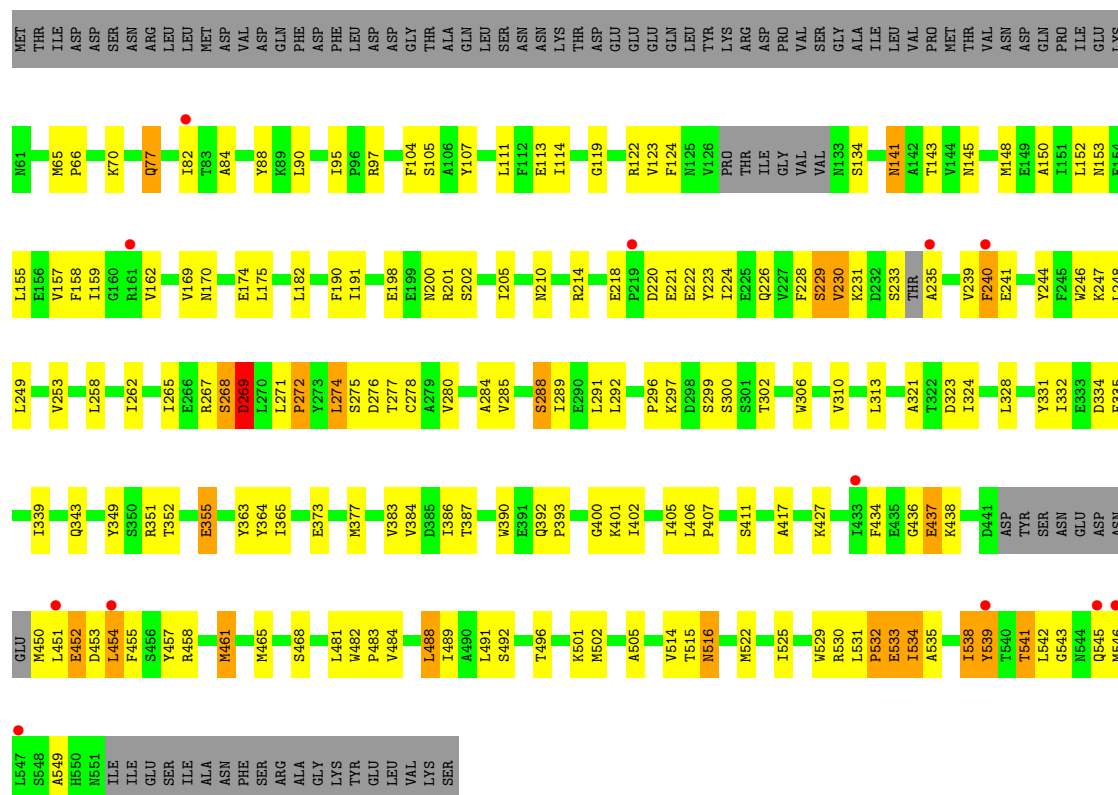


• Molecule 2: Nucleoporin NUP85

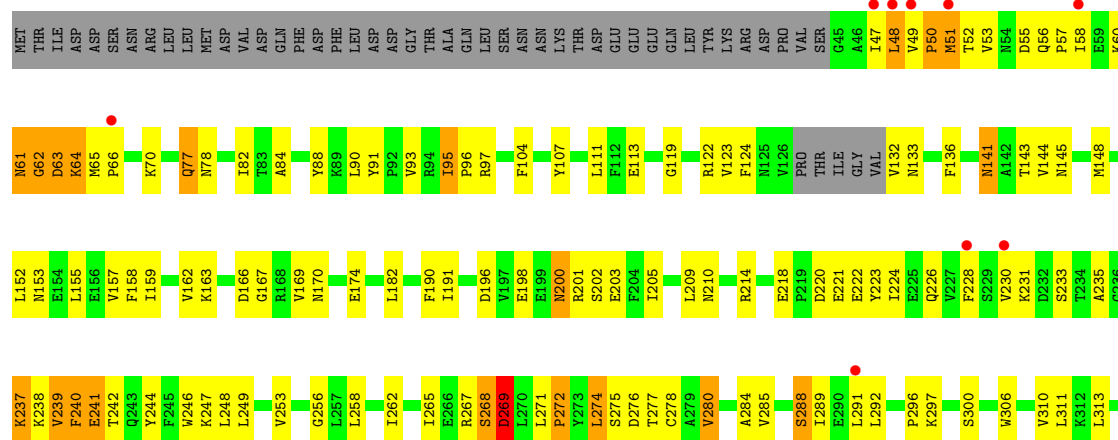


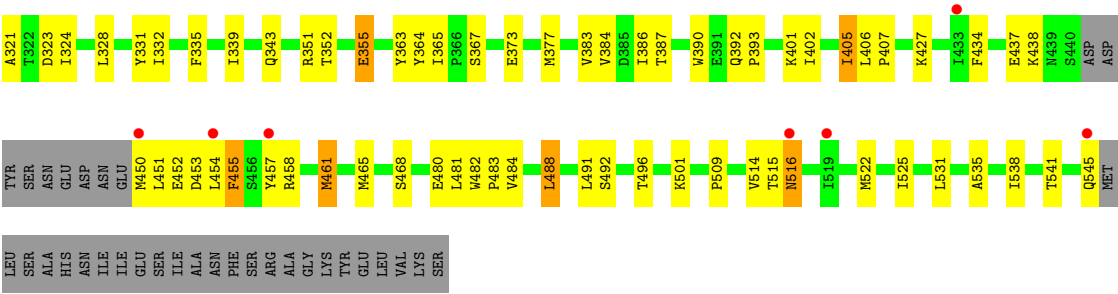


• Molecule 2: Nucleoporin NUP85



• Molecule 2: Nucleoporin NUP85





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.84Å 166.19Å 188.90Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 89.6 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.246 , 0.265 0.248 , 0.267	Depositor DCC
R_{free} test set	10747 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25239	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

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	0.54	0/2510	1.03	13/3403 (0.4%)
1	B	0.48	1/2501 (0.0%)	1.01	10/3391 (0.3%)
1	E	0.54	0/2495	1.02	9/3383 (0.3%)
1	F	0.50	0/2492	1.00	10/3379 (0.3%)
2	C	0.53	1/3889 (0.0%)	1.04	18/5265 (0.3%)
2	D	0.50	0/4037	1.06	20/5463 (0.4%)
2	G	0.56	0/3896	1.02	19/5268 (0.4%)
2	H	0.51	0/3978	1.00	15/5384 (0.3%)
All	All	0.52	2/25798 (0.0%)	1.02	114/34936 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	MET	SD-CE	5.14	1.92	1.79
2	C	377	MET	SD-CE	5.04	1.92	1.79

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	454	LEU	N-CA-C	11.64	126.26	111.24
2	D	228	PHE	N-CA-C	9.16	122.57	111.40
2	C	453	ASP	N-CA-C	8.85	122.33	108.79
2	H	288	SER	N-CA-C	-8.65	100.85	111.40
2	G	461	MET	N-CA-C	-8.57	102.60	113.23
2	C	288	SER	N-CA-C	-8.49	101.04	111.40
2	G	288	SER	N-CA-C	-8.45	101.30	111.69
2	D	288	SER	N-CA-C	-8.42	101.33	111.69
2	C	461	MET	N-CA-C	-8.40	102.81	113.23
2	D	56	GLN	CA-C-N	8.34	130.27	119.84
2	D	56	GLN	C-N-CA	8.34	130.27	119.84
2	C	166	ASP	N-CA-C	8.32	121.91	108.76
1	B	163	ASN	N-CA-C	-8.28	103.17	113.18
2	D	461	MET	N-CA-C	-8.19	103.07	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	449	GLU	N-CA-C	8.13	122.33	109.65
2	G	438	LYS	N-CA-C	-7.91	103.12	114.12
2	H	461	MET	N-CA-C	-7.89	102.56	112.90
1	A	291	ASN	N-CA-C	-7.69	101.56	113.02
2	C	61	ASN	N-CA-C	-7.64	102.82	113.37
1	E	59	VAL	N-CA-C	7.64	118.38	111.81
2	H	61	ASN	N-CA-C	-7.63	103.86	113.01
2	G	541	THR	N-CA-C	-7.40	103.30	111.36
1	A	59	VAL	N-CA-C	7.38	118.15	111.81
1	F	59	VAL	N-CA-C	7.31	118.09	111.81
1	A	146	ARG	N-CA-C	-7.23	105.64	114.75
2	D	452	GLU	N-CA-C	-7.23	101.63	110.88
1	E	166	GLN	N-CA-C	-7.14	101.77	111.55
2	G	241	GLU	N-CA-C	-7.12	104.33	113.16
1	B	338	GLU	N-CA-C	-7.05	100.62	110.35
1	A	338	GLU	N-CA-C	-7.04	100.38	110.59
1	B	146	ARG	N-CA-C	-7.01	105.92	114.75
1	F	146	ARG	N-CA-C	-6.78	106.20	114.75
2	D	544	ASN	N-CA-C	-6.77	103.96	111.82
2	C	268	SER	N-CA-C	6.67	121.28	111.34
2	G	268	SER	N-CA-C	6.67	121.28	111.34
1	E	146	ARG	N-CA-C	-6.65	106.37	114.75
2	G	535	ALA	N-CA-C	-6.62	104.46	112.54
2	G	538	ILE	N-CA-C	-6.61	104.07	110.42
2	G	134	SER	N-CA-C	-6.58	105.26	113.28
2	H	268	SER	N-CA-C	6.57	121.14	111.34
1	F	338	GLU	N-CA-C	-6.54	101.11	110.59
2	D	268	SER	N-CA-C	6.44	120.93	111.34
1	A	290	SER	N-CA-C	6.40	118.79	110.53
1	E	338	GLU	N-CA-C	-6.33	100.55	110.36
2	H	405	ILE	N-CA-C	-6.22	106.14	113.42
2	D	53	VAL	N-CA-C	6.19	116.16	107.37
1	E	162	ALA	N-CA-C	6.11	120.07	112.24
1	F	160	PRO	N-CA-C	6.08	118.12	110.70
2	H	516	ASN	N-CA-C	-6.07	104.01	112.45
1	B	314	LEU	N-CA-C	-6.06	105.71	113.23
1	B	59	VAL	N-CA-C	5.99	117.93	111.58
2	D	166	ASP	N-CA-C	-5.99	107.20	114.75
1	F	2	GLN	CA-C-N	5.99	126.82	120.11
1	F	2	GLN	C-N-CA	5.99	126.82	120.11
2	G	82	ILE	N-CA-C	5.96	116.70	108.12
2	D	355	GLU	N-CA-C	-5.93	104.40	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	516	ASN	N-CA-C	-5.92	104.23	112.45
2	C	355	GLU	N-CA-C	-5.91	104.42	111.69
2	D	405	ILE	N-CA-C	-5.90	106.51	113.42
1	E	314	LEU	N-CA-C	-5.90	105.92	113.23
2	G	516	ASN	N-CA-C	-5.90	104.25	112.45
2	C	56	GLN	CA-C-N	5.87	127.17	119.84
2	C	56	GLN	C-N-CA	5.87	127.17	119.84
1	F	314	LEU	N-CA-C	-5.84	105.98	113.23
2	C	274	LEU	N-CA-C	5.81	118.73	111.24
2	D	516	ASN	N-CA-C	-5.77	104.42	112.45
2	H	274	LEU	N-CA-C	5.73	118.64	111.24
2	H	535	ALA	N-CA-C	-5.70	104.99	111.14
2	D	274	LEU	N-CA-C	5.69	118.58	111.24
1	A	165	LEU	N-CA-C	-5.64	105.90	112.89
2	G	269	ASP	N-CA-C	5.64	119.36	111.30
1	A	314	LEU	N-CA-C	-5.63	106.24	113.23
2	G	355	GLU	N-CA-C	-5.63	104.76	111.69
1	E	208	LEU	CA-C-N	5.62	125.60	120.03
1	E	208	LEU	C-N-CA	5.62	125.60	120.03
2	C	82	ILE	N-CA-C	5.59	116.18	108.12
2	D	60	LYS	N-CA-C	5.59	117.75	110.43
2	H	82	ILE	N-CA-C	5.58	116.16	108.12
2	D	269	ASP	N-CA-C	5.57	119.27	111.30
2	D	82	ILE	N-CA-C	5.56	116.13	108.12
2	H	363	TYR	N-CA-C	5.55	120.71	113.88
1	B	174	CYS	N-CA-C	-5.53	101.24	109.42
2	C	269	ASP	N-CA-C	5.49	119.15	111.30
2	G	274	LEU	N-CA-C	5.48	118.31	111.24
2	H	269	ASP	N-CA-C	5.48	119.14	111.30
2	G	363	TYR	N-CA-C	5.41	120.53	113.88
1	B	296	LEU	N-CA-C	-5.38	99.74	108.52
2	C	531	LEU	CA-C-N	5.34	125.15	119.28
2	C	531	LEU	C-N-CA	5.34	125.15	119.28
1	F	208	LEU	CA-C-N	5.34	125.63	119.92
1	F	208	LEU	C-N-CA	5.34	125.63	119.92
1	A	174	CYS	N-CA-C	-5.33	101.53	109.42
2	G	437	GLU	N-CA-C	5.29	117.11	108.76
1	F	174	CYS	N-CA-C	-5.28	101.61	109.42
2	C	363	TYR	N-CA-C	5.25	120.33	113.88
2	D	400	GLY	N-CA-C	5.24	122.06	114.67
2	C	400	GLY	N-CA-C	5.21	122.01	114.67
1	A	208	LEU	CA-C-N	5.20	125.49	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LEU	C-N-CA	5.20	125.49	119.92
1	B	292	LEU	N-CA-C	5.17	117.91	109.59
1	A	71	ILE	N-CA-C	5.17	115.56	108.12
1	A	296	LEU	N-CA-C	-5.16	100.11	108.52
1	E	296	LEU	N-CA-C	-5.12	100.17	108.52
2	D	312	LYS	N-CA-C	-5.11	105.62	111.14
1	A	239	ARG	N-CA-C	5.10	117.76	109.24
2	H	355	GLU	N-CA-C	-5.09	105.43	111.69
2	G	400	GLY	N-CA-C	5.07	121.82	114.67
2	H	133	ASN	N-CA-C	5.06	116.48	110.97
2	H	95	ILE	CA-C-N	5.04	126.14	119.84
2	H	95	ILE	C-N-CA	5.04	126.14	119.84
1	B	208	LEU	CA-C-N	5.04	125.31	119.92
1	B	208	LEU	C-N-CA	5.04	125.31	119.92
2	G	95	ILE	CA-C-N	5.02	126.11	119.84
2	G	95	ILE	C-N-CA	5.02	126.11	119.84

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	2448	0	2385	118	0
1	B	2438	0	2373	145	0
1	E	2432	0	2368	126	0
1	F	2430	0	2366	157	0
2	C	3812	0	3761	162	0
2	D	3959	0	3892	182	0
2	G	3820	0	3750	162	0
2	H	3900	0	3846	177	0
All	All	25239	0	24741	1157	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 23.

