



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 01:25 PM EST

PDB ID : 3JRO
Title : NUP84-NUP145C-SEC13 edge element of the NPC lattice
Authors : Brohawn, S.G.; Schwartz, T.U.
Deposited on : 2009-09-08
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

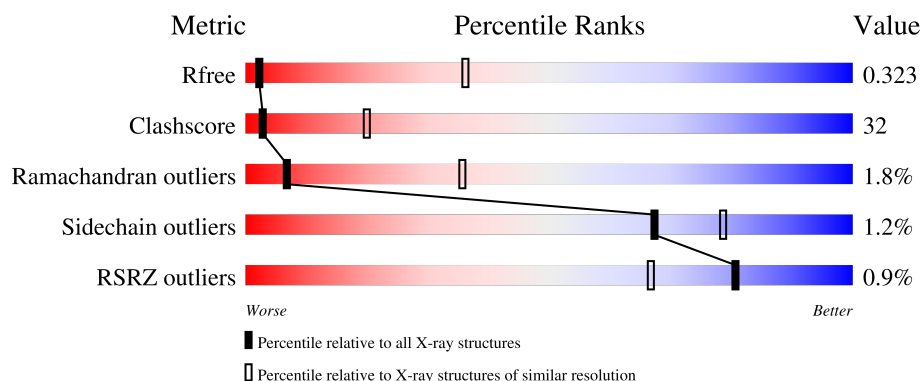
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


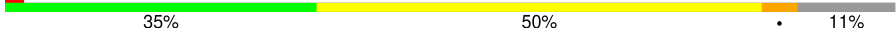
The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1028 (4.22-3.78)
Clashscore	180529	1055 (4.20-3.80)
Ramachandran outliers	177936	1004 (4.20-3.80)
Sidechain outliers	177891	1027 (4.22-3.78)
RSRZ outliers	164620	1029 (4.22-3.78)

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	753	
2	C	426	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8671 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 Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	Se	0	0	0
			5623	3598	943	1068	9	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1100	GLY	-	linker	UNP P49687
A	1101	GLY	-	linker	UNP P49687
A	1102	GLY	-	linker	UNP P49687
A	1103	GLY	-	linker	UNP P49687
A	1104	SER	-	linker	UNP P49687
A	1105	GLY	-	linker	UNP P49687
A	1106	GLY	-	linker	UNP P49687
A	1107	GLY	-	linker	UNP P49687
A	1108	GLY	-	linker	UNP P49687

- Molecule 2 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	379	Total	C	N	O	S	Se	0	0	0
			3048	1949	504	584	4	7			

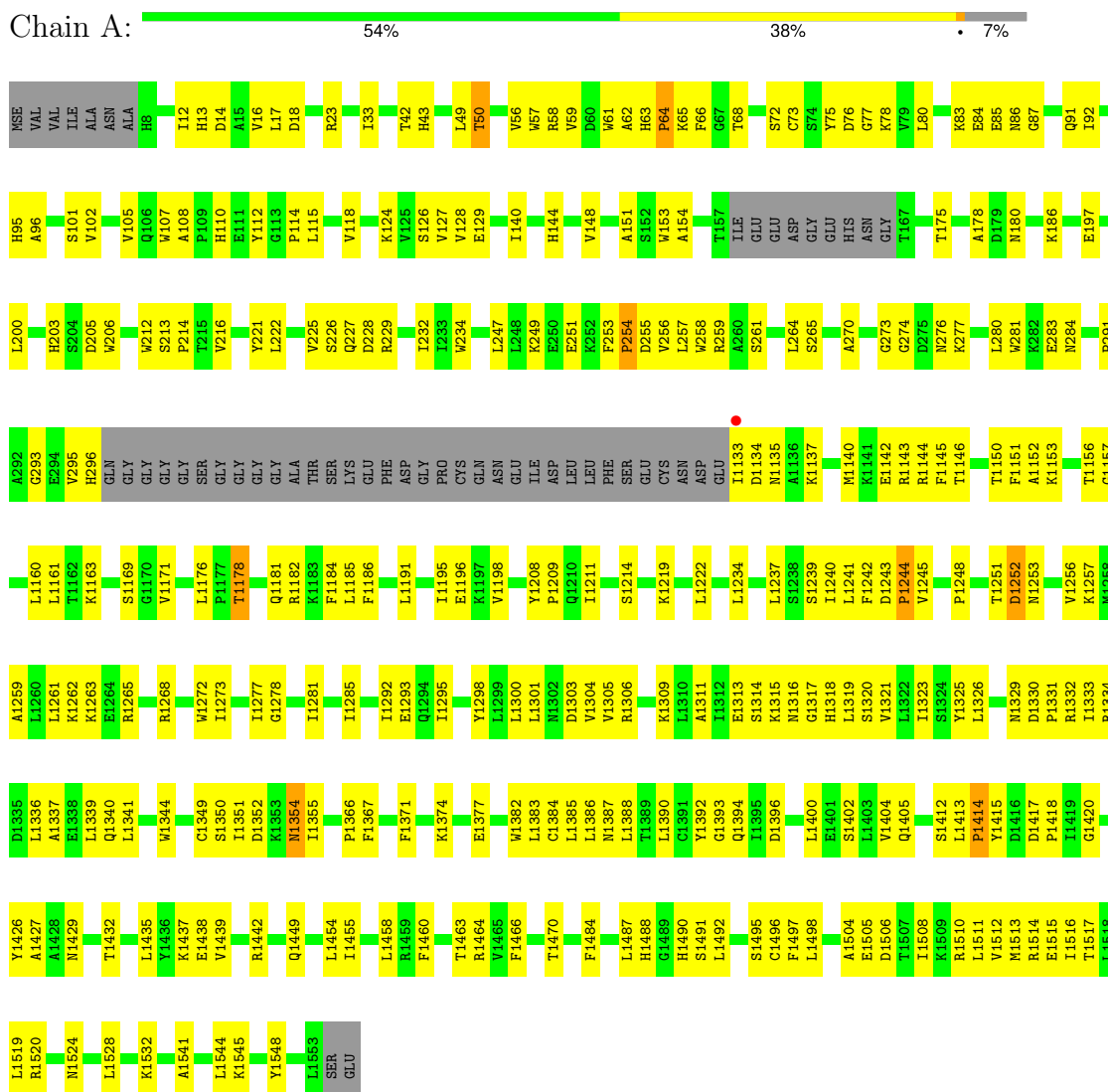
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P52891
C	0	SER	-	expression tag	UNP P52891

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: Fusion Protein of Protein Transport Protein SEC13 and Nucleoporin NUP145



