



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:56 AM UTC

PDB ID : 3JRO / pdb_00003jro
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

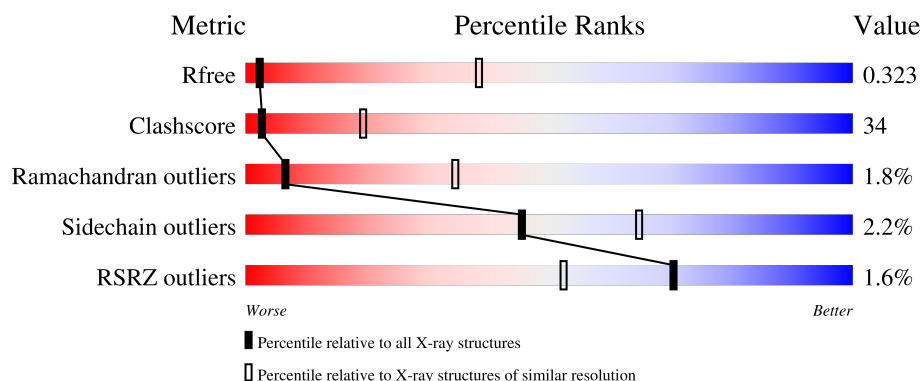
1 Overall quality at a glance

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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



I417	E340	S968	A200	V132	V62	GLY
S418	H341	G269	K201	M133	I63	SER
L419	P342	A270	L202	E134	S64	MSE
K421	I343	I271		R135	S65	GLU
L422	R344	P272	N205	P136	K66	LEU
Q423	V345	N273	I206	LYS	D67	SER
G424	L346		S907	ASN	U68	PRO
	M347	V276	I208	VAL		THR
		L277	C209	P140	A72	TYR
	I351	Q278	M210	T141	R73	GLN
	L355	Y279	I211	S142	F74	THR
	P356	S280	L212	K143	W75	GLU
		D281	C213	V144	H76	ARG
	I359	W282	G214	L145		PHE
	H360	E283	I215	N146	E79	THR
		S284	Q216	S147	L80	LYS
	V363	D285	E217		L81	PHE
		L286	Y218	G151	L82	SER
	V370	H287	L219	G152	W83	ASP
LYS	GLY	I288	W220	L153	F84	THR
THR	ALA	H289	P221	K154	R85	LEU
GLU	SER	L290	I223	S155	N86	LYS
ILE	ASN	N291		C156		GLU
D381	ASP	Q292	I227	D157	L89	PHE
	ILE	I293		L158		LYS
		L294	F231	D159	N94	ILE
		Q295	N232	F160	E95	GLU
			T233	P161	L96	GLN
		I298	Q234	L162	H97	ASN
		E299	Q235	R163	P98	ASN
		N300	Q236	E164	Y99	ASN
		Y301	I237		N100	GLU
			K238	V168	S101	ASN
		E304	N305	L169	R102	PRO
		N306	H240	D170	G103	I33
		Q307	S241	V171	L104	D34
		V308	L242	K172	F105	P35
			W243	D173	E106	F36
		E312	R244	K174	K107	F37
		L313	R245		K108	I38
		I314	T246	D177	L109	I39
		L315			M10	R40
		P316	S249	F180		E41
		L317	L250	F181	K114	F42
		S318	S251	K182	Q115	R43
		H320	Q252	Y183	L116	
		A321	Q253	I184	Y117	A46
		L322	A254	Y185	Q118	
			G255	E186	I119	L49
		V331	L256	L187	W120	A50
		S332		I188	I121	
		R333	E260	L189	V122	L53
		H334	R261		M123	A54
		P335	A262	A192		N55
		S337	I263	I193	L126	S56
		E338	Y264		K127	G57
		Y416	S265	A196	E128	D58
			Y266	L197	N129	E59
				E198	T130	S60
				E199	Y131	N61