All (1157) 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:D:450:MET:HG3	2:D:451:LEU:H	1.26	0.99
2:D:59:GLU:HG3	2:D:60:LYS:H	1.28	0.98
2:G:169:VAL:HG12	2:G:170:ASN:H	1.25	0.97
2:C:240:PHE:O	2:C:241:GLU:HG3	1.66	0.95
1:B:159:ILE:C	1:B:161:PRO:HD3	1.93	0.94
2:D:515:THR:HG22	2:D:516:ASN:H	1.32	0.92
1:F:221:ALA:HB2	1:F:312:TRP:CE2	2.08	0.88
1:E:221:ALA:HB2	1:E:312:TRP:CE2	2.07	0.88
2:H:50:PRO:HB2	2:H:53:VAL:HG22	1.54	0.88
2:C:515:THR:HG22	2:C:516:ASN:H	1.39	0.88
2:H:515:THR:HG22	2:H:516:ASN:H	1.36	0.87
1:A:221:ALA:HB2	1:A:312:TRP:CE2	2.10	0.86
2:G:515:THR:HG22	2:G:516:ASN:H	1.39	0.86
1:B:221:ALA:HB2	1:B:312:TRP:CE2	2.10	0.86
2:D:227:VAL:HG12	2:D:239:VAL:HG13	1.59	0.85
2:C:280:VAL:HG21	2:C:321:ALA:HB3	1.59	0.84
2:H:280:VAL:HG21	2:H:321:ALA:HB3	1.61	0.82
2:G:280:VAL:HG21	2:G:321:ALA:HB3	1.61	0.82
2:C:522:MET:HE1	2:C:538:ILE:HD12	1.62	0.81
2:G:538:ILE:O	2:G:542:LEU:HG	1.80	0.81
2:D:280:VAL:HG21	2:D:321:ALA:HB3	1.62	0.81
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.62	0.80
1:B:329:ARG:HG2	1:B:344:VAL:HG22	1.63	0.80
2:D:163:LYS:O	2:D:167:GLY:HA2	1.82	0.79
1:B:208:LEU:HD11	1:B:231:ILE:HD11	1.62	0.79
2:G:532:PRO:HG2	2:G:533:GLU:H	1.45	0.79
1:B:3:PRO:CG	2:D:52:THR:HG21	2.13	0.79
1:F:329:ARG:HG2	1:F:344:VAL:HG22	1.66	0.78
1:B:208:LEU:HD11	1:B:231:ILE:CD1	2.13	0.78
1:A:225:GLY:O	2:C:453:ASP:HB3	1.83	0.78
2:H:265:ILE:HG21	2:H:289:ILE:HD11	1.65	0.78
2:H:163:LYS:O	2:H:167:GLY:HA2	1.84	0.78
2:C:265:ILE:HG21	2:C:289:ILE:HD11	1.64	0.78
2:D:534:ILE:O	2:D:538:ILE:HG12	1.83	0.78
1:F:157:LEU:HD11	1:F:187:ALA:HB1	1.66	0.77
2:H:239:VAL:HB	2:H:268:SER:HB2	1.67	0.77
1:E:329:ARG:HG2	1:E:344:VAL:HG22	1.66	0.77
2:G:169:VAL:HG12	2:G:170:ASN:N	2.00	0.76
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.67	0.76
1:F:208:LEU:HD11	1:F:231:ILE:HD11	1.67	0.76
2:H:541:THR:O	2:H:545:GLN:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:265:ILE:HG21	2:D:289:ILE:HD11	1.65	0.76
2:G:265:ILE:HG21	2:G:289:ILE:HD11	1.66	0.76
1:E:225:GLY:HA2	2:G:452:GLU:OE2	1.85	0.75
1:F:1:MET:HE1	2:H:77:GLN:OE1	1.87	0.75
2:C:60:LYS:C	2:C:62:GLY:H	1.94	0.74
1:E:208:LEU:HD11	1:E:231:ILE:HD11	1.69	0.74
2:G:240:PHE:CD1	2:G:240:PHE:C	2.65	0.74
2:C:454:LEU:O	2:C:456:SER:N	2.21	0.73
1:F:208:LEU:HD11	1:F:231:ILE:CD1	2.18	0.73
1:B:248:LYS:HG3	2:D:450:MET:HE1	1.70	0.73
1:F:227:TRP:CZ3	2:H:452:GLU:HB2	2.24	0.73
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.70	0.73
1:B:1:MET:HE2	1:B:1:MET:HA	1.68	0.73
1:E:238:GLY:HA2	1:E:305:GLY:O	1.88	0.73
2:H:132:VAL:O	2:H:136:PHE:HB2	1.89	0.73
2:H:278:CYS:SG	2:H:323:ASP:HB2	2.29	0.72
1:F:81:VAL:HG23	1:F:111:LEU:HD13	1.71	0.72
2:H:509:PRO:HA	2:H:538:ILE:HD11	1.71	0.72
2:H:198:GLU:HG2	2:H:300:SER:CB	2.19	0.71
1:F:220:TRP:HA	1:F:231:ILE:HG22	1.72	0.71
2:G:522:MET:HE1	2:G:538:ILE:HD12	1.73	0.71
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.20	0.71
2:C:278:CYS:SG	2:C:323:ASP:HB2	2.31	0.70
1:A:68:TYR:OH	1:A:122:GLY:HA2	1.91	0.70
1:E:236:LYS:HG3	1:E:306:GLU:OE1	1.92	0.69
1:B:68:TYR:OH	1:B:122:GLY:HA2	1.93	0.69
1:A:220:TRP:HA	1:A:231:ILE:HG22	1.75	0.68
1:B:81:VAL:HG23	1:B:111:LEU:HD13	1.74	0.68
2:G:152:LEU:HD21	2:G:182:LEU:HB3	1.75	0.68
2:H:246:TRP:CD1	2:H:331:TYR:CD2	2.81	0.68
2:G:278:CYS:SG	2:G:323:ASP:HB2	2.33	0.68
2:G:246:TRP:CD1	2:G:331:TYR:CD2	2.82	0.68
2:C:240:PHE:CD1	2:C:268:SER:HB3	2.29	0.68
2:D:258:LEU:HD22	2:D:292:LEU:HD22	1.75	0.68
1:E:208:LEU:HD11	1:E:231:ILE:CD1	2.23	0.68
2:D:97:ARG:NH2	2:D:411:SER:O	2.28	0.67
1:E:68:TYR:OH	1:E:122:GLY:HA2	1.94	0.67
2:H:242:THR:HG22	2:H:244:TYR:H	1.59	0.67
2:G:169:VAL:CG1	2:G:170:ASN:H	2.05	0.67
2:H:50:PRO:CB	2:H:53:VAL:HG22	2.24	0.67
2:D:515:THR:HG22	2:D:516:ASN:N	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:258:LEU:HD22	2:H:292:LEU:HD22	1.76	0.67
1:B:196:ARG:HH11	1:B:202:LEU:HD21	1.60	0.67
2:D:169:VAL:HG12	2:D:170:ASN:H	1.60	0.67
1:E:81:VAL:HG23	1:E:111:LEU:HD13	1.77	0.67
1:A:178:PHE:CG	2:C:502:MET:HE3	2.29	0.67
2:C:227:VAL:C	2:C:229:SER:H	2.02	0.67
2:G:119:GLY:O	2:G:122:ARG:HG2	1.95	0.67
2:H:231:LYS:HE2	2:H:233:SER:OG	1.94	0.67
2:C:228:PHE:HE1	2:C:267:ARG:HB3	1.58	0.67
2:D:246:TRP:CD1	2:D:331:TYR:CD2	2.82	0.67
2:C:58:ILE:HG22	2:C:59:GLU:N	2.10	0.66
2:D:202:SER:HA	2:D:297:LYS:O	1.95	0.66
1:F:238:GLY:HA2	1:F:305:GLY:O	1.96	0.66
2:H:373:GLU:O	2:H:377:MET:HG3	1.94	0.66
2:C:280:VAL:HG21	2:C:321:ALA:CB	2.26	0.66
2:D:119:GLY:O	2:D:122:ARG:HG2	1.96	0.66
2:D:373:GLU:O	2:D:377:MET:HG3	1.96	0.66
2:G:258:LEU:HD22	2:G:292:LEU:HD22	1.77	0.66
2:D:450:MET:CG	2:D:451:LEU:H	2.05	0.66
2:H:515:THR:HG22	2:H:516:ASN:N	2.08	0.66
2:C:244:TYR:O	2:C:248:LEU:HG	1.96	0.65
1:A:238:GLY:HA2	1:A:305:GLY:O	1.97	0.65
2:H:280:VAL:HG21	2:H:321:ALA:CB	2.27	0.65
1:B:31:GLN:HG2	1:B:56:SER:O	1.96	0.65
2:C:246:TRP:CD1	2:C:331:TYR:CD2	2.84	0.65
2:D:306:TRP:O	2:D:310:VAL:HG23	1.97	0.65
2:G:198:GLU:HG2	2:G:300:SER:CB	2.27	0.65
2:H:50:PRO:HB2	2:H:53:VAL:CG2	2.24	0.65
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.78	0.65
2:C:155:LEU:O	2:C:159:ILE:HG13	1.97	0.65
2:C:258:LEU:HD22	2:C:292:LEU:HD22	1.78	0.65
1:B:345:ILE:HG22	2:D:51:MET:HA	1.78	0.65
2:C:198:GLU:HG2	2:C:300:SER:CB	2.27	0.65
2:D:278:CYS:SG	2:D:323:ASP:HB2	2.37	0.65
2:G:148:MET:HE1	2:G:182:LEU:HD22	1.77	0.65
2:H:119:GLY:O	2:H:122:ARG:HG2	1.96	0.65
2:H:450:MET:HG3	2:H:451:LEU:H	1.62	0.65
2:H:383:VAL:HG12	2:H:384:VAL:N	2.12	0.65
2:C:373:GLU:O	2:C:377:MET:HG3	1.97	0.64
2:D:60:LYS:HB2	2:D:63:ASP:OD2	1.96	0.64
1:E:220:TRP:HA	1:E:231:ILE:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:ASP:OD2	2:H:169:VAL:HG11	1.97	0.64
1:E:31:GLN:HG2	1:E:56:SER:O	1.97	0.64
1:A:196:ARG:HH11	1:A:202:LEU:HD21	1.62	0.64
1:B:238:GLY:HA2	1:B:305:GLY:O	1.98	0.64
2:D:155:LEU:O	2:D:159:ILE:HG13	1.98	0.64
2:H:148:MET:HE1	2:H:182:LEU:HD22	1.80	0.64
2:H:306:TRP:O	2:H:310:VAL:HG23	1.98	0.64
2:H:522:MET:HE1	2:H:538:ILE:HG13	1.79	0.64
1:B:85:GLU:HB2	1:B:101:LEU:HD11	1.79	0.64
2:C:241:GLU:HG2	2:C:328:LEU:HD13	1.80	0.64
2:C:454:LEU:HG	2:C:455:PHE:N	2.13	0.64
2:H:240:PHE:C	2:H:242:THR:H	2.06	0.64
1:B:313:ASN:HB2	1:B:318:ILE:H	1.63	0.64
2:H:155:LEU:O	2:H:159:ILE:HG13	1.98	0.64
2:G:244:TYR:O	2:G:248:LEU:HG	1.98	0.63
2:D:231:LYS:C	2:D:233:SER:H	2.05	0.63
1:F:314:LEU:HD12	1:F:314:LEU:O	1.97	0.63
1:A:159:ILE:O	1:A:161:PRO:HD3	1.98	0.63
2:C:170:ASN:O	2:C:174:GLU:HG3	1.99	0.63
2:D:198:GLU:HG2	2:D:300:SER:CB	2.29	0.63
2:C:242:THR:HG22	2:C:243:GLN:N	2.14	0.63
2:D:59:GLU:HG3	2:D:60:LYS:N	2.07	0.63
2:H:240:PHE:HD2	2:H:241:GLU:N	1.96	0.63
2:G:373:GLU:O	2:G:377:MET:HG3	1.97	0.63
2:G:383:VAL:HG12	2:G:384:VAL:N	2.14	0.63
2:C:515:THR:HG22	2:C:516:ASN:N	2.10	0.63
1:F:151:THR:HG21	1:F:196:ARG:HH22	1.63	0.63
2:G:545:GLN:O	2:G:549:ALA:HB3	1.98	0.63
2:D:390:TRP:O	2:D:393:PRO:HD2	1.99	0.62
2:G:280:VAL:HG21	2:G:321:ALA:CB	2.28	0.62
2:C:434:PHE:CD1	2:C:458:ARG:HA	2.34	0.62
1:F:42:THR:O	1:F:44:ASN:N	2.31	0.62
2:D:383:VAL:HG12	2:D:384:VAL:N	2.15	0.62
1:F:158:SER:C	1:F:160:PRO:HD3	2.24	0.62
2:G:240:PHE:CD1	2:G:269:ASP:OD2	2.53	0.62
1:B:53:ALA:HB1	1:B:84:TRP:CZ2	2.35	0.62
1:E:196:ARG:HH11	1:E:202:LEU:HD21	1.65	0.62
1:A:15:VAL:O	2:C:70:LYS:HD2	2.00	0.62
1:B:178:PHE:CG	2:D:502:MET:HE3	2.34	0.62
1:E:125:LEU:C	1:E:125:LEU:HD12	2.25	0.62
1:E:313:ASN:HB2	1:E:318:ILE:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:239:VAL:CG1	2:H:268:SER:HB3	2.30	0.62
2:C:406:LEU:HB2	2:C:407:PRO:HD3	1.82	0.61
1:B:10:ASP:HB3	1:B:29:SER:HB2	1.83	0.61
1:F:68:TYR:OH	1:F:122:GLY:HA2	2.00	0.61
2:C:241:GLU:HG2	2:C:328:LEU:CD1	2.30	0.61
1:E:53:ALA:HB1	1:E:84:TRP:CZ2	2.35	0.61
2:G:515:THR:HG22	2:G:516:ASN:N	2.11	0.61
2:H:202:SER:HA	2:H:297:LYS:O	2.00	0.61
2:H:244:TYR:O	2:H:248:LEU:HG	2.00	0.61
2:D:163:LYS:HA	2:D:167:GLY:O	2.00	0.61
2:D:265:ILE:C	2:D:267:ARG:H	2.07	0.61
1:E:306:GLU:N	1:E:324:ASP:OD2	2.32	0.61
1:F:313:ASN:HB2	1:F:318:ILE:H	1.63	0.61
1:F:196:ARG:HH11	1:F:202:LEU:HD21	1.66	0.61
2:C:306:TRP:O	2:C:310:VAL:HG23	2.00	0.61
1:F:10:ASP:HB3	1:F:29:SER:HB2	1.82	0.61
2:C:119:GLY:O	2:C:122:ARG:HG2	1.99	0.61
2:C:148:MET:HE1	2:C:182:LEU:HD22	1.81	0.61
1:F:85:GLU:HB2	1:F:101:LEU:HD11	1.82	0.61
2:D:280:VAL:HG21	2:D:321:ALA:CB	2.30	0.61
1:E:42:THR:O	1:E:44:ASN:N	2.30	0.60
2:H:406:LEU:HB2	2:H:407:PRO:HD3	1.83	0.60
2:D:240:PHE:HA	2:D:245:PHE:CB	2.31	0.60
1:F:344:VAL:O	2:H:48:LEU:HA	2.01	0.60
2:D:244:TYR:O	2:D:248:LEU:HG	2.01	0.60
2:H:240:PHE:O	2:H:242:THR:N	2.34	0.60