- Molecule 2: Nucleoporin NUP84



L420	K421	G424	I343	R344	V345	L346	P347	M347	I351	L355	P356	I359	H360	V363	L370	LYS	GLY	THR	GLU	ALA	SER	ASN	ASP	ILE	ILE	D381	R387	I388	V389	T390	H391	L392	A393	I394	C395	L396	D397	I398	I399	N400	P401	V404	E405	E406	V407	D408	K411	L412	I413	T414	T415	Y416	I417	S418	L419	G269	A270	I271	P272	N273	V276	S280	D281	W282	E283	S284	D285	L286	H287	I288	L290	N291	Q292	I293	L294	Q295	I298	E299	N300	Y301	E304	N305	N306	Q307	V308	E312	L313	L314	L315	P316	L317	P318	S319	H320	A321	L322	V331	A332	S333	R334	H335	P336	S337	E338	S339	E340	H341	P342	K201	L202	N205	I206	S207	T208	C209	M210	I211	L212	C213	G214	I215	Q216	E217	Y218	L219	N220	P221	V222	I223	I227	F231	N232	T233	Q234	Q235	Q236	T237	K238	H239	H240	S241	L242	V243	R244	R245	T246	S249	L250	S251	Q252	Q253	A254	G255	L256	E260	R261	A262	I263	V264	S265	V266	L267	S268	V62	M133	E134	R135	P136	LYS	ASN	VAL	P140	T141	S142	K143	W144	L145	M146	S147	G151	G152	L153	K154	S155	C156	D157	L158	D159	F160	P161	L162	R163	E164	V168	L169	D170	V171	K172	D173	K174	D177	F180	F181	K182	Y183	I184	Y185	E186	L187	I188	A192	I193	A196	L197	E198	E199	A200	V62	I63	S64	S65	K66	D67	W68	A72	R73	F74	W75	H76	E79	L80	L81	L82	V83	F84	R85	N86	L89	M94	E95	L96	H97	P98	Y99	N100	S101	R102	G103	L104	F105	E106	K107	K108	L109	M110	K114	Q115	L116	Y117	Q118	I119	W120	I121	M123	L126	K127	F128	N129	T130	S60	N61	GLY	SER	MSE	GLU	LEU	SER	PRO	THR	TYR	GLN	THR	GLU	ARG	PHE	THR	LYS	PHE	SER	ASP	THR	LEU	LYS	GLU	PHE	LYS	ILE	GLU	GLN	ASN	ASN	GLU	GLN	ASN	PRO	I33	D34	P35	F36	R37	I38	I39	R40	E41	F42	R43	A46	L49	A50	L53	A54	N55	S56	G57	D58	E59	S60	N61
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4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.47Å 170.47Å 270.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.89 – 4.00 49.89 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.89-4.00) 99.8 (49.89-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.282 , 0.329 0.276 , 0.323	Depositor DCC
R_{free} test set	1586 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å ²)	133.7	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 144.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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	0.24	0/5744	0.41	0/7776
2	C	0.28	0/3101	0.49	0/4202
All	All	0.25	0/8845	0.44	0/11978

There are no bond length outliers.

There are no bond angle outliers.

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	5623	0	5577	286	0
2	C	3048	0	3033	306	0
All	All	8671	0	8610	555	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 32.