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 (7.82%)	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 [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/5744	0.74	6/7776 (0.1%)
2	C	0.38	0/3101	0.82	4/4202 (0.1%)
All	All	0.33	0/8845	0.77	10/11978 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	34	ASP	CA-C-N	7.80	127.44	119.56
2	C	34	ASP	C-N-CA	7.80	127.44	119.56
2	C	282	TRP	N-CA-C	-7.36	101.85	111.71
1	A	1165	ILE	N-CA-C	-6.91	106.57	113.20
1	A	1208	TYR	CA-C-N	6.50	126.46	119.76
1	A	1208	TYR	C-N-CA	6.50	126.46	119.76
2	C	308	VAL	N-CA-C	5.63	115.99	108.11
1	A	1443	THR	N-CA-C	5.13	116.95	108.13
1	A	1243	ASP	CA-C-N	5.10	126.22	119.84
1	A	1243	ASP	C-N-CA	5.10	126.22	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5623	0	5577	298	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3048	0	3033	319	0
All	All	8671	0	8610	579	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 34.

All (579) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:158:LEU:C	2:C:161:PRO:HD2	2.18	0.68
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:163:ARG:HH22	2:C:253:GLN:CD	2.04	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
1:A:1277:ILE:HD13	1:A:1384:CYS:SG	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1332:ARG:HH22	2:C:235:GLN:C	2.09	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: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:100:ASN:CG	2:C:102:ARG:HB3	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:336:PRO:HD2	2:C:338:GLU:CD	2.28	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
1:A:258:TRP:HH2	1:A:1146:THR:HG23	1.69	0.57
1:A:1516:ILE:HG13	1:A:1517:THR:N	2.18	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:234:GLN:O	2:C:234:GLN:HG3	2.03	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:98:PRO:C	2:C:100:ASN:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:270:ALA:C	2:C:272:PRO:HD3	2.31	0.55
1:A:1304:VAL:HG22	1:A:1326:LEU:HD23	1.89	0.55
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:301:TYR:CD1	2:C:301:TYR:C	2.85	0.54
2:C:215:ILE:HD12	2:C:267:LEU:HD22	1.89	0.54
1:A:205:ASP:CG	1:A:206:TRP:H	2.16	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
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
2:C:301:TYR:C	2:C:301:TYR:HD1	2.16	0.53
1:A:264:LEU:HD11	1:A:1156:THR:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:151:GLY:C	2:C:153:LEU:H	2.15	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
1:A:1316:ASN:CG	2:C:160:PHE:CZ	2.88	0.52
2:C:152:GLY:C	2:C:154:LYS:H	2.16	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
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: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:1354:ASN:C	1:A:1354:ASN:HD22	2.17	0.52
2:C:109:LEU:HD13	2:C:300:ASN:CG	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:127:LYS:C	2:C:129:ASN:H	2.19	0.50
2:C:169:LEU:HD13	2:C:174:LYS:HG3	1.92	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
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
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
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:227:GLN:C	1:A:229:ARG:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:ASN:C	2:C:160:PHE:CE1	2.91	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:1458:LEU:CB	1:A:1466:PHE:CZ	2.97	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
1:A:212:TRP:CD1	1:A:213:SER:H	2.32	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
2:C:57:GLY:O	2:C:58:ASP:OD1	2.33	0.47
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
1:A:1496:CYS:C	1:A:1498:LEU:H	2.22	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
1:A:1196:GLU:C	1:A:1198:VAL:H	2.22	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
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
1:A:1143:ARG:O	1:A:1144:ARG:C	2.58	0.47
2:C:85:ARG:O	2:C:86:ASN:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:274:GLY:C	1:A:276:ASN:H	2.23	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:162:LEU:C	2:C:164:GLU:N	2.73	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
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
2:C:95:GLU:C	2:C:98:PRO:HD2	2.40	0.46
1:A:270:ALA:HA	1:A:280:LEU:HD23	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:192:ALA:O	2:C:193:ILE:C	2.59	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
1:A:1334:ARG:HH12	1:A:1397:GLU:CD	2.24	0.45
2:C:157:ASP:C	2:C:157:ASP:OD1	2.60	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:152:GLY:C	2:C:154:LYS:N	2.75	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:242:LEU:HD23	2:C:242:LEU:C	2.42	0.44
2:C:245:ARG:HD3	2:C:315:LEU:O	2.18	0.44
1:A:1336:LEU:C	2:C:210:MSE:HE2	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:HD21	1:A:290:GLU:CD	2.26	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
1:A:1349:CYS:HB3	2:C:157:ASP:CG	2.42	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:151:GLY:C	2:C:153:LEU:N	2.76	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:9:ASN:O	1:A:10:GLU:C	2.62	0.43
1:A:31:LYS:HG2	1:A:54:GLY:C	2.44	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: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
1:A:1214:SER:HB3	1:A:1460:PHE:CD2	2.54	0.43
1:A:1269:LEU:C	1:A:1269:LEU:HD23	2.43	0.43
1:A:1341:LEU:HD23	1:A:1344:TRP:HD1	1.84	0.43
2:C:50:ALA:C	2:C:53:LEU:HD13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:MSE:HE3	1:A:1146:THR:C	2.44	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:82:LEU:C	2:C:84:PHE:N	2.75	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
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: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
2:C:99:TYR:C	2:C:99:TYR:CD2	2.97	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:1330:ASP:CG	1:A:1332:ARG:HG2	2.45	0.42
1:A:1512:VAL:O	1:A:1516:ILE:HG23	2.20	0.42
2:C:193:ILE:O	2:C:196:ALA:HB3	2.20	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
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:276:ASN:HA	1:A:1150:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1524:ASN:N	1:A:1524:ASN:ND2	2.65	0.41
2:C:82:LEU:O	2:C:83:VAL:C	2.62	0.41
2:C:340:GLU:O	2:C:341:HIS:C	2.63	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:73:ARG:HH11	2:C:129:ASN:CG	2.25	0.41
1:A:68:THR:C	1:A:69:ILE:HD12	2.46	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:227:GLN:C	1:A:229:ARG:N	2.79	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
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:277:LEU:O	2:C:278:GLN:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1185:LEU:C	1:A:1187:ASP:H	2.29	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:298:ILE:HA	2:C:301:TYR:CZ	2.56	0.40
2:C:400:ASN:CG	2:C:407:VAL:HG21	2.47	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%)	9	41
2	C	373/426 (88%)	297 (80%)	66 (18%)	10 (3%)	4	28
All	All	1068/1179 (91%)	905 (85%)	144 (14%)	19 (2%)	6	34