2:H:390:TRP:C	2:H:393:PRO:HD2	2.27	0.60
1:A:31:GLN:HG2	1:A:56:SER:O	2.01	0.60
2:H:265:ILE:C	2:H:267:ARG:H	2.08	0.60
1:A:125:LEU:HD12	1:A:125:LEU:C	2.27	0.60
2:D:169:VAL:HG12	2:D:170:ASN:N	2.16	0.60
2:G:265:ILE:C	2:G:267:ARG:H	2.09	0.60
1:B:125:LEU:C	1:B:125:LEU:HD12	2.27	0.60
1:A:313:ASN:HB2	1:A:318:ILE:H	1.65	0.60
2:C:60:LYS:C	2:C:62:GLY:N	2.58	0.60
2:C:158:PHE:O	2:C:162:VAL:HG23	2.02	0.60
2:C:383:VAL:HG12	2:C:384:VAL:N	2.16	0.60
2:C:201:ARG:CZ	2:C:205:ILE:HD11	2.32	0.60
1:A:53:ALA:HB1	1:A:84:TRP:CZ2	2.37	0.59
1:B:306:GLU:N	1:B:324:ASP:OD2	2.34	0.59
2:D:227:VAL:HG12	2:D:239:VAL:CG1	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:SER:O	2:D:272:PRO:HG2	2.01	0.59
2:H:166:ASP:OD2	2:H:169:VAL:CG1	2.51	0.59
2:H:291:LEU:HD13	2:H:310:VAL:HG22	1.83	0.59
2:C:265:ILE:C	2:C:267:ARG:H	2.09	0.59
2:G:268:SER:O	2:G:272:PRO:HG2	2.03	0.59
2:G:534:ILE:O	2:G:538:ILE:HG12	2.02	0.59
2:H:230:VAL:HG12	2:H:230:VAL:O	2.03	0.59
1:A:207:LYS:O	1:A:209:PRO:HD3	2.02	0.59
1:B:42:THR:O	1:B:44:ASN:N	2.32	0.59
1:F:347:ALA:HB3	2:H:58:ILE:HB	1.84	0.59
2:G:401:LYS:HE2	2:H:401:LYS:HE2	1.84	0.59
2:D:170:ASN:O	2:D:174:GLU:HG3	2.02	0.59
1:E:218:ILE:HG22	1:E:233:THR:HG22	1.84	0.59
2:G:306:TRP:O	2:G:310:VAL:HG23	2.03	0.59
2:C:226:GLN:O	2:C:230:VAL:HG23	2.02	0.59
1:E:10:ASP:HB3	1:E:29:SER:HB2	1.85	0.59
2:G:170:ASN:O	2:G:174:GLU:HG3	2.02	0.59
2:H:390:TRP:O	2:H:393:PRO:HD2	2.02	0.59
1:A:10:ASP:HB3	1:A:29:SER:HB2	1.85	0.59
2:G:406:LEU:HB2	2:G:407:PRO:HD3	1.83	0.59
2:C:268:SER:O	2:C:272:PRO:HG2	2.01	0.59
1:F:53:ALA:HB1	1:F:84:TRP:CZ2	2.37	0.59
1:F:306:GLU:N	1:F:324:ASP:OD2	2.35	0.59
2:G:198:GLU:OE1	2:H:437:GLU:HA	2.03	0.59
2:D:291:LEU:HD13	2:D:310:VAL:HG22	1.83	0.59
1:F:123:LEU:HB2	1:F:139:ALA:HB3	1.85	0.59
2:G:450:MET:O	2:G:451:LEU:HD23	2.03	0.59
2:G:542:LEU:O	2:G:546:MET:N	2.35	0.59
2:H:239:VAL:HG11	2:H:268:SER:HB3	1.85	0.59
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.32	0.59
1:A:314:LEU:HD12	1:A:314:LEU:O	2.03	0.59
1:F:207:LYS:O	1:F:209:PRO:HD3	2.03	0.59
2:H:240:PHE:HD2	2:H:241:GLU:H	1.49	0.59
2:C:242:THR:CG2	2:C:243:GLN:N	2.65	0.59
1:F:77:TYR:HD2	1:F:110:SER:HB3	1.67	0.59
1:F:157:LEU:CD1	1:F:187:ALA:HB1	2.33	0.59
2:H:240:PHE:CD2	2:H:241:GLU:N	2.70	0.59
1:B:311:SER:O	1:B:319:LEU:HD12	2.02	0.58
2:C:132:VAL:HG12	2:C:132:VAL:O	2.03	0.58
1:F:31:GLN:HG2	1:F:56:SER:O	2.03	0.58
2:H:49:VAL:HG21	2:H:96:PRO:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TRP:HA	1:B:231:ILE:HG22	1.84	0.58
2:C:63:ASP:O	2:C:64:LYS:C	2.43	0.58
1:F:191:ALA:HB2	1:F:215:ILE:CD1	2.33	0.58
1:A:101:LEU:O	1:A:102:CYS:HB2	2.03	0.58
2:D:201:ARG:CZ	2:D:205:ILE:HD11	2.33	0.58
1:F:4:PHE:CE1	2:H:90:LEU:HD12	2.39	0.58
2:H:434:PHE:CD1	2:H:458:ARG:O	2.56	0.58
1:E:166:GLN:O	1:E:166:GLN:HG2	2.04	0.58
1:F:101:LEU:O	1:F:102:CYS:HB2	2.04	0.58
1:F:125:LEU:HD12	1:F:125:LEU:C	2.28	0.58
2:C:53:VAL:O	2:C:53:VAL:HG13	2.03	0.58
2:C:291:LEU:HD13	2:C:310:VAL:HG22	1.84	0.58
2:D:390:TRP:C	2:D:393:PRO:HD2	2.28	0.58
2:D:406:LEU:HB2	2:D:407:PRO:HD3	1.85	0.58
2:D:450:MET:HG3	2:D:451:LEU:N	2.09	0.58
1:F:81:VAL:HG23	1:F:111:LEU:CD1	2.34	0.58
2:G:268:SER:HB2	2:G:269:ASP:OD1	2.04	0.58
2:H:285:VAL:O	2:H:289:ILE:HG13	2.04	0.58
1:A:4:PHE:CE1	2:C:90:LEU:HD12	2.39	0.58
1:A:191:ALA:HB2	1:A:215:ILE:CD1	2.34	0.58
1:F:118:PRO:HD2	1:F:121:LEU:HD12	1.86	0.57
2:G:201:ARG:CZ	2:G:205:ILE:HD11	2.32	0.57
1:E:314:LEU:HD12	1:E:314:LEU:O	2.03	0.57
1:F:218:ILE:HG22	1:F:233:THR:HG22	1.85	0.57
2:G:539:TYR:HA	2:G:542:LEU:HD12	1.87	0.57
1:B:96:ARG:HG2	1:E:96:ARG:HG3	1.86	0.57
1:B:191:ALA:HB2	1:B:215:ILE:CD1	2.34	0.57
2:H:170:ASN:O	2:H:174:GLU:HG3	2.05	0.57
2:H:246:TRP:CD1	2:H:331:TYR:HD2	2.21	0.57
2:H:268:SER:O	2:H:272:PRO:HG2	2.04	0.57
2:H:201:ARG:CZ	2:H:205:ILE:HD11	2.35	0.57
1:F:77:TYR:HA	1:F:110:SER:HB3	1.84	0.57
2:G:453:ASP:O	2:G:455:PHE:N	2.38	0.57
2:D:158:PHE:O	2:D:162:VAL:HG23	2.05	0.57
1:A:183:LEU:C	1:A:183:LEU:HD12	2.29	0.57
1:E:128:LEU:HD23	1:E:169:PHE:HB3	1.87	0.57
1:A:213:SER:OG	1:A:236:LYS:HD3	2.04	0.57
1:A:218:ILE:HG22	1:A:233:THR:HG22	1.87	0.57
1:B:207:LYS:O	1:B:209:PRO:HD3	2.05	0.57
1:F:15:VAL:O	2:H:70:LYS:HD2	2.04	0.57
2:G:365:ILE:HG21	2:H:457:TYR:OH	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:CYS:HB3	1:A:61:ILE:HD12	1.87	0.56
2:C:522:MET:CE	2:C:538:ILE:HD12	2.34	0.56
1:F:30:ASP:OD1	1:F:32:HIS:HB2	2.04	0.56
1:A:161:PRO:HB2	1:A:164:HIS:CD2	2.39	0.56
2:C:285:VAL:O	2:C:289:ILE:HG13	2.05	0.56
2:D:148:MET:HE1	2:D:182:LEU:HD22	1.86	0.56
2:G:97:ARG:HB3	2:G:97:ARG:NH1	2.20	0.56
1:E:101:LEU:O	1:E:102:CYS:HB2	2.04	0.56
1:E:164:HIS:O	1:E:166:GLN:N	2.38	0.56
2:G:240:PHE:CE2	2:G:269:ASP:HB2	2.40	0.56
1:B:101:LEU:O	1:B:102:CYS:HB2	2.06	0.56
1:B:314:LEU:O	1:B:314:LEU:HD12	2.04	0.56
2:H:386:ILE:HG22	2:H:386:ILE:O	2.04	0.56
2:D:209:LEU:CD2	2:D:256:GLY:HA3	2.36	0.56
2:D:230:VAL:HG12	2:D:230:VAL:O	2.06	0.56
1:A:311:SER:O	1:A:319:LEU:HD12	2.06	0.56
1:B:118:PRO:HD2	1:B:121:LEU:HD12	1.87	0.56
1:E:123:LEU:HB2	1:E:139:ALA:HB3	1.88	0.56
1:A:42:THR:O	1:A:44:ASN:N	2.33	0.56
1:A:123:LEU:HB2	1:A:139:ALA:HB3	1.86	0.56
2:C:152:LEU:HD21	2:C:182:LEU:HB3	1.87	0.56
2:C:268:SER:HB2	2:C:269:ASP:OD1	2.06	0.56
2:C:386:ILE:HG22	2:C:386:ILE:O	2.06	0.56
2:H:268:SER:HB2	2:H:269:ASP:OD1	2.06	0.56
1:A:324:ASP:HB3	2:C:64:LYS:HB3	1.88	0.56
2:D:97:ARG:HB3	2:D:97:ARG:NH1	2.20	0.56
2:D:246:TRP:CD1	2:D:331:TYR:HD2	2.22	0.56
1:E:207:LYS:O	1:E:209:PRO:HD3	2.04	0.56
1:B:27:CYS:HB3	1:B:61:ILE:HD12	1.88	0.56
1:F:27:CYS:HB3	1:F:61:ILE:HD12	1.88	0.56
2:G:246:TRP:CD1	2:G:331:TYR:HD2	2.22	0.56
2:G:386:ILE:O	2:G:386:ILE:HG22	2.06	0.56
1:F:77:TYR:CD2	1:F:110:SER:HB3	2.42	0.55
2:G:453:ASP:O	2:G:454:LEU:C	2.47	0.55
2:D:166:ASP:OD2	2:D:169:VAL:CG2	2.54	0.55
2:D:285:VAL:O	2:D:289:ILE:HG13	2.06	0.55
2:D:386:ILE:O	2:D:386:ILE:HG22	2.05	0.55
1:F:324:ASP:HB3	2:H:64:LYS:HB3	1.88	0.55
2:G:505:ALA:HB1	2:G:534:ILE:HD11	1.87	0.55
2:H:49:VAL:HG21	2:H:96:PRO:HG3	1.88	0.55
2:C:390:TRP:C	2:C:393:PRO:HD2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ALA:HB2	1:E:215:ILE:CD1	2.37	0.55
2:G:228:PHE:HE1	2:G:267:ARG:HG3	1.71	0.55
1:B:218:ILE:HG13	1:B:218:ILE:O	2.06	0.55
1:E:15:VAL:O	2:G:70:LYS:HD2	2.06	0.55
1:A:218:ILE:O	1:A:218:ILE:HG13	2.06	0.55
2:D:461:MET:O	2:D:465:MET:HG3	2.06	0.55
1:F:314:LEU:HD12	1:F:314:LEU:C	2.32	0.55
1:A:306:GLU:N	1:A:324:ASP:OD2	2.36	0.55
2:D:249:LEU:O	2:D:253:VAL:HG23	2.06	0.55
2:H:57:PRO:HG3	2:H:91:TYR:CZ	2.41	0.55
2:C:271:LEU:N	2:C:272:PRO:CD	2.70	0.55
1:F:335:TYR:HB3	2:G:373:GLU:HG3	1.88	0.55
2:C:246:TRP:CD1	2:C:331:TYR:HD2	2.24	0.55
2:G:202:SER:HA	2:G:297:LYS:O	2.07	0.55
2:G:230:VAL:HG12	2:G:230:VAL:O	2.07	0.55
2:G:271:LEU:N	2:G:272:PRO:CD	2.69	0.55
2:G:291:LEU:HD13	2:G:310:VAL:HG22	1.88	0.55
2:H:158:PHE:O	2:H:162:VAL:HG23	2.06	0.55
1:E:311:SER:O	1:E:319:LEU:HD12	2.06	0.55
2:G:390:TRP:C	2:G:393:PRO:HD2	2.32	0.55
2:G:390:TRP:O	2:G:393:PRO:HD2	2.07	0.55
1:B:128:LEU:HD23	1:B:169:PHE:HB3	1.89	0.55
1:E:85:GLU:HB2	1:E:101:LEU:HD11	1.88	0.55
2:G:240:PHE:CE1	2:G:269:ASP:OD2	2.60	0.55
2:H:240:PHE:CZ	2:H:269:ASP:OD2	2.60	0.55
2:D:271:LEU:N	2:D:272:PRO:CD	2.70	0.54
2:C:249:LEU:O	2:C:253:VAL:HG23	2.06	0.54
1:E:247:GLU:HB3	1:E:292:LEU:HD23	1.90	0.54
2:H:49:VAL:HG21	2:H:96:PRO:CG	2.37	0.54
2:H:152:LEU:HD21	2:H:182:LEU:HB3	1.88	0.54
1:A:30:ASP:OD1	1:A:32:HIS:HB2	2.07	0.54
2:D:152:LEU:HD21	2:D:182:LEU:HB3	1.89	0.54
2:D:271:LEU:O	2:D:275:SER:HB3	2.08	0.54
1:E:140:LEU:O	1:E:142:PRO:HD3	2.08	0.54
1:F:126:ALA:HB2	1:F:136:LEU:CD2	2.38	0.54
2:G:240:PHE:CZ	2:G:328:LEU:HD11	2.43	0.54
2:H:352:THR:OG1	2:H:355:GLU:HG3	2.07	0.54
2:C:202:SER:HA	2:C:297:LYS:O	2.08	0.54
2:D:335:PHE:CZ	2:D:339:ILE:HD11	2.42	0.54
2:G:97:ARG:HB3	2:G:97:ARG:HH11	1.73	0.54
2:G:436:GLY:O	2:H:198:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:383:VAL:HG12	2:H:384:VAL:H	1.72	0.54
2:G:343:GLN:NE2	2:G:364:TYR:CZ	2.72	0.54
1:B:159:ILE:C	1:B:161:PRO:CD	2.74	0.54
2:C:58:ILE:HG22	2:C:59:GLU:H	1.72	0.54
1:B:221:ALA:HB2	1:B:312:TRP:CD2	2.42	0.53
1:E:183:LEU:C	1:E:183:LEU:HD12	2.32	0.53
2:D:97:ARG:HB3	2:D:97:ARG:HH11	1.73	0.53
1:E:218:ILE:HG13	1:E:218:ILE:O	2.08	0.53
1:F:347:ALA:CB	2:H:58:ILE:HB	2.38	0.53
2:D:231:LYS:C	2:D:233:SER:N	2.67	0.53
1:E:335:TYR:HB3	2:H:373:GLU:HG3	1.90	0.53
2:G:539:TYR:HA	2:G:542:LEU:HB2	1.90	0.53
2:H:228:PHE:HE2	2:H:267:ARG:HB3	1.73	0.53
1:A:308:TRP:CD1	2:C:66:PRO:HA	2.43	0.53
2:C:271:LEU:O	2:C:275:SER:HB3	2.09	0.53