All (555) 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:C:104:LEU:HA	2:C:219:LEU:HD12	1.19	1.09
2:C:215:ILE:HG21	2:C:267:LEU:HD13	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:HIS:HB2	2:C:160:PHE:HB2	1.44	0.99
2:C:412:LEU:HB3	2:C:416:TYR:HE2	1.32	0.94
1:A:1251:THR:H	1:A:1257:LYS:HE2	1.35	0.91
2:C:217:GLU:O	2:C:219:LEU:HD23	1.69	0.91
2:C:104:LEU:HD12	2:C:219:LEU:HG	1.52	0.90
1:A:1513:MSE:HE3	1:A:1544:LEU:HD22	1.55	0.88
1:A:12:ILE:HG22	1:A:13:HIS:H	1.42	0.83
2:C:102:ARG:HH21	2:C:105:PHE:HA	1.43	0.83
2:C:256:LEU:HD23	2:C:256:LEU:H	1.45	0.82
2:C:97:HIS:O	2:C:100:ASN:HB2	1.81	0.81
1:A:115:LEU:HD13	1:A:129:GLU:HG2	1.61	0.81
2:C:415:THR:O	2:C:419:LEU:HG	1.81	0.81
2:C:282:TRP:O	2:C:285:ASP:HB3	1.81	0.80
1:A:216:VAL:HG21	1:A:1506:ASP:HB3	1.63	0.79
1:A:1414:PRO:HB2	1:A:1417:ASP:HB2	1.65	0.78
2:C:82:LEU:HD11	2:C:399:ILE:HD13	1.64	0.78
1:A:1341:LEU:HA	1:A:1344:TRP:CD1	2.18	0.78
2:C:74:PHE:HD1	2:C:347:MSE:HG2	1.49	0.77
2:C:237:ILE:HG13	2:C:237:ILE:O	1.83	0.77
2:C:104:LEU:HA	2:C:219:LEU:CD1	2.09	0.77
2:C:342:PRO:HB3	2:C:389:VAL:HG22	1.67	0.77
2:C:94:MSE:HE1	2:C:107:LYS:HE2	1.67	0.76
1:A:225:VAL:HG13	1:A:257:LEU:HB2	1.67	0.75
2:C:53:LEU:HD11	2:C:65:SER:HB3	1.67	0.75
2:C:338:GLU:O	2:C:344:ARG:HD3	1.87	0.74
2:C:397:ASP:HB3	2:C:416:TYR:CE1	2.23	0.73
1:A:1253:ASN:HB2	1:A:1256:VAL:HG23	1.69	0.73
1:A:200:LEU:HB3	1:A:234:TRP:CZ3	2.25	0.72
2:C:75:TRP:CH2	2:C:395:CYS:HB2	2.25	0.72
2:C:97:HIS:ND1	2:C:98:PRO:HD3	2.04	0.72
2:C:134:GLU:HA	2:C:183:TYR:HE1	1.55	0.71
2:C:147:SER:HB3	2:C:170:ASP:OD2	1.91	0.71
2:C:412:LEU:HB3	2:C:416:TYR:CE2	2.21	0.71
1:A:1437:LYS:HE2	1:A:1470:THR:HG21	1.70	0.71
2:C:334:ARG:O	2:C:336:PRO:HD3	1.90	0.71
1:A:1492:LEU:HD13	1:A:1511:LEU:HD23	1.71	0.71
2:C:290:LEU:HA	2:C:293:ILE:HG22	1.73	0.70
2:C:331:VAL:HG12	2:C:335:HIS:CE1	2.26	0.70
2:C:301:TYR:CE1	2:C:308:VAL:HG21	2.26	0.70
2:C:162:LEU:HD21	2:C:169:LEU:HG	1.74	0.70
1:A:1273:ILE:HG21	1:A:1387:ASN:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:LEU:HG	2:C:312:GLU:O	1.92	0.69
1:A:1332:ARG:NH2	2:C:217:GLU:HG3	2.08	0.69
1:A:1344:TRP:CE2	1:A:1351:ILE:HD11	2.27	0.69
2:C:359:ILE:HG12	2:C:396:LEU:HD13	1.73	0.69
1:A:1341:LEU:HA	1:A:1344:TRP:HD1	1.56	0.68
1:A:1326:LEU:HG	1:A:1392:TYR:CE1	2.28	0.68
1:A:1513:MSE:CE	1:A:1544:LEU:HD22	2.23	0.68
2:C:390:THR:HG23	2:C:419:LEU:HD13	1.74	0.67
1:A:1198:VAL:HG11	1:A:1211:ILE:HG13	1.76	0.67
1:A:16:VAL:HG12	1:A:61:TRP:HD1	1.60	0.67
2:C:94:MSE:HG3	2:C:97:HIS:CE1	2.29	0.67
1:A:1429:ASN:HA	1:A:1464:ARG:HH12	1.57	0.67
1:A:77:GLY:HA2	1:A:102:VAL:HG23	1.75	0.67
2:C:347:MSE:O	2:C:351:ILE:HG12	1.95	0.66
1:A:1429:ASN:HA	1:A:1464:ARG:NH1	2.11	0.66
2:C:244:ARG:HD3	2:C:298:ILE:HD11	1.77	0.66
2:C:160:PHE:HB3	2:C:161:PRO:HD3	1.78	0.66
2:C:288:ILE:HD11	2:C:334:ARG:NH1	2.10	0.65
1:A:18:ASP:OD2	1:A:23:ARG:HB2	1.96	0.65
2:C:181:PHE:CG	2:C:260:GLU:HB2	2.31	0.65
2:C:104:LEU:HD12	2:C:219:LEU:CG	2.26	0.65
1:A:1240:ILE:HD13	1:A:1268:ARG:HB3	1.77	0.65
2:C:181:PHE:CD2	2:C:260:GLU:HB2	2.32	0.65
1:A:213:SER:CB	1:A:221:TYR:HB2	2.28	0.64
1:A:108:ALA:HB2	1:A:153:TRP:CE2	2.33	0.64
1:A:62:ALA:HB2	1:A:107:TRP:CD2	2.32	0.64
1:A:1245:VAL:HG21	1:A:1265:ARG:HB2	1.79	0.64
2:C:158:LEU:C	2:C:161:PRO:HD2	2.18	0.64
1:A:1277:ILE:HD13	1:A:1384:CYS:SG	2.38	0.63
1:A:1318:HIS:N	2:C:160:PHE:HD1	1.96	0.63
1:A:1329:ASN:HB3	2:C:234:GLN:HE22	1.63	0.63
1:A:213:SER:HB2	1:A:221:TYR:HB2	1.79	0.63
1:A:1329:ASN:ND2	1:A:1393:GLY:O	2.32	0.63
2:C:205:ASN:HB3	2:C:208:ILE:HD12	1.79	0.63
2:C:245:ARG:HH12	2:C:317:LEU:HB2	1.64	0.63
2:C:102:ARG:NH1	2:C:227:ILE:HD11	2.14	0.63
1:A:1366:PRO:HG2	1:A:1367:PHE:CD1	2.34	0.62
1:A:1435:LEU:O	1:A:1439:VAL:HG23	1.99	0.62
2:C:75:TRP:HH2	2:C:395:CYS:HB2	1.64	0.62
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.82	0.62
2:C:103:GLY:HA2	2:C:307:GLN:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:TRP:CZ3	2:C:169:LEU:HD21	2.35	0.62
2:C:222:VAL:HG12	2:C:234:GLN:CB	2.29	0.62
1:A:23:ARG:CZ	1:A:1548:TYR:HE1	2.13	0.62
2:C:341:HIS:HB3	2:C:344:ARG:HD2	1.82	0.62
1:A:1156:THR:HG22	1:A:1514:ARG:HD3	1.82	0.61
2:C:408:ASP:HB2	2:C:411:LYS:HG2	1.82	0.61
1:A:1285:ILE:HD13	1:A:1298:TYR:CE1	2.35	0.61
2:C:341:HIS:O	2:C:345:VAL:HG23	2.00	0.61
2:C:82:LEU:HD11	2:C:399:ILE:CD1	2.31	0.61
1:A:1495:SER:O	1:A:1498:LEU:HG	2.00	0.61
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.36	0.60
2:C:280:SER:OG	2:C:280:SER:O	2.19	0.60
1:A:17:LEU:HG	1:A:1161:LEU:HD11	1.82	0.60
2:C:359:ILE:HG23	2:C:396:LEU:HD13	1.84	0.60
1:A:1151:PHE:CE2	1:A:1163:LYS:HB3	2.36	0.60
1:A:1332:ARG:O	1:A:1336:LEU:HG	2.01	0.60
2:C:62:VAL:O	2:C:66:LYS:HE3	2.00	0.60
1:A:203:HIS:ND1	1:A:226:SER:HB2	2.17	0.60
2:C:163:ARG:HH22	2:C:253:GLN:CD	2.04	0.60
2:C:104:LEU:HD11	2:C:221:PRO:HG3	1.83	0.59
2:C:332:ALA:HA	2:C:335:HIS:ND1	2.16	0.59
2:C:156:CYS:SG	2:C:162:LEU:HA	2.42	0.59
2:C:158:LEU:HD22	2:C:159:ASP:OD1	2.02	0.59
2:C:266:TYR:CZ	2:C:290:LEU:HD22	2.37	0.59
2:C:271:ILE:N	2:C:272:PRO:HD3	2.18	0.59