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

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Mol	Chain	Res	Type
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%)	615 (99%)	6 (1%)	68	76
2	C	345/384 (90%)	330 (96%)	15 (4%)	26	48
All	All	966/1039 (93%)	945 (98%)	21 (2%)	45	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	216	VAL
1	A	1252	ASP
1	A	1333	ILE
1	A	1354	ASN
1	A	1533	ILE
2	C	38	ILE
2	C	58	ASP

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Mol	Chain	Res	Type
2	C	163	ARG
2	C	189	LEU
2	C	227	ILE
2	C	249	SER
2	C	256	LEU
2	C	280	SER
2	C	298	ILE
2	C	301	TYR
2	C	359	ILE
2	C	390	THR
2	C	394	ILE
2	C	395	CYS
2	C	396	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	284	ASN
1	A	1276	GLN
1	A	1290	ASN
1	A	1354	ASN
1	A	1424	GLN
1	A	1481	GLN
1	A	1486	GLN
1	A	1488	HIS
2	C	118	GLN
2	C	234	GLN
2	C	240	HIS
2	C	273	ASN
2	C	295	GLN
2	C	300	ASN
2	C	320	HIS
2	C	360	HIS

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 [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%)	-0.09	1 (0%) 92 87	159, 188, 244, 325	0
2	C	372/426 (87%)	0.30	16 (4%) 40 31	134, 171, 248, 370	0
All	All	1068/1179 (90%)	0.05	17 (1%) 70 52	134, 183, 246, 370	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	287	HIS	3.8
2	C	289	HIS	3.5
2	C	416	TYR	3.5
2	C	397	ASP	3.2
2	C	391	HIS	2.7
1	A	1133	ILE	2.7
2	C	185	TYR	2.6
2	C	223	ILE	2.6
2	C	270	ALA	2.5
2	C	301	TYR	2.2
2	C	285	ASP	2.2
2	C	213	CYS	2.2
2	C	292	GLN	2.2
2	C	41	GLU	2.2
2	C	423	GLN	2.1
2	C	163	ARG	2.0
2	C	80	LEU	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.