2:C:534:ILE:O	2:C:538:ILE:HG12	2.08	0.53
2:H:97:ARG:NH1	2:H:97:ARG:HB3	2.23	0.53
1:A:209:PRO:HB2	2:D:318:GLY:HA3	1.91	0.53
2:D:268:SER:HB2	2:D:269:ASP:OD1	2.07	0.53
1:F:221:ALA:HB2	1:F:312:TRP:CD2	2.42	0.53
2:H:239:VAL:HB	2:H:268:SER:CB	2.35	0.53
2:H:249:LEU:O	2:H:253:VAL:HG23	2.09	0.53
2:H:271:LEU:N	2:H:272:PRO:CD	2.71	0.53
1:A:92:GLU:O	1:A:93:CYS:HB2	2.08	0.53
1:B:236:LYS:HG3	1:B:306:GLU:OE1	2.08	0.53
2:C:97:ARG:NH1	2:C:97:ARG:HB3	2.24	0.53
1:F:74:SER:O	1:F:81:VAL:HA	2.09	0.53
1:A:85:GLU:OE2	1:A:145:LEU:HD12	2.08	0.53
1:B:92:GLU:O	1:B:93:CYS:HB2	2.09	0.53
1:B:157:LEU:O	1:B:158:SER:C	2.51	0.53
1:F:205:ALA:O	1:F:206:ALA:HB2	2.07	0.53
2:H:335:PHE:O	2:H:339:ILE:HG13	2.09	0.53
1:A:314:LEU:HD12	1:A:314:LEU:C	2.34	0.53
1:B:1(A):PRO:O	1:B:1(B):HIS:HB3	2.08	0.53
1:B:192:ILE:HD11	1:B:194:TYR:CE1	2.44	0.53
2:D:343:GLN:NE2	2:D:364:TYR:CZ	2.71	0.53
2:D:352:THR:OG1	2:D:355:GLU:HG3	2.09	0.53
1:E:205:ALA:O	1:E:206:ALA:HB2	2.09	0.53
2:H:271:LEU:O	2:H:275:SER:HB3	2.09	0.53
1:B:30:ASP:OD1	1:B:32:HIS:HB2	2.09	0.53
1:B:123:LEU:HB2	1:B:139:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:HIS:HA	1:B:325:ASP:OD2	2.08	0.53
1:B:345:ILE:CG2	2:D:51:MET:HA	2.39	0.53
1:F:119:ALA:C	1:F:121:LEU:H	2.17	0.53
1:F:151:THR:CG2	1:F:196:ARG:HH22	2.21	0.53
1:F:218:ILE:O	1:F:218:ILE:HG13	2.08	0.53
1:B:85:GLU:OE2	1:B:145:LEU:HD12	2.09	0.52
1:B:183:LEU:HD12	1:B:183:LEU:C	2.34	0.52
1:F:311:SER:O	1:F:319:LEU:HD12	2.09	0.52
2:G:271:LEU:O	2:G:275:SER:HB3	2.09	0.52
2:H:335:PHE:CZ	2:H:339:ILE:HD11	2.44	0.52
2:H:364:TYR:CD2	2:H:365:ILE:HG13	2.44	0.52
2:D:240:PHE:CE2	2:D:269:ASP:OD2	2.62	0.52
2:G:269:ASP:OD1	2:G:269:ASP:N	2.41	0.52
2:G:285:VAL:O	2:G:289:ILE:HG13	2.09	0.52
2:G:155:LEU:O	2:G:159:ILE:HG13	2.09	0.52
2:G:158:PHE:O	2:G:162:VAL:HG23	2.09	0.52
2:G:352:THR:OG1	2:G:355:GLU:HG3	2.08	0.52
2:H:292:LEU:HD11	2:H:335:PHE:HZ	1.74	0.52
1:B:247:GLU:HB3	1:B:292:LEU:HD23	1.91	0.52
2:C:451:LEU:HD22	2:C:458:ARG:NE	2.24	0.52
2:C:461:MET:O	2:C:465:MET:HG3	2.09	0.52
1:E:29:SER:C	1:E:31:GLN:H	2.18	0.52
2:C:169:VAL:HG12	2:C:169:VAL:O	2.10	0.52
1:E:68:TYR:CD1	1:E:123:LEU:HD11	2.45	0.52
2:G:383:VAL:HG12	2:G:384:VAL:H	1.74	0.52
1:B:126:ALA:HB2	1:B:136:LEU:CD2	2.39	0.52
2:C:364:TYR:CD2	2:C:365:ILE:HG13	2.45	0.52
1:F:291:ASN:N	1:F:291:ASN:HD22	2.08	0.52
1:A:212:LYS:NZ	2:D:330:ASP:OD1	2.38	0.52
2:C:335:PHE:CZ	2:C:339:ILE:HD11	2.45	0.52
1:E:303:HIS:HA	1:E:325:ASP:OD2	2.09	0.52
1:F:162:ALA:O	1:F:164:HIS:N	2.43	0.52
1:A:140:LEU:O	1:A:142:PRO:HD3	2.09	0.52
2:C:390:TRP:O	2:C:393:PRO:HD2	2.09	0.52
2:D:383:VAL:HG12	2:D:384:VAL:H	1.74	0.52
2:D:533:GLU:CD	2:D:533:GLU:H	2.16	0.52
1:E:126:ALA:HB2	1:E:136:LEU:CD2	2.40	0.52
1:E:157:LEU:HD13	1:E:161:PRO:HD2	1.92	0.52
1:F:303:HIS:HA	1:F:325:ASP:OD2	2.10	0.52
1:A:335:TYR:HB3	2:D:373:GLU:HG3	1.92	0.51
1:E:314:LEU:HD12	1:E:314:LEU:C	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:THR:OG1	1:F:347:ALA:N	2.39	0.51
2:G:364:TYR:CD2	2:G:365:ILE:HG13	2.45	0.51
1:A:131:ASP:OD1	1:A:135:ARG:NH2	2.43	0.51
1:B:140:LEU:O	1:B:142:PRO:HD3	2.10	0.51
2:G:153:ASN:O	2:G:157:VAL:HG23	2.10	0.51
2:G:190:PHE:CE2	2:G:427:LYS:HG3	2.45	0.51
1:A:178:PHE:CB	2:C:502:MET:HE3	2.39	0.51
2:C:352:THR:OG1	2:C:355:GLU:HG3	2.11	0.51
1:F:160:PRO:N	1:F:161:PRO:CD	2.73	0.51
2:G:249:LEU:O	2:G:253:VAL:HG23	2.09	0.51
1:A:119:ALA:C	1:A:121:LEU:H	2.19	0.51
1:B:119:ALA:C	1:B:121:LEU:H	2.18	0.51
2:C:141:ASN:O	2:C:145:ASN:ND2	2.43	0.51
2:C:292:LEU:HD11	2:C:335:PHE:HZ	1.75	0.51
2:G:539:TYR:O	2:G:543:GLY:N	2.44	0.51
2:H:269:ASP:OD1	2:H:269:ASP:N	2.42	0.51
2:D:269:ASP:OD1	2:D:269:ASP:N	2.43	0.51
2:G:532:PRO:CG	2:G:533:GLU:H	2.21	0.51
2:H:223:TYR:O	2:H:226:GLN:HB2	2.11	0.51
1:B:29:SER:C	1:B:31:GLN:H	2.19	0.51
1:B:81:VAL:HG23	1:B:111:LEU:CD1	2.40	0.51
1:B:239:ARG:HG3	1:B:239:ARG:HH11	1.75	0.51
1:F:167:SER:HA	1:F:188:LEU:HD21	1.91	0.51
1:E:178:PHE:CG	2:G:502:MET:HE3	2.46	0.51
1:F:140:LEU:O	1:F:142:PRO:HD3	2.10	0.51
1:B:3:PRO:CD	2:D:52:THR:HG21	2.41	0.51
1:B:159:ILE:O	1:B:161:PRO:HD3	2.09	0.51
2:D:262:ILE:HG12	2:D:289:ILE:HG23	1.93	0.51
1:E:77:TYR:HD2	1:E:110:SER:HB3	1.76	0.51
1:A:192:ILE:HD11	1:A:194:TYR:CE1	2.46	0.51
1:B:151:THR:HG21	1:B:196:ARG:HH22	1.76	0.51
2:D:536:LYS:C	2:D:538:ILE:N	2.69	0.51
1:F:7:GLY:C	1:F:34:LYS:HE3	2.36	0.51
2:H:49:VAL:HG21	2:H:96:PRO:CB	2.40	0.51
1:B:153:GLU:O	1:B:154:MET:HE3	2.11	0.51
2:D:364:TYR:CD2	2:D:365:ILE:HG13	2.46	0.51
1:E:30:ASP:OD1	1:E:32:HIS:HB2	2.10	0.51
1:E:124:LYS:HG3	1:E:138:ASP:OD1	2.11	0.51
1:F:3:PRO:HG3	2:H:52:THR:HG21	1.92	0.51
1:F:29:SER:C	1:F:31:GLN:H	2.19	0.51
1:F:159:ILE:HG22	1:F:159:ILE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:LEU:C	1:F:183:LEU:HD12	2.36	0.51
2:D:51:MET:HE1	2:D:57:PRO:HD2	1.92	0.50
2:D:515:THR:CG2	2:D:516:ASN:H	2.13	0.50
1:F:92:GLU:O	1:F:93:CYS:HB2	2.11	0.50
1:A:239:ARG:HG3	1:A:239:ARG:HH11	1.76	0.50
1:B:314:LEU:HD12	1:B:314:LEU:C	2.36	0.50
1:A:68:TYR:CD1	1:A:123:LEU:HD11	2.46	0.50
1:A:225:GLY:O	2:C:453:ASP:CB	2.56	0.50
2:D:523:LEU:CD2	2:D:535:ALA:HB1	2.41	0.50
1:E:136:LEU:HD11	1:E:202:LEU:HD11	1.93	0.50
2:H:163:LYS:HA	2:H:167:GLY:O	2.10	0.50
1:A:102:CYS:SG	1:A:103:THR:N	2.85	0.50
1:E:27:CYS:HB3	1:E:61:ILE:HD12	1.92	0.50
1:F:88:PRO:HA	1:F:97:ARG:HH12	1.76	0.50
1:F:247:GLU:HB3	1:F:292:LEU:HD23	1.94	0.50
1:A:303:HIS:HA	1:A:325:ASP:OD2	2.11	0.50
1:A:324:ASP:HB3	2:C:64:LYS:HD3	1.93	0.50
1:B:74:SER:O	1:B:81:VAL:HA	2.11	0.50
2:C:262:ILE:HG12	2:C:289:ILE:HG23	1.93	0.50
2:C:269:ASP:OD1	2:C:269:ASP:N	2.44	0.50
2:C:343:GLN:NE2	2:C:364:TYR:CZ	2.68	0.50
1:F:131:ASP:OD1	1:F:135:ARG:NH2	2.44	0.50
1:A:154:MET:HE2	1:A:154:MET:HA	1.93	0.50
1:A:183:LEU:HD12	1:A:183:LEU:O	2.11	0.50
2:D:235:ALA:C	2:D:237:LYS:H	2.18	0.50
2:D:240:PHE:HA	2:D:245:PHE:CG	2.47	0.50
1:E:131:ASP:OD1	1:E:135:ARG:NH2	2.44	0.50
1:A:77:TYR:HA	1:A:110:SER:HB3	1.92	0.50
1:B:154:MET:HA	1:B:154:MET:HE2	1.94	0.50
1:E:92:GLU:O	1:E:93:CYS:HB2	2.11	0.50
1:F:236:LYS:HG3	1:F:306:GLU:OE1	2.12	0.50
1:F:131:ASP:O	1:F:159:ILE:HD11	2.11	0.50
1:A:126:ALA:HB2	1:A:136:LEU:CD2	2.41	0.50
1:B:102:CYS:SG	1:B:103:THR:N	2.85	0.50
1:E:7:GLY:C	1:E:34:LYS:HE3	2.37	0.50
1:E:308:TRP:CD1	2:G:66:PRO:HA	2.47	0.50
2:H:60:LYS:C	2:H:62:GLY:H	2.20	0.50
2:H:509:PRO:HA	2:H:538:ILE:CD1	2.42	0.49
1:B:213:SER:OG	1:B:236:LYS:HD3	2.12	0.49
2:C:218:GLU:HA	2:C:220:ASP:N	2.27	0.49
2:C:240:PHE:CD1	2:C:268:SER:CB	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:LEU:HD11	2:D:335:PHE:HZ	1.76	0.49
1:E:221:ALA:HB2	1:E:312:TRP:CD2	2.47	0.49
1:E:239:ARG:HG3	1:E:239:ARG:HH11	1.77	0.49
1:F:114:VAL:HA	1:F:126:ALA:O	2.11	0.49
1:F:239:ARG:HH11	1:F:239:ARG:HG3	1.76	0.49
1:B:65:SER:HB2	1:B:119:ALA:HB2	1.94	0.49
2:C:105:SER:HB2	2:C:481:LEU:HD21	1.95	0.49
1:E:81:VAL:HG23	1:E:111:LEU:CD1	2.40	0.49
1:F:97:ARG:HG3	1:F:97:ARG:HH11	1.77	0.49
2:H:65:MET:HE2	2:H:84:ALA:HB1	1.93	0.49
2:H:343:GLN:NE2	2:H:364:TYR:CZ	2.68	0.49
1:B:76:SER:HB3	1:B:78:ASP:OD1	2.12	0.49
1:E:220:TRP:CG	1:E:231:ILE:HG22	2.48	0.49
1:F:162:ALA:C	1:F:164:HIS:N	2.70	0.49
2:G:218:GLU:HA	2:G:220:ASP:N	2.28	0.49
1:B:61:ILE:O	1:B:62:ASP:HB2	2.12	0.49
2:D:491:LEU:O	2:D:492:SER:C	2.54	0.49
1:E:151:THR:HG21	1:E:196:ARG:HH22	1.78	0.49
1:F:189:GLU:HA	1:F:213:SER:O	2.13	0.49
2:H:231:LYS:O	2:H:237:LYS:HD3	2.13	0.49
1:A:221:ALA:HB2	1:A:312:TRP:CD2	2.47	0.49
1:B:189:GLU:HA	1:B:213:SER:O	2.12	0.49
2:D:153:ASN:O	2:D:157:VAL:HG23	2.12	0.49
2:D:218:GLU:HA	2:D:220:ASP:N	2.28	0.49
2:D:221:GLU:HA	2:D:224:ILE:HG13	1.94	0.49
1:A:29:SER:C	1:A:31:GLN:H	2.19	0.49
1:A:74:SER:O	1:A:81:VAL:HA	2.12	0.49
1:B:4:PHE:CE1	2:D:90:LEU:HD12	2.47	0.49
2:D:225:GLU:HA	2:D:228:PHE:HB2	1.94	0.49
1:E:293:GLN:OE1	2:H:311:LEU:HD12	2.13	0.49
1:F:161:PRO:HB2	1:F:165:LEU:HB2	1.94	0.49
2:H:451:LEU:O	2:H:458:ARG:NH1	2.45	0.49
1:A:205:ALA:O	1:A:206:ALA:HB2	2.13	0.49
1:A:144:ASP:C	1:A:146:ARG:H	2.21	0.49
1:B:150:LEU:HD23	1:B:150:LEU:C	2.37	0.49
2:C:58:ILE:CG2	2:C:59:GLU:N	2.75	0.49
2:D:240:PHE:CD2	2:D:269:ASP:OD2	2.66	0.49
1:E:118:PRO:HD2	1:E:121:LEU:HD12	1.95	0.49
1:F:311:SER:HB3	1:F:320:SER:OG	2.13	0.49
2:G:292:LEU:HD11	2:G:335:PHE:HZ	1.77	0.49
2:G:530:ARG:O	2:G:532:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ALA:O	1:B:206:ALA:HB2	2.12	0.49
2:C:434:PHE:CD2	2:C:457:TYR:HE1	2.30	0.49
2:D:190:PHE:CE2	2:D:427:LYS:HG3	2.48	0.49
1:F:128:LEU:HD23	1:F:169:PHE:HB3	1.95	0.49
2:H:491:LEU:O	2:H:492:SER:C	2.56	0.49
1:A:76:SER:HB3	1:A:78:ASP:OD1	2.13	0.48