1:A:1516:ILE:HG13	1:A:1517:THR:N	2.18	0.59
2:C:218:TYR:O	2:C:219:LEU:HB3	2.03	0.59
2:C:158:LEU:O	2:C:161:PRO:HD2	2.02	0.59
2:C:222:VAL:HG23	2:C:223:ILE:H	1.68	0.59
2:C:244:ARG:NH1	2:C:317:LEU:HD13	2.17	0.59
2:C:97:HIS:CE1	2:C:108:LYS:HD2	2.38	0.58
2:C:234:GLN:O	2:C:234:GLN:HG3	2.03	0.58
1:A:12:ILE:HG22	1:A:13:HIS:N	2.16	0.58
1:A:1332:ARG:HH21	2:C:217:GLU:HG3	1.68	0.58
2:C:159:ASP:O	2:C:162:LEU:HB3	2.03	0.58
1:A:1157:GLY:HA2	1:A:1514:ARG:HH11	1.69	0.58
1:A:1234:LEU:HD13	1:A:1418:PRO:HB2	1.86	0.58
1:A:280:LEU:HD12	1:A:293:GLY:O	2.04	0.58
1:A:1382:TRP:NE1	1:A:1414:PRO:HG3	2.18	0.58
1:A:1300:LEU:HD23	1:A:1388:LEU:HD21	1.85	0.58
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TRP:HH2	1:A:1146:THR:HG23	1.69	0.57
2:C:318:PRO:HB2	2:C:320:HIS:CE1	2.38	0.57
1:A:259:ARG:NH1	1:A:1153:LYS:HE3	2.20	0.57
2:C:245:ARG:NH1	2:C:317:LEU:HB2	2.19	0.57
2:C:146:ASN:OD1	2:C:173:ASP:HB2	2.04	0.57
2:C:407:VAL:HG12	2:C:412:LEU:HG	1.85	0.57
1:A:1432:THR:HG21	1:A:1464:ARG:HD3	1.86	0.57
1:A:1458:LEU:HB3	1:A:1466:PHE:CZ	2.40	0.57
2:C:49:LEU:HD13	2:C:68:TRP:CD1	2.40	0.57
1:A:1176:LEU:HD12	1:A:1484:PHE:CD2	2.39	0.57
2:C:343:ILE:O	2:C:347:MSE:HG3	2.04	0.57
1:A:1292:ILE:HG21	1:A:1355:ILE:CG1	2.35	0.57
2:C:53:LEU:N	2:C:53:LEU:HD12	2.19	0.57
2:C:94:MSE:HE1	2:C:107:LYS:CE	2.35	0.57
2:C:359:ILE:HD13	2:C:396:LEU:HB3	1.86	0.57
2:C:59:GLU:O	2:C:62:VAL:HG12	2.05	0.56
2:C:241:SER:OG	2:C:308:VAL:HG22	2.06	0.56
2:C:98:PRO:O	2:C:99:TYR:CG	2.58	0.56
2:C:245:ARG:NE	2:C:313:LEU:HD22	2.20	0.56
2:C:62:VAL:O	2:C:66:LYS:HG3	2.06	0.56
1:A:1432:THR:HB	1:A:1464:ARG:HH11	1.69	0.56
1:A:203:HIS:CE1	1:A:226:SER:HB2	2.41	0.56
1:A:1516:ILE:HD11	1:A:1545:LYS:HB3	1.86	0.56
2:C:158:LEU:HB3	2:C:161:PRO:HD2	1.88	0.56
2:C:168:VAL:HG22	2:C:168:VAL:O	2.05	0.56
2:C:245:ARG:HE	2:C:313:LEU:HD22	1.71	0.56
1:A:1513:MSE:SE	1:A:1541:ALA:HB2	2.56	0.55
1:A:23:ARG:NH1	1:A:68:THR:HG23	2.21	0.55
1:A:1142:GLU:O	1:A:1142:GLU:HG2	2.07	0.55
2:C:102:ARG:HH12	2:C:227:ILE:HD11	1.71	0.55
2:C:153:LEU:HD21	2:C:168:VAL:HG13	1.88	0.55
2:C:359:ILE:O	2:C:363:VAL:HG23	2.05	0.55
2:C:100:ASN:OD1	2:C:102:ARG:HB3	2.05	0.55
1:A:1332:ARG:HH22	2:C:235:GLN:C	2.09	0.55
1:A:1400:LEU:O	1:A:1404:VAL:HG23	2.07	0.55
2:C:413:ILE:HA	2:C:416:TYR:HD2	1.71	0.55
1:A:1334:ARG:NH2	1:A:1394:GLN:HG2	2.21	0.55
1:A:1528:LEU:HD23	1:A:1528:LEU:H	1.71	0.55
2:C:134:GLU:HA	2:C:183:TYR:CE1	2.40	0.55
2:C:240:HIS:HA	2:C:243:TRP:HB3	1.89	0.55
1:A:1304:VAL:HG22	1:A:1326:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:TYR:HD1	2:C:263:ILE:HG22	1.72	0.55
2:C:185:TYR:CD1	2:C:263:ILE:HG22	2.42	0.55
1:A:1319:LEU:HD23	1:A:1323:ILE:HG13	1.88	0.55
1:A:1344:TRP:HH2	2:C:158:LEU:HD21	1.72	0.55
2:C:53:LEU:HD11	2:C:65:SER:CB	2.36	0.55
1:A:281:TRP:CZ3	1:A:291:PRO:HG3	2.42	0.55
2:C:298:ILE:HG12	2:C:301:TYR:OH	2.07	0.55
2:C:100:ASN:CG	2:C:102:ARG:HB3	2.26	0.54
2:C:215:ILE:HD12	2:C:267:LEU:HD22	1.89	0.54
1:A:1182:ARG:HG3	1:A:1449:GLN:OE1	2.07	0.54
1:A:1181:GLN:HG2	1:A:1181:GLN:O	2.08	0.54
1:A:1214:SER:HB3	1:A:1460:PHE:CG	2.43	0.54
1:A:1514:ARG:HE	1:A:1515:GLU:HG2	1.73	0.54
1:A:115:LEU:CD1	1:A:129:GLU:HG2	2.36	0.54
1:A:1273:ILE:HG22	1:A:1277:ILE:HD12	1.89	0.53
1:A:1367:PHE:HE2	1:A:1385:LEU:HD22	1.73	0.53
2:C:394:ILE:HA	2:C:397:ASP:OD2	2.08	0.53
2:C:46:ALA:HB3	2:C:72:ALA:HB2	1.90	0.53
1:A:105:VAL:HG12	1:A:118:VAL:HG22	1.91	0.53
2:C:50:ALA:O	2:C:53:LEU:HD13	2.09	0.53
2:C:254:ALA:HA	2:C:261:ARG:CD	2.38	0.53
2:C:336:PRO:HD2	2:C:338:GLU:CD	2.28	0.53
1:A:1292:ILE:HG21	1:A:1355:ILE:HG12	1.89	0.53
1:A:1329:ASN:ND2	1:A:1394:GLN:HA	2.23	0.53
1:A:264:LEU:HD11	1:A:1156:THR:HA	1.91	0.53
2:C:215:ILE:HG22	2:C:243:TRP:CH2	2.44	0.53
2:C:244:ARG:NH1	2:C:298:ILE:HD12	2.23	0.53
2:C:250:LEU:HA	2:C:253:GLN:OE1	2.09	0.53
1:A:1329:ASN:OD1	1:A:1334:ARG:HD2	2.08	0.53
2:C:390:THR:CG2	2:C:419:LEU:HD22	2.39	0.53
2:C:193:ILE:O	2:C:197:LEU:HD12	2.09	0.53
1:A:1326:LEU:HG	1:A:1392:TYR:CD1	2.43	0.53
1:A:264:LEU:CD1	1:A:1156:THR:HA	2.39	0.52
2:C:242:LEU:O	2:C:242:LEU:HD23	2.09	0.52
1:A:18:ASP:OD2	1:A:23:ARG:NE	2.43	0.52
1:A:78:LYS:HG2	1:A:96:ALA:CB	2.39	0.52
1:A:1186:PHE:HA	1:A:1487:LEU:HD11	1.90	0.52
1:A:1326:LEU:HG	1:A:1392:TYR:HE1	1.75	0.52
2:C:222:VAL:HG12	2:C:234:GLN:HB2	1.90	0.52
1:A:1412:SER:O	1:A:1413:LEU:HD23	2.10	0.52
2:C:198:GLU:O	2:C:202:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:413:ILE:O	2:C:417:ILE:HG13	2.10	0.52
2:C:49:LEU:HD13	2:C:68:TRP:NE1	2.25	0.52
2:C:98:PRO:C	2:C:100:ASN:H	2.12	0.52
2:C:249:SER:HB2	2:C:315:LEU:HD11	1.92	0.52
1:A:1259:ALA:HB3	2:C:223:ILE:HD13	1.90	0.52
1:A:1323:ILE:O	1:A:1326:LEU:HB2	2.10	0.52
1:A:283:GLU:HG2	1:A:284:ASN:N	2.25	0.52
2:C:163:ARG:HH22	2:C:253:GLN:CG	2.23	0.52
2:C:304:GLU:HB3	2:C:306:ASN:ND2	2.24	0.52
1:A:1374:LYS:NZ	1:A:1374:LYS:HB3	2.25	0.51
1:A:1209:PRO:HB3	1:A:1532:LYS:HB3	1.92	0.51
2:C:109:LEU:HB3	2:C:300:ASN:ND2	2.24	0.51
2:C:116:LEU:O	2:C:119:ILE:HB	2.10	0.51
2:C:177:ASP:O	2:C:180:PHE:HB3	2.10	0.51