1:B:218:ILE:HG22	1:B:233:THR:HG22	1.95	0.48
2:C:392:GLN:HB3	2:C:393:PRO:HD3	1.95	0.48
1:E:48:SER:O	1:E:92:GLU:HB3	2.13	0.48
2:G:262:ILE:HG12	2:G:289:ILE:HG23	1.95	0.48
2:G:454:LEU:HD21	2:G:489:ILE:HG23	1.94	0.48
2:H:240:PHE:C	2:H:242:THR:N	2.70	0.48
1:B:15:VAL:O	2:D:70:LYS:HD2	2.12	0.48
1:B:48:SER:O	1:B:92:GLU:HB3	2.12	0.48
2:C:220:ASP:OD2	2:C:222:GLU:HB3	2.13	0.48
1:E:119:ALA:C	1:E:121:LEU:H	2.20	0.48
1:E:153:GLU:O	1:E:154:MET:HE3	2.13	0.48
2:G:461:MET:O	2:G:465:MET:HG3	2.14	0.48
2:H:218:GLU:HA	2:H:220:ASP:N	2.28	0.48
2:H:220:ASP:OD2	2:H:222:GLU:HB3	2.13	0.48
1:A:131:ASP:O	1:A:133:ILE:HG13	2.13	0.48
2:D:234:THR:HG22	2:D:234:THR:O	2.13	0.48
2:D:265:ILE:C	2:D:267:ARG:N	2.71	0.48
2:H:107:TYR:CZ	2:H:111:LEU:HD11	2.48	0.48
1:B:68:TYR:CD1	1:B:123:LEU:HD11	2.48	0.48
1:B:227:TRP:CD1	2:D:450:MET:HB2	2.49	0.48
2:C:141:ASN:N	2:C:141:ASN:HD22	2.11	0.48
2:C:515:THR:CG2	2:C:516:ASN:H	2.20	0.48
2:D:220:ASP:OD2	2:D:222:GLU:HB3	2.12	0.48
2:D:335:PHE:O	2:D:339:ILE:HG13	2.14	0.48
1:F:101:LEU:HB3	1:F:145:LEU:O	2.13	0.48
1:F:154:MET:HE2	1:F:154:MET:HA	1.94	0.48
1:B:159:ILE:O	1:B:161:PRO:CD	2.61	0.48
2:C:153:ASN:O	2:C:157:VAL:HG23	2.13	0.48
2:C:383:VAL:HG12	2:C:384:VAL:H	1.75	0.48
2:C:491:LEU:O	2:C:492:SER:C	2.56	0.48
2:D:65:MET:HE2	2:D:84:ALA:HB1	1.96	0.48
1:E:74:SER:O	1:E:81:VAL:HA	2.13	0.48
1:E:187:ALA:O	1:E:188:LEU:HB2	2.13	0.48
2:H:97:ARG:HB3	2:H:97:ARG:HH11	1.78	0.48
1:A:196:ARG:NH1	1:A:202:LEU:HD21	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:TYR:HA	1:B:110:SER:HB3	1.96	0.48
2:H:221:GLU:HA	2:H:224:ILE:HG13	1.95	0.48
1:F:192:ILE:HD11	1:F:194:TYR:CE1	2.48	0.48
1:F:247:GLU:HB3	1:F:292:LEU:CD2	2.44	0.48
2:G:220:ASP:OD2	2:G:222:GLU:HB3	2.13	0.48
2:G:522:MET:HE1	2:G:538:ILE:CD1	2.43	0.48
1:B:114:VAL:HA	1:B:126:ALA:O	2.14	0.48
2:D:223:TYR:O	2:D:226:GLN:HB2	2.14	0.48
1:F:131:ASP:O	1:F:133:ILE:HG13	2.14	0.48
1:F:312:TRP:CZ3	1:F:319:LEU:HB2	2.49	0.48
1:F:346:THR:HG22	2:H:49:VAL:O	2.13	0.48
2:H:57:PRO:CG	2:H:91:TYR:CZ	2.97	0.48
2:H:63:ASP:O	2:H:64:LYS:C	2.57	0.48
2:H:141:ASN:N	2:H:141:ASN:HD22	2.12	0.48
2:H:148:MET:HE3	2:H:152:LEU:HG	1.96	0.48
2:H:484:VAL:O	2:H:488:LEU:HB2	2.13	0.48
2:C:223:TYR:HA	2:C:226:GLN:HB2	1.95	0.48
1:F:213:SER:OG	1:F:236:LYS:HD3	2.14	0.48
2:G:491:LEU:O	2:G:492:SER:C	2.56	0.48
2:G:532:PRO:HG2	2:G:533:GLU:N	2.23	0.48
2:H:190:PHE:CE2	2:H:427:LYS:HG3	2.48	0.48
1:A:189:GLU:HA	1:A:213:SER:O	2.14	0.48
1:B:7:GLY:C	1:B:34:LYS:HE3	2.39	0.48
2:G:148:MET:HE3	2:G:152:LEU:HG	1.95	0.48
2:G:436:GLY:O	2:G:437:GLU:HG3	2.13	0.48
2:H:461:MET:O	2:H:465:MET:HG3	2.14	0.48
1:A:118:PRO:HD2	1:A:121:LEU:HD12	1.96	0.47
1:B:131:ASP:OD1	1:B:135:ARG:NH2	2.47	0.47
1:B:193:ILE:CD1	1:B:245:ILE:HD13	2.44	0.47
1:B:296:LEU:HD21	1:B:299:GLU:HG3	1.96	0.47
2:C:97:ARG:HB3	2:C:97:ARG:HH11	1.77	0.47
2:C:453:ASP:OD1	2:C:499:ALA:HB1	2.13	0.47
1:E:1:MET:O	1:E:3:PRO:HD3	2.14	0.47
1:E:164:HIS:O	1:E:165:LEU:C	2.56	0.47
1:E:189:GLU:HA	1:E:213:SER:O	2.14	0.47
2:G:240:PHE:C	2:G:240:PHE:HD1	2.20	0.47
2:G:265:ILE:C	2:G:267:ARG:N	2.72	0.47
2:G:335:PHE:CZ	2:G:339:ILE:HD11	2.49	0.47
1:E:20:TYR:OH	2:G:541:THR:HG21	2.14	0.47
1:E:101:LEU:HB3	1:E:145:LEU:O	2.13	0.47
2:G:198:GLU:HG2	2:G:300:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:198:GLU:HG2	2:H:300:SER:HB2	1.92	0.47
1:A:187:ALA:O	1:A:188:LEU:HB2	2.13	0.47
1:E:192:ILE:HD11	1:E:194:TYR:CE1	2.49	0.47
1:F:166:GLN:HB3	1:F:214:LEU:HD11	1.96	0.47
2:G:453:ASP:C	2:G:455:PHE:N	2.69	0.47
1:B:131:ASP:O	1:B:133:ILE:HG13	2.14	0.47
1:E:247:GLU:HB3	1:E:292:LEU:CD2	2.44	0.47
1:F:153:GLU:O	1:F:154:MET:HE3	2.15	0.47
2:H:153:ASN:O	2:H:157:VAL:HG23	2.14	0.47
1:A:48:SER:O	1:A:92:GLU:HB3	2.15	0.47
2:D:196:ASP:OD1	2:D:367:SER:HA	2.14	0.47
1:F:86:GLU:HB2	1:F:98:TRP:CZ2	2.49	0.47
2:G:65:MET:HE2	2:G:84:ALA:HB1	1.97	0.47
2:G:223:TYR:HA	2:G:226:GLN:HB2	1.96	0.47
2:H:60:LYS:C	2:H:62:GLY:N	2.71	0.47
2:H:480:GLU:O	2:H:483:PRO:HD2	2.15	0.47
2:H:240:PHE:CE2	2:H:269:ASP:OD2	2.68	0.47
2:H:455:PHE:HE1	2:H:468:SER:OG	1.96	0.47
1:B:196:ARG:HD2	1:B:202:LEU:HD23	1.97	0.47
2:C:223:TYR:O	2:C:226:GLN:HB2	2.15	0.47
2:C:240:PHE:C	2:C:241:GLU:HG3	2.38	0.47
2:C:265:ILE:C	2:C:267:ARG:N	2.73	0.47
2:C:454:LEU:CG	2:C:455:PHE:N	2.78	0.47
1:F:20:TYR:OH	2:H:541:THR:HG21	2.15	0.47
1:F:48:SER:O	1:F:92:GLU:HB3	2.14	0.47
2:G:392:GLN:HB3	2:G:393:PRO:HD3	1.96	0.47
2:G:505:ALA:HA	2:G:534:ILE:HD12	1.96	0.47
2:H:262:ILE:HG12	2:H:289:ILE:HG23	1.96	0.47
2:H:265:ILE:C	2:H:267:ARG:N	2.72	0.47
1:A:123:LEU:HD12	1:A:123:LEU:H	1.80	0.47
1:A:296:LEU:HD21	1:A:299:GLU:HG3	1.96	0.47
1:B:187:ALA:O	1:B:188:LEU:HB2	2.14	0.47
2:D:134:SER:C	2:D:136:PHE:N	2.72	0.47
1:F:144:ASP:C	1:F:146:ARG:H	2.23	0.47
2:G:223:TYR:O	2:G:226:GLN:HB2	2.15	0.47
2:G:228:PHE:C	2:G:230:VAL:H	2.23	0.47
1:B:144:ASP:C	1:B:146:ARG:H	2.23	0.47
2:C:221:GLU:HA	2:C:224:ILE:HG13	1.96	0.47
2:D:402:ILE:O	2:D:405:ILE:HG12	2.14	0.47
2:D:455:PHE:O	2:D:455:PHE:CD2	2.68	0.47
2:D:484:VAL:O	2:D:488:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:HD12	1:E:183:LEU:O	2.15	0.47
1:B:9:ASP:O	2:D:88:TYR:CZ	2.68	0.47
1:B:301:ASP:OD1	1:B:301:ASP:N	2.47	0.47
2:G:457:TYR:OH	2:H:365:ILE:HG21	2.15	0.47
2:H:196:ASP:OD1	2:H:367:SER:HA	2.15	0.47
2:H:223:TYR:HA	2:H:226:GLN:HB2	1.95	0.47
2:H:515:THR:CG2	2:H:516:ASN:H	2.17	0.47
2:C:335:PHE:O	2:C:339:ILE:HG13	2.15	0.46
2:C:484:VAL:O	2:C:488:LEU:HB2	2.15	0.46
2:D:123:VAL:HG12	2:D:124:PHE:N	2.30	0.46
2:D:134:SER:C	2:D:136:PHE:H	2.23	0.46
2:D:482:TRP:N	2:D:483:PRO:CD	2.78	0.46
1:E:4:PHE:CE1	2:G:90:LEU:HD12	2.50	0.46
2:G:105:SER:HB2	2:G:481:LEU:HD21	1.96	0.46
1:A:124:LYS:HG3	1:A:138:ASP:OD1	2.16	0.46
2:C:57:PRO:HB2	2:C:82:ILE:HD11	1.97	0.46
2:D:105:SER:HB2	2:D:481:LEU:HD21	1.96	0.46
1:E:154:MET:HA	1:E:154:MET:HE2	1.97	0.46
1:E:324:ASP:C	1:E:326:GLY:H	2.23	0.46
1:A:114:VAL:HA	1:A:126:ALA:O	2.16	0.46
1:B:107:SER:HA	1:B:135:ARG:HH21	1.80	0.46
2:D:59:GLU:CG	2:D:60:LYS:H	2.10	0.46
1:E:144:ASP:C	1:E:146:ARG:H	2.23	0.46
1:E:296:LEU:HD21	1:E:299:GLU:HG3	1.97	0.46
2:H:209:LEU:HD21	2:H:256:GLY:HA3	1.97	0.46
1:A:150:LEU:C	1:A:150:LEU:HD23	2.40	0.46
1:B:196:ARG:NH1	1:B:202:LEU:HD21	2.27	0.46
2:C:198:GLU:HG2	2:C:300:SER:HB2	1.97	0.46
2:D:480:GLU:O	2:D:483:PRO:HD2	2.15	0.46
1:E:157:LEU:HD13	1:E:161:PRO:CD	2.46	0.46
1:F:11:LEU:O	1:F:28:SER:HB2	2.14	0.46
1:F:113:SER:O	1:F:127:CYS:HA	2.15	0.46
1:F:167:SER:HA	1:F:188:LEU:CD2	2.46	0.46
1:F:296:LEU:HD21	1:F:299:GLU:HG3	1.97	0.46
2:G:107:TYR:CZ	2:G:111:LEU:HD11	2.51	0.46
1:B:1(B):HIS:O	1:B:1(B):HIS:ND1	2.45	0.46
2:C:57:PRO:HB2	2:C:82:ILE:CD1	2.45	0.46
2:C:61:ASN:O	2:C:63:ASP:N	2.49	0.46
2:C:123:VAL:HG12	2:C:124:PHE:N	2.31	0.46
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.50	0.46
2:D:223:TYR:HA	2:D:226:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:ARG:HG3	1:E:97:ARG:HH11	1.81	0.46
1:F:134:LEU:HD11	1:F:183:LEU:HD11	1.97	0.46
2:G:233:SER:C	2:G:235:ALA:N	2.74	0.46
2:G:484:VAL:O	2:G:488:LEU:HB2	2.15	0.46
1:A:301:ASP:O	1:A:303:HIS:N	2.49	0.46
2:C:58:ILE:CG2	2:C:59:GLU:H	2.28	0.46
2:C:243:GLN:O	2:C:247:LYS:HG3	2.16	0.46
2:D:210:ASN:OD1	2:D:214:ARG:HD2	2.16	0.46
1:F:68:TYR:CD1	1:F:123:LEU:HD11	2.51	0.46
1:E:77:TYR:CD2	1:E:110:SER:HB3	2.50	0.46
2:H:209:LEU:CD2	2:H:256:GLY:HA3	2.46	0.46
2:H:242:THR:CG2	2:H:244:TYR:HB2	2.46	0.46
1:A:117:ALA:HB3	1:A:124:LYS:HB3	1.98	0.46
1:B:87:ASP:OD2	1:B:90:GLN:HG2	2.15	0.46
1:B:124:LYS:HG3	1:B:138:ASP:OD1	2.16	0.46
2:D:209:LEU:HD21	2:D:256:GLY:HA3	1.97	0.46
1:F:225:GLY:O	2:H:453:ASP:HA	2.16	0.46
1:F:308:TRP:CD1	2:H:66:PRO:HA	2.51	0.46
2:G:335:PHE:O	2:G:339:ILE:HG13	2.16	0.46
2:G:532:PRO:C	2:G:534:ILE:H	2.24	0.46
2:H:50:PRO:O	2:H:51:MET:C	2.59	0.46
2:H:392:GLN:HB3	2:H:393:PRO:HD3	1.98	0.46
1:B:83:LEU:HD13	1:B:148:TRP:CE2	2.51	0.46
1:E:76:SER:HB3	1:E:78:ASP:OD1	2.16	0.46
2:G:278:CYS:HB2	2:G:323:ASP:O	2.16	0.46
1:B:236:LYS:C	1:B:238:GLY:H	2.23	0.45
2:C:455:PHE:CD2	2:C:455:PHE:O	2.69	0.45
2:D:141:ASN:O	2:D:145:ASN:ND2	2.49	0.45
1:E:150:LEU:C	1:E:150:LEU:HD23	2.41	0.45
1:F:159:ILE:N	1:F:160:PRO:CD	2.79	0.45
1:F:220:TRP:CG	1:F:231:ILE:HG22	2.51	0.45
2:C:65:MET:HE2	2:C:84:ALA:HB1	1.99	0.45
1:E:45:TRP:HZ2	2:G:77:GLN:HG2	1.81	0.45
2:G:296:PRO:HD3	2:G:306:TRP:CD1	2.50	0.45
2:G:515:THR:CG2	2:G:516:ASN:H	2.20	0.45
2:H:278:CYS:HB2	2:H:323:ASP:O	2.16	0.45
2:C:296:PRO:HD3	2:C:306:TRP:CD1	2.51	0.45
2:C:533:GLU:H	2:C:533:GLU:HG2	1.29	0.45
1:E:102:CYS:SG	1:E:103:THR:N	2.89	0.45
1:E:301:ASP:O	1:E:303:HIS:N	2.49	0.45
2:G:221:GLU:HA	2:G:224:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:O	1:B:303:HIS:N	2.50	0.45
2:C:434:PHE:CE2	2:C:457:TYR:CE1	3.04	0.45
2:C:482:TRP:N	2:C:483:PRO:CD	2.78	0.45
2:G:141:ASN:N	2:G:141:ASN:HD22	2.14	0.45
2:H:481:LEU:O	2:H:484:VAL:HB	2.17	0.45
1:A:209:PRO:HG3	2:D:315:GLN:HA	1.99	0.45
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.81	0.45
1:B:324:ASP:C	1:B:326:GLY:H	2.25	0.45
2:C:434:PHE:CE2	2:C:457:TYR:HE1	2.34	0.45
2:D:417:ALA:HB1	2:D:465:MET:HE1	1.98	0.45
1:F:128:LEU:HD22	1:F:185:VAL:HG13	1.97	0.45
1:F:161:PRO:HA	1:F:165:LEU:HD12	1.99	0.45
2:H:296:PRO:HD3	2:H:306:TRP:CD1	2.51	0.45
1:A:114:VAL:O	1:A:114:VAL:HG13	2.16	0.45
1:B:114:VAL:O	1:B:114:VAL:HG13	2.17	0.45
1:B:247:GLU:HB3	1:B:292:LEU:CD2	2.46	0.45
2:D:163:LYS:O	2:D:167:GLY:CA	2.60	0.45
2:D:328:LEU:O	2:D:332:ILE:HG13	2.16	0.45
1:F:87:ASP:OD2	1:F:90:GLN:HG2	2.16	0.45
2:G:152:LEU:CD2	2:G:182:LEU:HB3	2.43	0.45
2:H:78:ASN:HB2	2:H:93:VAL:O	2.17	0.45
2:H:210:ASN:OD1	2:H:214:ARG:HD2	2.16	0.45
1:A:7:GLY:C	1:A:34:LYS:HE3	2.41	0.45
1:B:3:PRO:HG2	2:D:52:THR:HG21	1.95	0.45
1:B:123:LEU:HD12	1:B:123:LEU:H	1.82	0.45
2:C:148:MET:HE3	2:C:152:LEU:HG	1.99	0.45
2:C:278:CYS:HB2	2:C:323:ASP:O	2.17	0.45
2:D:501:LYS:HG2	2:D:531:LEU:HD21	1.98	0.45
1:E:196:ARG:NH1	1:E:202:LEU:HD21	2.32	0.45
2:G:97:ARG:NH2	2:G:411:SER:O	2.50	0.45
2:D:235:ALA:C	2:D:237:LYS:N	2.74	0.45
2:D:447:ASP:O	2:D:448:ASN:HB2	2.17	0.45
1:E:114:VAL:HA	1:E:126:ALA:O	2.16	0.45
1:E:236:LYS:C	1:E:238:GLY:H	2.24	0.45
1:A:87:ASP:OD2	1:A:90:GLN:HG2	2.16	0.45
1:A:236:LYS:C	1:A:238:GLY:H	2.25	0.45
2:C:49:VAL:CG1	2:C:50:PRO:HD2	2.47	0.45
2:C:209:LEU:HD21	2:C:256:GLY:HA3	1.99	0.45
2:D:278:CYS:HB2	2:D:323:ASP:O	2.16	0.45
1:E:77:TYR:HA	1:E:110:SER:HB3	1.98	0.45
1:E:107:SER:HA	1:E:135:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:159:ILE:HG12	2:G:175:LEU:HB3	1.99	0.45
2:G:457:TYR:CD1	2:G:457:TYR:C	2.95	0.45
2:G:481:LEU:O	2:G:484:VAL:HB	2.17	0.45
2:H:123:VAL:HG12	2:H:124:PHE:N	2.32	0.45
2:H:402:ILE:O	2:H:405:ILE:HG12	2.17	0.45
2:C:49:VAL:HG13	2:C:50:PRO:HD2	1.99	0.45
2:D:454:LEU:HD13	2:D:503:VAL:HG21	1.98	0.45
1:F:76:SER:HB3	1:F:78:ASP:OD1	2.16	0.45
1:B:308:TRP:CD1	2:D:66:PRO:HA	2.52	0.44
2:C:269:ASP:HA	2:C:272:PRO:HB2	1.99	0.44
2:D:209:LEU:HD22	2:D:256:GLY:HA3	1.99	0.44
2:D:274:LEU:C	2:D:276:ASP:N	2.74	0.44
2:G:402:ILE:O	2:G:405:ILE:HG12	2.17	0.44
1:B:117:ALA:HB3	1:B:124:LYS:HB3	2.00	0.44
2:D:240:PHE:CZ	2:D:269:ASP:OD2	2.70	0.44
2:D:242:THR:O	2:D:243:GLN:C	2.60	0.44
1:E:123:LEU:H	1:E:123:LEU:HD12	1.82	0.44
1:E:196:ARG:HD2	1:E:202:LEU:HD23	1.99	0.44
1:F:150:LEU:C	1:F:150:LEU:HD23	2.43	0.44
2:H:482:TRP:N	2:H:483:PRO:CD	2.80	0.44
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.82	0.44
1:B:313:ASN:HD22	1:B:313:ASN:HA	1.62	0.44
2:C:230:VAL:O	2:C:235:ALA:HB2	2.18	0.44
2:D:166:ASP:OD2	2:D:169:VAL:HG21	2.17	0.44
2:D:457:TYR:CD1	2:D:457:TYR:C	2.95	0.44
1:E:131:ASP:O	1:E:133:ILE:HG13	2.17	0.44
1:F:117:ALA:HB3	1:F:124:LYS:HB3	1.99	0.44
2:C:501:LYS:HG2	2:C:531:LEU:HD21	1.99	0.44
2:D:392:GLN:HB3	2:D:393:PRO:HD3	2.00	0.44
1:E:85:GLU:OE2	1:E:145:LEU:HD12	2.17	0.44
1:F:124:LYS:HG3	1:F:138:ASP:OD1	2.17	0.44
1:F:196:ARG:NH1	1:F:202:LEU:HD21	2.32	0.44
2:G:228:PHE:N	2:G:228:PHE:CD2	2.85	0.44
1:B:80:THR:HG22	1:B:104:LEU:O	2.18	0.44
2:D:141:ASN:N	2:D:141:ASN:HD22	2.16	0.44
1:F:102:CYS:SG	1:F:103:THR:N	2.90	0.44
2:G:505:ALA:HB1	2:G:534:ILE:CD1	2.48	0.44
2:H:65:MET:HE2	2:H:84:ALA:CB	2.47	0.44
1:A:236:LYS:HG3	1:A:306:GLU:OE1	2.18	0.44
1:B:311:SER:HB3	1:B:320:SER:OG	2.18	0.44
2:C:402:ILE:O	2:C:405:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ASN:HB2	2:D:93:VAL:O	2.17	0.44
1:E:126:ALA:HB2	1:E:136:LEU:HD22	2.00	0.44
1:F:291:ASN:N	1:F:291:ASN:ND2	2.66	0.44
2:G:148:MET:CE	2:G:152:LEU:HG	2.47	0.44
2:G:437:GLU:OE1	2:G:458:ARG:NH2	2.47	0.44
2:H:241:GLU:O	2:H:241:GLU:HG2	2.18	0.44
2:H:274:LEU:C	2:H:276:ASP:N	2.75	0.44
2:H:328:LEU:O	2:H:332:ILE:HG13	2.17	0.44
1:A:180:PRO:O	1:A:182:LYS:HG2	2.18	0.44
1:B:20:TYR:OH	2:D:541:THR:HG21	2.17	0.44
1:B:79:LYS:HG2	1:B:109:GLY:C	2.43	0.44
1:B:136:LEU:HD11	1:B:202:LEU:HD11	1.98	0.44
2:C:351:ARG:HB3	2:C:355:GLU:OE1	2.17	0.44
2:C:481:LEU:O	2:C:484:VAL:HB	2.18	0.44
1:F:183:LEU:HD12	1:F:183:LEU:O	2.17	0.44
2:H:141:ASN:O	2:H:145:ASN:ND2	2.50	0.44
2:C:107:TYR:CZ	2:C:111:LEU:HD11	2.53	0.44
2:C:228:PHE:CE1	2:C:267:ARG:HB3	2.46	0.44
2:C:274:LEU:C	2:C:276:ASP:N	2.75	0.44
2:D:57:PRO:HG3	2:D:91:TYR:CZ	2.53	0.44
2:D:148:MET:HE3	2:D:152:LEU:HG	1.99	0.44
2:G:141:ASN:O	2:G:145:ASN:ND2	2.50	0.44
2:G:482:TRP:N	2:G:483:PRO:CD	2.80	0.44
1:A:247:GLU:HB3	1:A:292:LEU:HD23	2.00	0.44
1:B:3:PRO:HG3	2:D:52:THR:HG21	1.96	0.44
1:B:101:LEU:HB3	1:B:145:LEU:O	2.18	0.44
1:B:130:ASN:C	1:B:132:GLY:H	2.26	0.44
1:B:313:ASN:HB3	1:B:316:GLY:H	1.83	0.44
2:C:210:ASN:OD1	2:C:214:ARG:HD2	2.17	0.44
2:C:242:THR:CG2	2:C:243:GLN:H	2.31	0.44
2:D:148:MET:CE	2:D:152:LEU:HG	2.48	0.44
2:D:228:PHE:HA	2:D:239:VAL:HG21	1.99	0.44
2:D:284:ALA:O	2:D:288:SER:HB3	2.18	0.44
1:F:130:ASN:C	1:F:132:GLY:H	2.26	0.44
1:A:130:ASN:C	1:A:132:GLY:H	2.25	0.43
1:A:196:ARG:HD2	1:A:202:LEU:HD23	2.00	0.43
1:B:220:TRP:CG	1:B:231:ILE:HG22	2.53	0.43
2:C:78:ASN:HB2	2:C:93:VAL:O	2.18	0.43
2:D:114:ILE:HD13	2:D:150:ALA:HB1	2.00	0.43
2:D:238:LYS:HB2	2:D:240:PHE:CD2	2.53	0.43
1:F:84:TRP:CD1	1:F:84:TRP:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:328:LEU:O	2:G:332:ILE:HG13	2.18	0.43
2:G:417:ALA:HB1	2:G:465:MET:HE1	1.99	0.43
2:G:501:LYS:HG2	2:G:531:LEU:HD21	2.00	0.43
2:H:453:ASP:O	2:H:454:LEU:C	2.60	0.43
1:A:301:ASP:OD1	1:A:301:ASP:N	2.51	0.43
1:B:117:ALA:HB2	1:B:173:TRP:CZ2	2.54	0.43
1:F:4:PHE:HE1	2:H:90:LEU:HD12	1.81	0.43
1:F:85:GLU:OE2	1:F:145:LEU:HD12	2.18	0.43
1:F:180:PRO:O	1:F:182:LYS:HG2	2.18	0.43
2:G:123:VAL:HG12	2:G:124:PHE:N	2.33	0.43
2:H:457:TYR:CD1	2:H:457:TYR:C	2.96	0.43
1:A:134:LEU:HD23	1:A:134:LEU:C	2.44	0.43
2:C:328:LEU:O	2:C:332:ILE:HG13	2.18	0.43
1:E:313:ASN:OD1	1:E:317:THR:HB	2.18	0.43
1:A:33:ILE:HG23	1:A:61:ILE:HD11	2.01	0.43
2:D:269:ASP:HA	2:D:272:PRO:HB2	2.00	0.43
1:E:113:SER:O	1:E:127:CYS:HA	2.19	0.43
1:F:31:GLN:HB3	1:F:54:HIS:O	2.18	0.43
2:G:145:ASN:OD1	2:G:190:PHE:HA	2.18	0.43
2:G:228:PHE:N	2:G:228:PHE:HD2	2.17	0.43
2:G:529:TRP:O	2:G:530:ARG:HB2	2.18	0.43
2:H:47:ILE:HD13	2:H:97:ARG:HG3	2.01	0.43
1:A:101:LEU:HB3	1:A:145:LEU:O	2.18	0.43
1:B:84:TRP:CD1	1:B:84:TRP:N	2.85	0.43
1:B:342:MET:O	1:B:343:SER:HB3	2.18	0.43
2:C:299:SER:HB3	2:C:302:THR:OG1	2.18	0.43
2:C:529:TRP:O	2:C:530:ARG:HB2	2.19	0.43
1:E:87:ASP:OD2	1:E:90:GLN:HG2	2.19	0.43
2:H:383:VAL:CG1	2:H:384:VAL:N	2.80	0.43
2:C:51:MET:HE2	2:C:91:TYR:HB2	2.01	0.43
2:C:531:LEU:HB3	2:C:534:ILE:CG1	2.48	0.43
1:E:301:ASP:C	1:E:303:HIS:N	2.77	0.43
1:F:324:ASP:HB3	2:H:64:LYS:HD3	2.00	0.43
1:F:324:ASP:C	1:F:326:GLY:H	2.26	0.43
2:G:455:PHE:HE1	2:G:468:SER:OG	2.02	0.43
2:G:455:PHE:O	2:G:455:PHE:CD2	2.72	0.43
1:A:107:SER:HA	1:A:135:ARG:HH21	1.83	0.43
1:B:338:GLU:HB2	2:C:343:GLN:OE1	2.18	0.43
1:B:345:ILE:HA	2:D:49:VAL:O	2.19	0.43
2:C:242:THR:C	2:C:244:TYR:N	2.76	0.43
2:D:299:SER:HB3	2:D:302:THR:OG1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:ARG:HB3	2:D:355:GLU:OE1	2.19	0.43
2:D:536:LYS:C	2:D:538:ILE:H	2.27	0.43
1:F:165:LEU:O	1:F:166:GLN:C	2.61	0.43
1:A:346:THR:C	2:C:51:MET:HB3	2.44	0.43
1:E:238:GLY:CA	1:E:305:GLY:O	2.63	0.43
2:G:269:ASP:HA	2:G:272:PRO:HB2	2.01	0.43
2:G:284:ALA:O	2:G:288:SER:HB3	2.19	0.43
2:H:242:THR:HG22	2:H:244:TYR:HB2	2.01	0.43
1:B:9:ASP:O	2:D:88:TYR:CE1	2.72	0.43
2:C:168:ARG:HD3	2:C:170:ASN:CB	2.49	0.43
1:F:134:LEU:CD1	1:F:185:VAL:HG21	2.49	0.43
1:F:301:ASP:O	1:F:303:HIS:N	2.52	0.43
2:H:313:LEU:C	2:H:313:LEU:HD23	2.44	0.43
2:H:501:LYS:HG2	2:H:531:LEU:HD21	2.01	0.43
1:A:301:ASP:C	1:A:303:HIS:N	2.77	0.43
1:A:324:ASP:C	1:A:326:GLY:H	2.26	0.43
1:B:11:LEU:O	1:B:28:SER:HB2	2.18	0.43
2:C:209:LEU:CD2	2:C:256:GLY:HA3	2.49	0.43
2:C:455:PHE:O	2:C:455:PHE:CG	2.71	0.43
2:D:57:PRO:CB	2:D:82:ILE:HD11	2.49	0.43
2:D:237:LYS:HB2	2:D:241:GLU:HG2	2.00	0.43
1:E:180:PRO:O	1:E:182:LYS:HG2	2.18	0.43
1:F:107:SER:HA	1:F:135:ARG:HH21	1.82	0.43
1:F:187:ALA:O	1:F:188:LEU:HB2	2.17	0.43
2:G:77:GLN:HE21	2:G:77:GLN:HB2	1.71	0.43
2:G:114:ILE:HD13	2:G:150:ALA:CB	2.49	0.43
2:G:228:PHE:O	2:G:230:VAL:HG23	2.19	0.43
2:G:383:VAL:CG1	2:G:384:VAL:N	2.82	0.43
2:H:455:PHE:CD2	2:H:455:PHE:O	2.71	0.43