1:A:1295:ILE:HD11	1:A:1311:ALA:HA	1.92	0.51
1:A:144:HIS:ND1	1:A:148:VAL:HG22	2.25	0.51
1:A:1344:TRP:CH2	2:C:158:LEU:HD21	2.46	0.51
2:C:341:HIS:CB	2:C:344:ARG:HD2	2.40	0.51
1:A:253:PHE:CD1	1:A:257:LEU:HD11	2.45	0.51
1:A:1435:LEU:HD12	1:A:1438:GLU:HB3	1.92	0.51
2:C:400:ASN:OD1	2:C:407:VAL:HG21	2.10	0.51
2:C:245:ARG:HB3	2:C:315:LEU:HB2	1.93	0.51
1:A:1281:ILE:HB	1:A:1301:LEU:HD21	1.93	0.51
1:A:1513:MSE:HE3	1:A:1544:LEU:CD2	2.35	0.51
2:C:144:TRP:CD1	2:C:144:TRP:N	2.78	0.51
2:C:355:LEU:N	2:C:356:PRO:CD	2.73	0.51
1:A:1219:LYS:HA	1:A:1222:LEU:HD12	1.93	0.51
2:C:390:THR:HG21	2:C:419:LEU:HD22	1.92	0.51
1:A:228:ASP:O	1:A:229:ARG:HB2	2.10	0.50
1:A:1198:VAL:CG1	1:A:1211:ILE:HG13	2.41	0.50
1:A:1251:THR:HG22	1:A:1252:ASP:N	2.24	0.50
1:A:1344:TRP:HZ3	2:C:143:LYS:NZ	2.08	0.50
1:A:1519:LEU:O	1:A:1528:LEU:HD22	2.11	0.50
1:A:1191:LEU:O	1:A:1195:ILE:HG13	2.11	0.50
1:A:83:LYS:HB2	1:A:92:ILE:HD13	1.93	0.50
1:A:1432:THR:HB	1:A:1464:ARG:NH1	2.26	0.50
2:C:158:LEU:HB3	2:C:161:PRO:CD	2.41	0.50
2:C:169:LEU:HD13	2:C:174:LYS:HG3	1.92	0.50
2:C:270:ALA:C	2:C:272:PRO:HD3	2.31	0.50
2:C:363:VAL:HG22	2:C:415:THR:HG21	1.93	0.50
1:A:249:LYS:HG3	1:A:251:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:LYS:HE2	1:A:1470:THR:CG2	2.42	0.50
2:C:38:ILE:HG23	2:C:39:ILE:N	2.26	0.50
2:C:231:PHE:O	2:C:232:ASN:HB2	2.12	0.50
2:C:245:ARG:HG2	2:C:317:LEU:HD12	1.94	0.50
2:C:335:HIS:O	2:C:337:SER:N	2.45	0.50
1:A:75:TYR:HA	1:A:101:SER:OG	2.12	0.50
2:C:146:ASN:ND2	2:C:172:LYS:HB2	2.26	0.50
2:C:392:LEU:O	2:C:395:CYS:HB3	2.12	0.50
1:A:1251:THR:N	1:A:1257:LYS:HE2	2.16	0.50
2:C:301:TYR:CD1	2:C:301:TYR:C	2.85	0.50
1:A:65:LYS:HE2	1:A:110:HIS:HB2	1.94	0.49
1:A:280:LEU:HD21	1:A:1160:LEU:HD22	1.93	0.49
1:A:295:VAL:O	1:A:296:HIS:HB2	2.12	0.49
2:C:183:TYR:HE2	2:C:187:LEU:HD22	1.77	0.49
2:C:254:ALA:HA	2:C:261:ARG:HD3	1.94	0.49
1:A:205:ASP:CG	1:A:206:TRP:H	2.16	0.49
2:C:117:TYR:O	2:C:121:ILE:HG13	2.11	0.49
1:A:1374:LYS:O	1:A:1377:GLU:HG3	2.12	0.49
2:C:104:LEU:CD1	2:C:221:PRO:HG3	2.42	0.49
1:A:1208:TYR:CE1	1:A:1505:GLU:HG3	2.47	0.49
1:A:1317:GLY:HA3	2:C:163:ARG:NH1	2.26	0.49
1:A:1133:ILE:HG22	1:A:1134:ASP:H	1.78	0.49
1:A:1504:ALA:O	1:A:1508:ILE:HG13	2.13	0.49
2:C:46:ALA:CB	2:C:72:ALA:HB2	2.43	0.49
2:C:123:MSE:HE1	2:C:290:LEU:HD13	1.95	0.49
1:A:229:ARG:HG2	1:A:255:ASP:O	2.12	0.49
1:A:1242:PHE:HB3	1:A:1458:LEU:HD21	1.95	0.49
1:A:253:PHE:HB3	1:A:254:PRO:HD2	1.93	0.49
2:C:151:GLY:C	2:C:153:LEU:H	2.15	0.49
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.94	0.49
1:A:1516:ILE:HD11	1:A:1545:LYS:CB	2.43	0.49
2:C:130:THR:HG22	2:C:131:TYR:H	1.78	0.49
2:C:244:ARG:HH12	2:C:317:LEU:HD13	1.78	0.49
1:A:1321:VAL:HG12	1:A:1325:TYR:HE2	1.78	0.49
2:C:276:VAL:HG12	2:C:276:VAL:O	2.12	0.49
1:A:66:PHE:CD2	1:A:114:PRO:HG3	2.48	0.49
2:C:184:ILE:O	2:C:188:ILE:HG12	2.12	0.49
2:C:109:LEU:HD13	2:C:300:ASN:ND2	2.28	0.48
1:A:1415:TYR:OH	1:A:1442:ARG:HB3	2.13	0.48
1:A:1455:ILE:HG23	1:A:1466:PHE:CD2	2.47	0.48
2:C:301:TYR:C	2:C:301:TYR:HD1	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD11	1:A:127:VAL:CG1	2.43	0.48
2:C:59:GLU:HG2	2:C:60:SER:H	1.77	0.48
2:C:133:MSE:HE1	2:C:182:LYS:HG2	1.95	0.48
2:C:184:ILE:HD11	2:C:200:ALA:HB2	1.95	0.48
2:C:215:ILE:CG2	2:C:267:LEU:HD13	2.22	0.48
1:A:83:LYS:HB3	1:A:92:ILE:HG21	1.96	0.48
1:A:265:SER:HB3	1:A:1510:ARG:NH2	2.28	0.48
2:C:218:TYR:CD2	2:C:219:LEU:HD22	2.48	0.48
1:A:1184:PHE:HZ	1:A:1449:GLN:HE22	1.62	0.48
2:C:35:PRO:HB2	2:C:398:ILE:HG12	1.96	0.48
2:C:215:ILE:HG22	2:C:243:TRP:HH2	1.79	0.48
2:C:290:LEU:HA	2:C:293:ILE:CG2	2.41	0.48
1:A:1252:ASP:OD2	2:C:96:LEU:HB3	2.13	0.48
1:A:1464:ARG:HB2	1:A:1466:PHE:CZ	2.49	0.48
2:C:97:HIS:N	2:C:98:PRO:CD	2.76	0.48
1:A:1176:LEU:HD12	1:A:1484:PHE:CE2	2.49	0.48
2:C:63:ILE:HA	2:C:66:LYS:HD2	1.96	0.48
2:C:109:LEU:HD21	2:C:304:GLU:OE2	2.13	0.48
2:C:254:ALA:HA	2:C:261:ARG:NE	2.29	0.48
2:C:256:LEU:HD23	2:C:256:LEU:N	2.23	0.48
2:C:390:THR:HG23	2:C:419:LEU:CD1	2.41	0.48
1:A:277:LYS:HG2	1:A:296:HIS:O	2.14	0.48
1:A:1426:TYR:HA	1:A:1464:ARG:NH2	2.28	0.48
2:C:283:GLU:HB3	2:C:287:HIS:CE1	2.49	0.48
1:A:1319:LEU:HB3	2:C:160:PHE:CZ	2.48	0.48
1:A:1331:PRO:HA	1:A:1334:ARG:HD3	1.95	0.48
1:A:1339:LEU:HB3	2:C:206:ILE:CD1	2.44	0.48
1:A:1354:ASN:C	1:A:1354:ASN:HD22	2.17	0.48
1:A:1458:LEU:CB	1:A:1466:PHE:CZ	2.97	0.48
2:C:152:GLY:C	2:C:154:LYS:H	2.16	0.48
1:A:1321:VAL:HG22	2:C:246:THR:HG22	1.96	0.47
1:A:1350:SER:HB2	2:C:154:LYS:O	2.14	0.47
2:C:241:SER:CB	2:C:301:TYR:OH	2.62	0.47
2:C:301:TYR:CE1	2:C:308:VAL:CG2	2.95	0.47
2:C:356:PRO:HA	2:C:359:ILE:HD12	1.94	0.47
1:A:108:ALA:HB2	1:A:153:TRP:CZ2	2.48	0.47
1:A:1344:TRP:CZ2	1:A:1351:ILE:HD11	2.49	0.47
2:C:341:HIS:CG	2:C:342:PRO:HD2	2.49	0.47
1:A:1237:LEU:HD22	1:A:1272:TRP:CH2	2.49	0.47
1:A:1316:ASN:CG	2:C:160:PHE:CZ	2.88	0.47
2:C:57:GLY:O	2:C:58:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:363:VAL:HG22	2:C:415:THR:CG2	2.44	0.47
1:A:33:ILE:HB	1:A:49:LEU:HD12	1.97	0.47
1:A:112:TYR:N	1:A:112:TYR:CD2	2.83	0.47
2:C:89:LEU:HD13	2:C:114:LYS:NZ	2.29	0.47
2:C:104:LEU:HD22	2:C:221:PRO:HA	1.97	0.47
1:A:85:GLU:HG3	1:A:86:ASN:OD1	2.14	0.47
1:A:178:ALA:HB1	1:A:206:TRP:NE1	2.30	0.47
2:C:109:LEU:HD13	2:C:300:ASN:CG	2.35	0.47
2:C:153:LEU:HD21	2:C:168:VAL:CG1	2.45	0.47
2:C:335:HIS:ND1	2:C:339:SER:HB3	2.30	0.47
1:A:1344:TRP:HZ3	2:C:143:LYS:HZ3	1.57	0.47
2:C:219:LEU:O	2:C:221:PRO:HD3	2.14	0.47
2:C:222:VAL:HG12	2:C:234:GLN:HB3	1.96	0.47
1:A:200:LEU:HB3	1:A:234:TRP:CH2	2.49	0.47
2:C:94:MSE:HG3	2:C:97:HIS:HE1	1.78	0.47
2:C:293:ILE:HG23	2:C:294:LEU:N	2.29	0.47
1:A:59:VAL:HG12	1:A:72:SER:HB3	1.97	0.47
1:A:124:LYS:HB3	1:A:140:ILE:HD11	1.97	0.47
1:A:1152:ALA:HA	1:A:1161:LEU:O	2.16	0.47
1:A:1163:LYS:O	1:A:1163:LYS:HG3	2.15	0.47
1:A:1382:TRP:CH2	1:A:1420:GLY:HA2	2.50	0.47
1:A:1516:ILE:HG13	1:A:1517:THR:H	1.80	0.47
1:A:76:ASP:O	1:A:78:LYS:HG3	2.15	0.46
1:A:1241:LEU:HB3	1:A:1426:TYR:CD1	2.51	0.46
1:A:1252:ASP:N	1:A:1252:ASP:OD1	2.48	0.46
2:C:34:ASP:HA	2:C:35:PRO:HD2	1.73	0.46
2:C:153:LEU:HD11	2:C:168:VAL:O	2.14	0.46
2:C:271:ILE:N	2:C:272:PRO:CD	2.78	0.46
1:A:1321:VAL:HG11	2:C:211:ILE:HG23	1.97	0.46
1:A:1325:TYR:CE1	2:C:237:ILE:HD13	2.50	0.46
1:A:1293:GLU:HB2	1:A:1354:ASN:OD1	2.15	0.46
1:A:80:LEU:HD22	1:A:91:GLN:NE2	2.30	0.46
1:A:1133:ILE:HG22	1:A:1134:ASP:N	2.29	0.46
1:A:1321:VAL:HA	2:C:246:THR:HG21	1.97	0.46
1:A:1332:ARG:CZ	2:C:217:GLU:HG3	2.45	0.46
2:C:183:TYR:CE2	2:C:187:LEU:HD22	2.51	0.46
1:A:227:GLN:NE2	1:A:256:VAL:HG11	2.31	0.46
1:A:265:SER:HB3	1:A:1510:ARG:HH21	1.80	0.46
1:A:1349:CYS:HB3	2:C:157:ASP:OD2	2.16	0.46
1:A:1400:LEU:O	1:A:1400:LEU:HD12	2.16	0.46
2:C:106:GLU:O	2:C:110:MSE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:CE1	1:A:128:VAL:HG21	2.51	0.46
1:A:257:LEU:HD23	1:A:273:GLY:HA2	1.96	0.46
1:A:1325:TYR:CD1	1:A:1333:ILE:HD11	2.50	0.46
2:C:221:PRO:HG2	2:C:231:PHE:CE2	2.49	0.46
1:A:258:TRP:CH2	1:A:1146:THR:HG23	2.51	0.46
1:A:1330:ASP:OD2	1:A:1332:ARG:HG2	2.16	0.46
2:C:187:LEU:HG	2:C:192:ALA:HB3	1.98	0.46
2:C:295:GLN:HB3	2:C:299:GLU:OE2	2.16	0.46
2:C:344:ARG:HA	2:C:347:MSE:HE2	1.98	0.46
1:A:270:ALA:HA	1:A:280:LEU:HD23	1.97	0.45
2:C:127:LYS:C	2:C:129:ASN:H	2.19	0.45
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.52	0.45
1:A:1330:ASP:OD1	1:A:1332:ARG:HG2	2.16	0.45
2:C:317:LEU:HA	2:C:318:PRO:HD3	1.79	0.45
1:A:1239:SER:O	1:A:1243:ASP:HB2	2.16	0.45
1:A:84:GLU:OE2	1:A:87:GLY:HA2	2.16	0.45
1:A:1344:TRP:CZ2	2:C:158:LEU:HD11	2.52	0.45
2:C:273:ASN:HB3	2:C:276:VAL:HG23	1.98	0.45
2:C:418:SER:O	2:C:421:LYS:HB2	2.16	0.45
1:A:227:GLN:C	1:A:229:ARG:H	2.20	0.45
1:A:1157:GLY:HA2	1:A:1514:ARG:NH1	2.29	0.45
1:A:1277:ILE:HD11	1:A:1384:CYS:HA	1.98	0.45
2:C:342:PRO:HB3	2:C:389:VAL:CG2	2.44	0.45
1:A:180:ASN:HA	1:A:205:ASP:O	2.16	0.45
1:A:1251:THR:HG23	2:C:99:TYR:OH	2.17	0.45
1:A:1313:GLU:HG2	1:A:1313:GLU:O	2.17	0.45
2:C:104:LEU:HD12	2:C:219:LEU:CD1	2.46	0.45
2:C:160:PHE:CB	2:C:161:PRO:HD3	2.45	0.45
2:C:76:HIS:O	2:C:80:LEU:HG	2.17	0.45
2:C:126:LEU:HD11	2:C:285:ASP:OD1	2.17	0.45
1:A:1243:ASP:HA	1:A:1244:PRO:HD2	1.79	0.45
1:A:1292:ILE:O	1:A:1295:ILE:HB	2.16	0.45
1:A:186:LYS:HB2	1:A:197:GLU:HG3	1.99	0.45
2:C:355:LEU:O	2:C:359:ILE:HG13	2.17	0.45
1:A:1520:ARG:HA	1:A:1520:ARG:HD3	1.65	0.44
2:C:68:TRP:HA	2:C:68:TRP:CE3	2.52	0.44
2:C:290:LEU:CA	2:C:293:ILE:HG22	2.45	0.44
1:A:1341:LEU:HD23	1:A:1344:TRP:CD1	2.52	0.44
2:C:245:ARG:HD3	2:C:315:LEU:O	2.18	0.44
1:A:1463:THR:O	1:A:1464:ARG:HG3	2.17	0.44
2:C:301:TYR:HE1	2:C:308:VAL:HG21	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:GLN:OE1	1:A:1427:ALA:HB1	2.17	0.44
2:C:36:PHE:O	2:C:40:ARG:HG3	2.17	0.44
2:C:249:SER:CB	2:C:315:LEU:HD11	2.47	0.44
1:A:33:ILE:HD11	1:A:56:VAL:HG11	2.00	0.44
1:A:78:LYS:HG2	1:A:96:ALA:HB1	1.99	0.44
1:A:1257:LYS:O	1:A:1261:LEU:HG	2.18	0.44
1:A:1285:ILE:HD13	1:A:1298:TYR:CD1	2.52	0.44
1:A:1340:GLN:NE2	1:A:1344:TRP:CZ2	2.85	0.44
1:A:1432:THR:HG21	1:A:1464:ARG:HB3	1.98	0.44
1:A:1524:ASN:N	1:A:1524:ASN:HD22	2.15	0.44
2:C:95:GLU:O	2:C:98:PRO:HD2	2.17	0.44
2:C:291:ASN:ND2	2:C:322:LEU:HD11	2.33	0.44
2:C:307:GLN:O	2:C:307:GLN:HG2	2.17	0.44
2:C:393:ALA:HA	2:C:396:LEU:HD12	2.00	0.44
1:A:112:TYR:N	1:A:112:TYR:HD2	2.16	0.44
1:A:151:ALA:HB2	1:A:175:THR:HG22	2.00	0.44
1:A:1524:ASN:N	1:A:1524:ASN:ND2	2.65	0.44
2:C:97:HIS:CG	2:C:98:PRO:HD3	2.52	0.44
2:C:241:SER:HB3	2:C:301:TYR:CZ	2.53	0.44
2:C:320:HIS:HB3	2:C:322:LEU:HG	1.99	0.44
2:C:404:VAL:HG12	2:C:404:VAL:O	2.18	0.44
2:C:94:MSE:HB2	2:C:97:HIS:ND1	2.33	0.44
1:A:1140:MSE:HG3	1:A:1145:PHE:HD2	1.83	0.44
1:A:1169:SER:O	1:A:1171:VAL:HG23	2.18	0.43
1:A:1413:LEU:HB3	1:A:1414:PRO:HD2	1.99	0.43
2:C:117:TYR:CE2	2:C:121:ILE:HD11	2.53	0.43
2:C:106:GLU:HG3	2:C:107:LYS:N	2.32	0.43
2:C:109:LEU:HD22	2:C:300:ASN:HD21	1.83	0.43
2:C:131:TYR:O	2:C:132:VAL:HB	2.18	0.43
1:A:1182:ARG:HB2	1:A:1185:LEU:HD12	2.00	0.43
2:C:158:LEU:HD23	2:C:158:LEU:HA	1.75	0.43
1:A:234:TRP:CD1	1:A:234:TRP:N	2.86	0.43
1:A:1390:LEU:HD21	1:A:1404:VAL:HG22	2.01	0.43