1:B:159:ILE:HG22	1:B:161:PRO:HD3	2.01	0.42
1:B:183:LEU:HD12	1:B:183:LEU:O	2.18	0.42
1:E:31:GLN:HG2	1:E:56:SER:C	2.44	0.42
1:A:61:ILE:O	1:A:62:ASP:HB2	2.18	0.42
1:A:128:LEU:HD23	1:A:169:PHE:HB3	2.01	0.42
1:B:134:LEU:CD1	1:B:185:VAL:HG21	2.48	0.42
1:B:180:PRO:O	1:B:182:LYS:HG2	2.19	0.42
2:C:313:LEU:C	2:C:313:LEU:HD23	2.43	0.42
1:F:193:ILE:CD1	1:F:245:ILE:HD13	2.49	0.42
2:G:65:MET:HE2	2:G:84:ALA:CB	2.49	0.42
2:H:57:PRO:HG3	2:H:91:TYR:CE2	2.54	0.42
2:H:61:ASN:O	2:H:62:GLY:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:O	1:A:28:SER:HB2	2.18	0.42
1:A:207:LYS:O	1:A:209:PRO:CD	2.67	0.42
1:B:31:GLN:HG2	1:B:56:SER:C	2.44	0.42
1:B:113:SER:O	1:B:127:CYS:HA	2.18	0.42
2:C:97:ARG:NH2	2:C:411:SER:O	2.52	0.42
2:C:168:ARG:HD3	2:C:170:ASN:HB3	2.00	0.42
2:C:455:PHE:HE1	2:C:468:SER:OG	2.02	0.42
2:D:462:ALA:O	2:D:463:SER:C	2.62	0.42
1:E:342:MET:O	1:E:343:SER:HB3	2.19	0.42
2:G:104:PHE:O	2:G:107:TYR:HB3	2.19	0.42
1:A:67:GLU:OE1	1:A:119:ALA:HB1	2.19	0.42
1:A:77:TYR:HD2	1:A:110:SER:HB3	1.84	0.42
1:A:177:ARG:NH1	2:C:534:ILE:HD13	2.35	0.42
1:B:126:ALA:HB2	1:B:136:LEU:HD22	2.00	0.42
1:F:162:ALA:C	1:F:164:HIS:H	2.27	0.42
2:H:65:MET:HA	2:H:66:PRO:HD3	1.79	0.42
1:E:11:LEU:O	1:E:28:SER:HB2	2.18	0.42
1:E:123:LEU:HD12	1:E:123:LEU:N	2.35	0.42
1:F:80:THR:HG22	1:F:104:LEU:O	2.19	0.42
2:G:246:TRP:O	2:G:247:LYS:C	2.62	0.42
2:G:299:SER:HB3	2:G:302:THR:OG1	2.19	0.42
1:F:136:LEU:HD11	1:F:202:LEU:HD11	2.02	0.42
1:F:236:LYS:C	1:F:238:GLY:H	2.26	0.42
2:G:210:ASN:OD1	2:G:214:ARG:HD2	2.19	0.42
2:G:228:PHE:C	2:G:230:VAL:N	2.78	0.42
2:G:268:SER:C	2:G:269:ASP:OD1	2.62	0.42
2:G:434:PHE:CD1	2:G:458:ARG:O	2.73	0.42
2:G:505:ALA:O	2:G:534:ILE:HD13	2.20	0.42
2:H:95:ILE:HA	2:H:96:PRO:HD3	1.90	0.42
2:H:182:LEU:HD23	2:H:182:LEU:HA	1.89	0.42
1:A:153:GLU:O	1:A:154:MET:HE3	2.19	0.42
1:F:61:ILE:O	1:F:62:ASP:HB2	2.19	0.42
1:F:157:LEU:HD11	1:F:187:ALA:CB	2.44	0.42
2:H:51:MET:HG3	2:H:93:VAL:HG22	2.02	0.42
2:H:104:PHE:O	2:H:107:TYR:HB3	2.20	0.42
1:A:123:LEU:HD12	1:A:123:LEU:N	2.35	0.42
2:C:457:TYR:CD1	2:C:457:TYR:C	2.97	0.42
2:C:480:GLU:O	2:C:483:PRO:HD2	2.19	0.42
2:D:242:THR:O	2:D:244:TYR:N	2.53	0.42
2:D:296:PRO:HD3	2:D:306:TRP:CD1	2.54	0.42
1:F:301:ASP:OD1	1:F:301:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:PHE:CE1	2:H:269:ASP:OD2	2.73	0.42
1:E:133:ILE:HG21	1:E:135:ARG:HH12	1.84	0.42
1:E:313:ASN:HD22	1:E:313:ASN:HA	1.62	0.42
1:F:9:ASP:O	2:H:88:TYR:CZ	2.73	0.42
1:F:133:ILE:HG21	1:F:135:ARG:HH12	1.85	0.42
2:G:228:PHE:O	2:G:230:VAL:N	2.53	0.42
2:H:268:SER:C	2:H:269:ASP:OD1	2.63	0.42
1:A:130:ASN:C	1:A:132:GLY:N	2.78	0.42
1:A:243:PHE:CD1	1:A:243:PHE:N	2.88	0.42
1:E:311:SER:HB3	1:E:320:SER:OG	2.20	0.42
1:F:158:SER:C	1:F:160:PRO:CD	2.92	0.42
2:G:313:LEU:HD23	2:G:313:LEU:C	2.45	0.42
1:B:33:ILE:HG23	1:B:61:ILE:HD11	2.02	0.41
1:B:192:ILE:HD11	1:B:194:TYR:CZ	2.55	0.41
2:C:227:VAL:C	2:C:229:SER:N	2.71	0.41
2:C:284:ALA:O	2:C:288:SER:HB3	2.20	0.41
1:E:301:ASP:OD1	1:E:301:ASP:N	2.52	0.41
1:F:136:LEU:HD12	1:F:196:ARG:HH12	1.84	0.41
1:A:81:VAL:CG2	1:A:111:LEU:HD13	2.44	0.41
2:D:65:MET:HE2	2:D:84:ALA:CB	2.49	0.41
2:D:313:LEU:C	2:D:313:LEU:HD23	2.45	0.41
1:E:130:ASN:C	1:E:132:GLY:H	2.28	0.41
1:E:164:HIS:C	1:E:166:GLN:N	2.78	0.41
1:E:324:ASP:C	1:E:326:GLY:N	2.78	0.41
1:F:162:ALA:O	1:F:163:ASN:C	2.63	0.41
2:D:56:GLN:HA	2:D:57:PRO:HD3	1.75	0.41
2:D:114:ILE:HD13	2:D:150:ALA:CB	2.50	0.41
2:D:246:TRP:O	2:D:247:LYS:C	2.62	0.41
1:F:114:VAL:O	1:F:114:VAL:HG13	2.21	0.41
1:F:313:ASN:HB3	1:F:316:GLY:H	1.83	0.41
1:F:347:ALA:HB1	2:H:58:ILE:H	1.84	0.41
2:H:240:PHE:CD2	2:H:240:PHE:N	2.87	0.41
1:A:313:ASN:HB3	1:A:316:GLY:H	1.85	0.41
1:A:345:ILE:HD13	2:C:93:VAL:HG11	2.01	0.41
1:B:207:LYS:O	1:B:209:PRO:CD	2.68	0.41
2:C:334:ASP:HB3	2:C:349:TYR:HE1	1.85	0.41
2:D:242:THR:HG22	2:D:244:TYR:HD1	1.86	0.41
2:D:455:PHE:O	2:D:455:PHE:CG	2.73	0.41
1:E:114:VAL:O	1:E:114:VAL:HG13	2.19	0.41
1:F:83:LEU:HD13	1:F:148:TRP:CE2	2.55	0.41
1:F:123:LEU:HD12	1:F:123:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:274:LEU:C	2:G:276:ASP:N	2.74	0.41
2:H:284:ALA:O	2:H:288:SER:HB3	2.20	0.41
1:A:193:ILE:CD1	1:A:245:ILE:HD13	2.51	0.41
2:C:113:GLU:HA	2:C:113:GLU:OE2	2.21	0.41
2:D:51:MET:HE1	2:D:57:PRO:CD	2.50	0.41
2:D:481:LEU:O	2:D:484:VAL:HB	2.21	0.41
2:D:536:LYS:O	2:D:538:ILE:N	2.54	0.41
1:F:221:ALA:HB2	1:F:312:TRP:NE1	2.33	0.41
2:G:65:MET:HA	2:G:66:PRO:HD3	1.86	0.41
2:H:269:ASP:HA	2:H:272:PRO:HB2	2.03	0.41
1:B:344:VAL:O	2:D:48:LEU:HA	2.21	0.41
2:D:182:LEU:HD23	2:D:182:LEU:HA	1.93	0.41
2:D:455:PHE:HE1	2:D:468:SER:OG	2.02	0.41
1:E:84:TRP:CD1	1:E:84:TRP:N	2.87	0.41
1:E:313:ASN:HB3	1:E:316:GLY:H	1.85	0.41
1:F:196:ARG:HD2	1:F:202:LEU:HD23	2.02	0.41
1:F:313:ASN:OD1	1:F:317:THR:HB	2.20	0.41
1:A:166:GLN:HG3	1:A:166:GLN:O	2.21	0.41
1:A:311:SER:HB3	1:A:320:SER:OG	2.20	0.41
1:B:31:GLN:HB3	1:B:54:HIS:O	2.20	0.41
2:C:104:PHE:O	2:C:107:TYR:HB3	2.20	0.41
2:D:449:GLU:HB3	2:D:450:MET:H	1.70	0.41
1:E:213:SER:OG	1:E:236:LYS:HD3	2.21	0.41
1:F:207:LYS:O	1:F:209:PRO:CD	2.68	0.41
2:H:56:GLN:HA	2:H:57:PRO:HD3	1.73	0.41
1:B:3:PRO:HD3	2:D:52:THR:HG21	2.01	0.41
2:C:322:THR:HG23	2:C:329:ARG:HD3	2.03	0.41
2:C:383:VAL:CG1	2:C:384:VAL:N	2.83	0.41
2:D:198:GLU:HG2	2:D:300:SER:HB2	2.02	0.41
2:D:511:TYR:HA	2:D:512:PRO:HD3	1.84	0.41
2:D:539:TYR:HA	2:D:542:LEU:HB2	2.02	0.41
1:E:9:ASP:O	2:G:88:TYR:CE1	2.74	0.41
1:E:101:LEU:O	1:E:102:CYS:CB	2.69	0.41
1:F:94:SER:C	1:F:96:ARG:H	2.28	0.41
1:F:342:MET:O	1:F:343:SER:HB3	2.21	0.41
2:G:182:LEU:HD23	2:G:182:LEU:HA	1.97	0.41
2:H:113:GLU:HA	2:H:113:GLU:OE2	2.20	0.41
2:H:246:TRP:O	2:H:247:LYS:C	2.63	0.41
2:H:351:ARG:HB3	2:H:355:GLU:OE1	2.21	0.41
1:A:342:MET:O	1:A:343:SER:HB3	2.21	0.41
1:B:4:PHE:HE1	2:D:90:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:C	1:B:132:GLY:N	2.78	0.41
1:B:178:PHE:CB	2:D:502:MET:HE3	2.50	0.41
2:D:169:VAL:CG1	2:D:170:ASN:N	2.84	0.41
1:F:125:LEU:O	1:F:136:LEU:HA	2.21	0.41
1:A:126:ALA:HB2	1:A:136:LEU:HD22	2.02	0.40
1:B:159:ILE:CB	1:B:161:PRO:HD3	2.51	0.40
2:C:65:MET:HE2	2:C:84:ALA:CB	2.51	0.40
2:C:196:ASP:OD1	2:C:367:SER:HA	2.21	0.40
2:D:50:PRO:O	2:D:51:MET:C	2.64	0.40
2:D:51:MET:CE	2:D:57:PRO:HD2	2.51	0.40
2:D:238:LYS:HB2	2:D:240:PHE:CE2	2.56	0.40
2:D:334:ASP:HB3	2:D:349:TYR:HE1	1.86	0.40
1:E:31:GLN:HB3	1:E:54:HIS:O	2.21	0.40
1:E:125:LEU:O	1:E:136:LEU:HA	2.22	0.40
1:E:312:TRP:CZ3	1:E:319:LEU:HB2	2.57	0.40
1:F:33:ILE:HG23	1:F:61:ILE:HD11	2.02	0.40
1:F:119:ALA:C	1:F:121:LEU:N	2.79	0.40
1:A:220:TRP:CG	1:A:231:ILE:HG22	2.56	0.40
1:B:123:LEU:HD12	1:B:123:LEU:N	2.37	0.40
2:C:228:PHE:CD1	2:C:240:PHE:CE2	3.09	0.40
1:F:2:GLN:H	1:F:2:GLN:HG2	1.72	0.40
2:G:532:PRO:C	2:G:534:ILE:N	2.78	0.40
2:H:278:CYS:CB	2:H:323:ASP:HB2	2.51	0.40
1:B:71:ILE:HD11	1:B:145:LEU:HD13	2.03	0.40
1:B:151:THR:CG2	1:B:196:ARG:HH22	2.34	0.40
1:B:193:ILE:HD11	1:B:208:LEU:HD21	2.04	0.40
1:B:324:ASP:C	1:B:326:GLY:N	2.79	0.40
2:C:57:PRO:HB3	2:C:91:TYR:OH	2.22	0.40
2:C:278:CYS:CB	2:C:323:ASP:HB2	2.51	0.40
1:E:117:ALA:HB3	1:E:124:LYS:HB3	2.03	0.40
1:E:134:LEU:CD1	1:E:185:VAL:HG21	2.50	0.40
1:F:126:ALA:HB2	1:F:136:LEU:HD22	2.03	0.40
2:G:113:GLU:OE2	2:G:113:GLU:HA	2.20	0.40
2:G:190:PHE:CE2	2:G:427:LYS:CG	3.04	0.40
2:G:229:SER:C	2:G:231:LYS:N	2.78	0.40
1:A:65:SER:HB2	1:A:119:ALA:HB2	2.04	0.40
1:B:344:VAL:O	2:D:48:LEU:HD12	2.21	0.40
2:D:227:VAL:O	2:D:239:VAL:CG2	2.69	0.40
1:F:336:SER:O	1:F:337:ASN:CB	2.68	0.40
2:H:144:VAL:HG11	2:H:427:LYS:HG2	2.03	0.40
2:H:148:MET:CE	2:H:152:LEU:HG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:GLN:HA	1:B:3:PRO:HD3	1.97	0.40
2:C:522:MET:HE2	2:C:522:MET:HB3	2.01	0.40
1:E:61:ILE:O	1:E:62:ASP:HB2	2.21	0.40
1:E:117:ALA:HB2	1:E:173:TRP:CZ2	2.57	0.40
1:F:81:VAL:CG2	1:F:111:LEU:HD13	2.46	0.40
2:G:334:ASP:HB3	2:G:349:TYR:HE1	1.87	0.40
2:G:351:ARG:HB3	2:G:355:GLU:OE1	2.21	0.40
2:H:163:LYS:O	2:H:167:GLY:CA	2.63	0.40
2:H:200:ASN:ND2	2:H:203:GLU:HB2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/351 (87%)	266 (88%)	31 (10%)	7 (2%)	5	19
1	B	303/351 (86%)	265 (88%)	33 (11%)	5 (2%)	7	26
1	E	302/351 (86%)	263 (87%)	30 (10%)	9 (3%)	3	14
1	F	302/351 (86%)	267 (88%)	26 (9%)	9 (3%)	3	14
2	C	467/570 (82%)	406 (87%)	53 (11%)	8 (2%)	7	26
2	D	489/570 (86%)	419 (86%)	58 (12%)	12 (2%)	4	17
2	G	468/570 (82%)	406 (87%)	52 (11%)	10 (2%)	5	21
2	H	481/570 (84%)	406 (84%)	60 (12%)	15 (3%)	3	14
All	All	3116/3684 (85%)	2698 (87%)	343 (11%)	75 (2%)	4	18