2:C:73:ARG:HD2	2:C:129:ASN:ND2	2.34	0.43
2:C:262:ALA:CB	2:C:276:VAL:HG11	2.48	0.43
2:C:280:SER:O	2:C:281:ASP:O	2.36	0.43
1:A:1133:ILE:N	1:A:1137:LYS:HE3	2.33	0.43
1:A:1292:ILE:HD12	1:A:1352:ASP:OD2	2.18	0.43
1:A:1316:ASN:C	2:C:160:PHE:CE1	2.91	0.43
1:A:1396:ASP:HB2	2:C:234:GLN:NE2	2.34	0.43
2:C:79:GLU:O	2:C:83:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:SER:HB3	1:A:1460:PHE:CD2	2.54	0.43
1:A:1341:LEU:HD23	1:A:1344:TRP:HD1	1.84	0.43
1:A:14:ASP:HB3	1:A:58:ARG:HA	2.01	0.43
2:C:36:PHE:CD2	2:C:36:PHE:N	2.86	0.43
2:C:227:ILE:HG22	2:C:227:ILE:O	2.19	0.43
1:A:213:SER:HA	1:A:214:PRO:HD2	1.87	0.43
1:A:1251:THR:CG2	1:A:1252:ASP:N	2.81	0.43
1:A:1316:ASN:HB2	2:C:160:PHE:CE1	2.54	0.43
1:A:1344:TRP:HH2	2:C:158:LEU:CD2	2.32	0.43
1:A:1318:HIS:N	2:C:160:PHE:CD1	2.82	0.43
1:A:78:LYS:HG2	1:A:96:ALA:HB2	2.01	0.42
1:A:1304:VAL:HG13	1:A:1323:ILE:HG22	2.00	0.42
1:A:57:TRP:HA	1:A:57:TRP:CE3	2.55	0.42
2:C:265:SER:O	2:C:269:GLY:O	2.38	0.42
2:C:413:ILE:HA	2:C:416:TYR:CD2	2.52	0.42
1:A:232:ILE:HD13	1:A:247:LEU:HA	2.02	0.42
1:A:1263:LYS:HD2	1:A:1263:LYS:HA	1.83	0.42
1:A:1496:CYS:C	1:A:1498:LEU:H	2.22	0.42
2:C:49:LEU:HD23	2:C:49:LEU:HA	1.79	0.42
2:C:64:SER:O	2:C:67:ASP:HB2	2.19	0.42
2:C:193:ILE:H	2:C:193:ILE:HG13	1.68	0.42
1:A:1196:GLU:C	1:A:1198:VAL:H	2.22	0.42
1:A:1277:ILE:CD1	1:A:1384:CYS:HA	2.48	0.42
2:C:341:HIS:CD2	2:C:342:PRO:HD2	2.54	0.42
1:A:253:PHE:CB	1:A:254:PRO:HD2	2.49	0.42
1:A:1208:TYR:CZ	1:A:1505:GLU:HG3	2.55	0.42
2:C:53:LEU:N	2:C:53:LEU:CD1	2.83	0.42
2:C:59:GLU:CG	2:C:60:SER:H	2.33	0.42
1:A:50:THR:O	1:A:50:THR:CG2	2.67	0.42
1:A:1259:ALA:HA	1:A:1262:LYS:HB3	2.00	0.42
1:A:1309:LYS:CE	2:C:314:ILE:HG12	2.49	0.42
1:A:1350:SER:O	2:C:157:ASP:HB2	2.19	0.42
1:A:1498:LEU:HD23	1:A:1498:LEU:HA	1.83	0.42
1:A:1512:VAL:O	1:A:1516:ILE:HG23	2.20	0.42
2:C:85:ARG:O	2:C:86:ASN:C	2.58	0.42
2:C:193:ILE:O	2:C:196:ALA:HB3	2.20	0.42
1:A:1143:ARG:O	1:A:1144:ARG:C	2.58	0.42
1:A:1337:ALA:HA	2:C:210:MSE:HE1	2.02	0.42
2:C:97:HIS:H	2:C:98:PRO:CD	2.33	0.42
2:C:185:TYR:CB	2:C:263:ILE:HG22	2.50	0.42
2:C:217:GLU:O	2:C:219:LEU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:CG1	1:A:257:LEU:HB2	2.44	0.42
2:C:185:TYR:HB2	2:C:263:ILE:HG22	2.02	0.42
2:C:197:LEU:HB3	2:C:209:CYS:SG	2.59	0.42
1:A:1304:VAL:HG13	1:A:1323:ILE:CG2	2.50	0.42
1:A:1344:TRP:HZ2	2:C:158:LEU:HD11	1.85	0.42
2:C:43:ARG:NH1	2:C:76:HIS:HB2	2.35	0.42
1:A:1314:SER:O	1:A:1315:LYS:HB2	2.20	0.41
2:C:74:PHE:CD1	2:C:347:MSE:HG2	2.40	0.41
2:C:142:SER:O	2:C:143:LYS:HG3	2.20	0.41
1:A:200:LEU:HD13	1:A:234:TRP:CE3	2.54	0.41
1:A:274:GLY:C	1:A:276:ASN:H	2.23	0.41
1:A:276:ASN:HA	1:A:1150:THR:OG1	2.19	0.41
1:A:1134:ASP:O	1:A:1135:ASN:HB2	2.20	0.41
2:C:85:ARG:HH12	2:C:404:VAL:CG2	2.32	0.41
1:A:1191:LEU:HD13	1:A:1490:HIS:CD2	2.55	0.41
1:A:1371:PHE:O	1:A:1371:PHE:CD2	2.74	0.41
2:C:162:LEU:C	2:C:164:GLU:N	2.73	0.41
2:C:215:ILE:CG1	2:C:216:GLN:N	2.83	0.41
2:C:222:VAL:HG23	2:C:223:ILE:N	2.34	0.41
1:A:1309:LYS:HG2	2:C:314:ILE:CG2	2.50	0.41
1:A:1317:GLY:O	1:A:1320:SER:HB3	2.21	0.41
1:A:73:CYS:HB2	1:A:102:VAL:HB	2.01	0.41
1:A:1325:TYR:HB3	1:A:1333:ILE:CD1	2.51	0.41
2:C:252:GLN:O	2:C:252:GLN:HG2	2.19	0.41
2:C:262:ALA:HB2	2:C:276:VAL:HG21	2.03	0.41
1:A:1178:THR:HG22	1:A:1484:PHE:HB2	2.03	0.41
1:A:1402:SER:O	1:A:1405:GLN:HB3	2.20	0.41
2:C:95:GLU:C	2:C:98:PRO:HD2	2.40	0.41
1:A:1488:HIS:HA	1:A:1491:SER:HB3	2.02	0.41
2:C:239:LYS:HD3	2:C:242:LEU:HD13	2.02	0.41
2:C:359:ILE:HG13	2:C:359:ILE:H	1.63	0.41
1:A:42:THR:HG22	1:A:43:HIS:N	2.36	0.41
1:A:126:SER:HB3	1:A:140:ILE:HD13	2.02	0.41
1:A:1340:GLN:HG3	1:A:1344:TRP:NE1	2.36	0.41
2:C:75:TRP:CZ3	2:C:395:CYS:HB2	2.55	0.41
2:C:267:LEU:H	2:C:267:LEU:HG	1.69	0.41
1:A:229:ARG:NH1	1:A:253:PHE:O	2.53	0.41
1:A:1325:TYR:OH	2:C:214:GLY:HA3	2.21	0.41
1:A:1332:ARG:HH22	2:C:236:GLY:N	2.18	0.41
2:C:360:HIS:HD2	2:C:411:LYS:HG3	1.86	0.41
1:A:63:HIS:HA	1:A:64:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:N	1:A:251:GLU:OE1	2.53	0.40
1:A:1492:LEU:HD11	1:A:1508:ILE:HG23	2.03	0.40
2:C:396:LEU:H	2:C:396:LEU:HG	1.63	0.40
1:A:1303:ASP:OD2	1:A:1306:ARG:HB2	2.21	0.40
2:C:187:LEU:HD12	2:C:187:LEU:HA	1.93	0.40
1:A:1181:GLN:O	1:A:1181:GLN:CG	2.69	0.40
1:A:1383:LEU:O	1:A:1386:LEU:HB3	2.21	0.40
2:C:73:ARG:NH1	2:C:129:ASN:HD21	2.19	0.40
2:C:315:LEU:HA	2:C:316:PRO:HD3	1.91	0.40
2:C:316:PRO:O	2:C:317:LEU:HG	2.21	0.40
2:C:344:ARG:HG2	2:C:347:MSE:HE2	2.02	0.40
1:A:151:ALA:CB	1:A:175:THR:HG22	2.51	0.40
1:A:261:SER:CB	1:A:1153:LYS:HA	2.51	0.40
2:C:401:PRO:HA	2:C:405:GLU:HA	2.04	0.40
1:A:1454:LEU:O	1:A:1458:LEU:HG	2.21	0.40
2:C:39:ILE:HA	2:C:42:PHE:HD2	1.85	0.40
2:C:162:LEU:O	2:C:164:GLU:N	2.55	0.40
2:C:185:TYR:HB2	2:C:263:ILE:CG2	2.52	0.40
2:C:192:ALA:O	2:C:193:ILE:C	2.59	0.40
2:C:298:ILE:HA	2:C:301:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/753 (92%)	608 (88%)	78 (11%)	9 (1%)	10	42
2	C	373/426 (88%)	297 (80%)	66 (18%)	10 (3%)	4	29
All	All	1068/1179 (91%)	905 (85%)	144 (14%)	19 (2%)	7	36