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER

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Mol	Chain	Res	Type
1	B	43	SER
2	C	272	PRO
2	C	455	PHE
2	D	272	PRO
2	D	450	MET
2	D	451	LEU
1	E	43	SER
1	E	165	LEU
1	F	43	SER
2	G	272	PRO
2	H	62	GLY
2	H	241	GLU
2	H	272	PRO
1	A	162	ALA
1	A	302	ASP
1	B	302	ASP
2	C	62	GLY
2	C	239	VAL
2	D	448	ASN
1	E	302	ASP
1	F	163	ASN
1	F	302	ASP
2	G	239	VAL
2	H	235	ALA
2	H	238	LYS
2	H	438	LYS
1	A	120	HIS
1	B	120	HIS
1	B	213	SER
2	D	243	GLN
2	D	455	PHE
1	E	120	HIS
1	E	164	HIS
1	F	120	HIS
1	F	166	GLN
1	F	213	SER
2	G	229	SER
2	G	454	LEU
1	A	213	SER
1	B	188	LEU
2	D	200	ASN
1	E	213	SER

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Mol	Chain	Res	Type
2	H	51	MET
2	H	455	PHE
1	A	188	LEU
2	C	53	VAL
2	C	200	ASN
2	C	364	TYR
2	D	277	THR
1	E	325	ASP
1	F	161	PRO
1	F	188	LEU
2	G	200	ASN
2	G	533	GLU
2	H	64	LYS
2	H	200	ASN
2	H	237	LYS
2	D	135	ASN
2	D	239	VAL
1	E	188	LEU
2	G	277	THR
2	G	532	PRO
2	H	50	PRO
2	H	63	ASP
2	H	277	THR
2	C	191	ILE
2	D	191	ILE
1	E	142	PRO
2	G	191	ILE
2	H	191	ILE
1	A	142	PRO
1	F	142	PRO
2	G	230	VAL
2	D	47	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	A	270/307 (88%)	256 (95%)	14 (5%)	21	52
1	B	269/307 (88%)	257 (96%)	12 (4%)	24	58
1	E	268/307 (87%)	255 (95%)	13 (5%)	22	54
1	F	267/307 (87%)	251 (94%)	16 (6%)	17	47
2	C	424/510 (83%)	409 (96%)	15 (4%)	32	66
2	D	441/510 (86%)	426 (97%)	15 (3%)	32	66
2	G	424/510 (83%)	410 (97%)	14 (3%)	33	67
2	H	434/510 (85%)	419 (96%)	15 (4%)	32	66
All	All	2797/3268 (86%)	2683 (96%)	114 (4%)	27	61

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(A)	HIS
1	A	1	MET
1	A	61	ILE
1	A	80	THR
1	A	125	LEU
1	A	154	MET
1	A	168	ASP
1	A	183	LEU
1	A	226	ARG
1	A	301	ASP
1	A	310	VAL
1	A	313	ASN
1	A	314	LEU
1	A	334	THR
1	B	61	ILE
1	B	80	THR
1	B	125	LEU
1	B	154	MET
1	B	168	ASP
1	B	183	LEU
1	B	226	ARG
1	B	301	ASP
1	B	310	VAL
1	B	313	ASN
1	B	314	LEU
1	B	334	THR
2	C	51	MET

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Mol	Chain	Res	Type
2	C	77	GLN
2	C	141	ASN
2	C	143	THR
2	C	239	VAL
2	C	269	ASP
2	C	280	VAL
2	C	324	ILE
2	C	387	THR
2	C	453	ASP
2	C	488	LEU
2	C	496	THR
2	C	514	VAL
2	C	525	ILE
2	C	539	TYR
2	D	55	ASP
2	D	77	GLN
2	D	134	SER
2	D	143	THR
2	D	269	ASP
2	D	280	VAL
2	D	324	ILE
2	D	387	THR
2	D	437	GLU
2	D	488	LEU
2	D	496	THR
2	D	514	VAL
2	D	525	ILE
2	D	542	LEU
2	D	544	ASN
1	E	61	ILE
1	E	80	THR
1	E	125	LEU
1	E	154	MET
1	E	164	HIS
1	E	168	ASP
1	E	183	LEU
1	E	226	ARG
1	E	301	ASP
1	E	310	VAL
1	E	313	ASN
1	E	314	LEU
1	E	334	THR

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Mol	Chain	Res	Type
1	F	1(A)	HIS
1	F	1	MET
1	F	61	ILE
1	F	80	THR
1	F	125	LEU
1	F	154	MET
1	F	161	PRO
1	F	168	ASP
1	F	183	LEU
1	F	226	ARG
1	F	291	ASN
1	F	301	ASP
1	F	310	VAL
1	F	313	ASN
1	F	314	LEU
1	F	334	THR
2	G	77	GLN
2	G	141	ASN
2	G	143	THR
2	G	240	PHE
2	G	269	ASP
2	G	324	ILE
2	G	387	THR
2	G	452	GLU
2	G	488	LEU
2	G	496	THR
2	G	514	VAL
2	G	525	ILE
2	G	534	ILE
2	G	539	TYR
2	H	48	LEU
2	H	55	ASP
2	H	77	GLN
2	H	141	ASN
2	H	143	THR
2	H	239	VAL
2	H	240	PHE
2	H	269	ASP
2	H	280	VAL
2	H	324	ILE
2	H	387	THR
2	H	488	LEU

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Mol	Chain	Res	Type
2	H	496	THR
2	H	514	VAL
2	H	525	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	90	GLN
1	A	195	GLN
1	B	23	HIS
1	B	44	ASN
1	B	90	GLN
1	B	313	ASN
2	C	170	ASN
2	C	260	GLN
2	C	467	ASN
2	D	61	ASN
2	D	260	GLN
2	D	294	GLN
2	D	308	ASN
2	D	342	ASN
2	D	432	ASN
1	E	90	GLN
1	E	163	ASN
1	E	164	HIS
1	E	313	ASN
1	F	90	GLN
1	F	313	ASN
2	G	170	ASN
2	G	260	GLN
2	G	308	ASN
2	G	342	ASN
2	G	467	ASN
2	H	260	GLN
2	H	342	ASN
2	H	545	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	308/351 (87%)	0.48	8 (2%) 57 48	77, 104, 136, 169	0
1	B	307/351 (87%)	0.21	3 (0%) 79 73	79, 107, 137, 180	0
1	E	306/351 (87%)	0.35	7 (2%) 61 52	75, 105, 134, 172	0
1	F	306/351 (87%)	0.40	8 (2%) 57 48	82, 107, 137, 180	0
2	C	475/570 (83%)	0.18	17 (3%) 46 38	74, 102, 159, 171	0
2	D	495/570 (86%)	0.19	13 (2%) 57 48	75, 106, 168, 191	0
2	G	476/570 (83%)	0.27	12 (2%) 58 48	70, 102, 159, 190	0
2	H	487/570 (85%)	0.23	16 (3%) 49 40	77, 106, 174, 192	0
All	All	3160/3684 (85%)	0.27	84 (2%) 56 47	70, 105, 160, 192	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	549	ALA	6.0
2	G	539	TYR	5.4
1	F	165	LEU	4.2
2	H	48	LEU	4.1
1	F	162	ALA	4.0
2	H	545	GLN	3.8
2	G	545	GLN	3.8
2	C	451	LEU	3.3
2	H	47	ILE	3.2
2	G	433	ILE	3.2
1	F	14	ASP	3.2
2	D	451	LEU	3.2
2	C	433	ILE	3.2
2	C	454	LEU	3.1
2	C	455	PHE	3.1
2	H	49	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	230	VAL	3.0
1	F	111	LEU	2.9
2	H	228	PHE	2.8
1	E	1(A)	PRO	2.8
2	H	454	LEU	2.7
2	D	265	ILE	2.7
1	A	162	ALA	2.6
2	H	230	VAL	2.6
1	E	165	LEU	2.6
2	C	453	ASP	2.6
1	B	342	MET	2.6
1	E	346	THR	2.6
2	H	433	ILE	2.5
1	E	243	PHE	2.5
1	F	26	THR	2.5
1	A	70	ARG	2.5
2	D	270	LEU	2.5
2	H	519	ILE	2.5
2	C	126	VAL	2.5
2	H	51	MET	2.4
1	A	341	CYS	2.4
2	H	58	ILE	2.4
1	A	156	VAL	2.4
2	C	132	VAL	2.4
2	G	240	PHE	2.4
1	E	248	LYS	2.4
1	F	36	PHE	2.4
1	E	295	GLU	2.4
2	D	224	ILE	2.4
2	G	219	PRO	2.4
2	C	335	PHE	2.3
2	H	291	LEU	2.3
2	C	49	VAL	2.3
2	G	547	LEU	2.3
2	H	66	PRO	2.3
1	A	36	PHE	2.3
1	B	165	LEU	2.3
2	D	75	SER	2.3
2	C	457	TYR	2.3
1	F	156	VAL	2.3
2	G	451	LEU	2.2
2	D	65	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	450	MET	2.2
2	C	238	LYS	2.2
2	H	516	ASN	2.2
1	A	331	TRP	2.2
1	A	288	LEU	2.2
1	E	156	VAL	2.2
2	C	285	VAL	2.2
2	G	546	MET	2.2
2	C	240	PHE	2.2
2	C	67	LEU	2.2
2	G	235	ALA	2.2
2	C	47	ILE	2.2
2	G	82	ILE	2.2
2	G	161	ARG	2.2
2	G	454	LEU	2.2
2	D	169	VAL	2.1
2	D	51	MET	2.1
2	D	228	PHE	2.1
2	D	44	SER	2.1
2	H	457	TYR	2.1
1	A	248	LYS	2.1
2	C	227	VAL	2.1
1	B	1(A)	PRO	2.0
2	D	53	VAL	2.0
2	D	58	ILE	2.0
1	F	119	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.