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	218	TYR
2	C	281	ASP
2	C	55	ASN
2	C	171	VAL
2	C	222	VAL
1	A	1178	THR
2	C	104	LEU
2	C	132	VAL
2	C	387	ARG
1	A	254	PRO
1	A	1244	PRO
1	A	1497	PHE
2	C	336	PRO
1	A	1278	GLY
2	C	223	ILE
1	A	1305	VAL
1	A	1414	PRO
1	A	1248	PRO
1	A	64	PRO

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	621/655 (95%)	618 (100%)	3 (0%)	86	89
2	C	345/384 (90%)	336 (97%)	9 (3%)	41	61
All	All	966/1039 (93%)	954 (99%)	12 (1%)	67	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	1252	ASP
1	A	1354	ASN
2	C	58	ASP
2	C	99	TYR

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Mol	Chain	Res	Type
2	C	163	ARG
2	C	170	ASP
2	C	249	SER
2	C	280	SER
2	C	301	TYR
2	C	390	THR
2	C	395	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1290	ASN
1	A	1354	ASN
2	C	118	GLN
2	C	234	GLN
2	C	240	HIS
2	C	273	ASN
2	C	300	ASN
2	C	360	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [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(Å ²)	Q<0.9
1	A	696/753 (92%)	-0.21	1 (0%) 92 89	159, 188, 244, 325	0
2	C	372/426 (87%)	0.15	9 (2%) 59 45	134, 171, 248, 370	0
All	All	1068/1179 (90%)	-0.09	10 (0%) 81 67	134, 183, 246, 370	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	287	HIS	3.4
2	C	416	TYR	3.1
2	C	289	HIS	3.1
2	C	397	ASP	2.7
1	A	1133	ILE	2.4
2	C	391	HIS	2.3
2	C	185	TYR	2.3
2	C	223	ILE	2.3
2	C	270	ALA	2.2
2	C	213	CYS	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 monosaccharides 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.