



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:22 PM UTC

PDB ID : 4I5S / pdb_00004i5s
Title : Structure and function of sensor histidine kinase
Authors : Cai, Y.
Deposited on : 2012-11-28
Resolution : 3.30 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

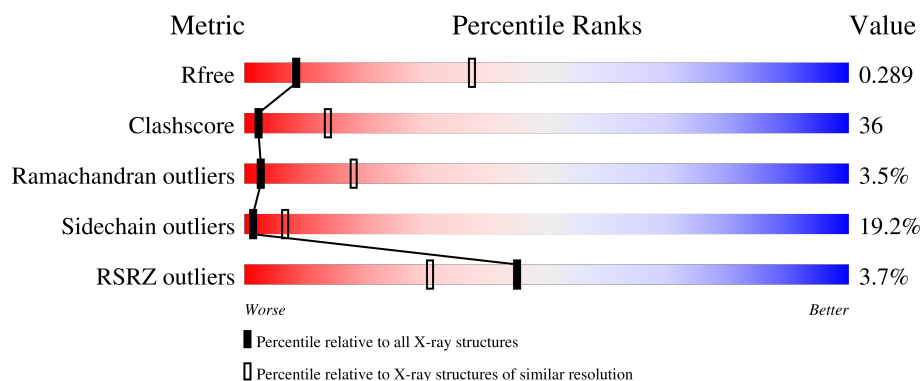
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

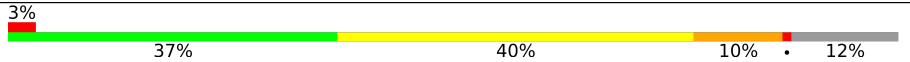
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	450	
1	B	450	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6233 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.

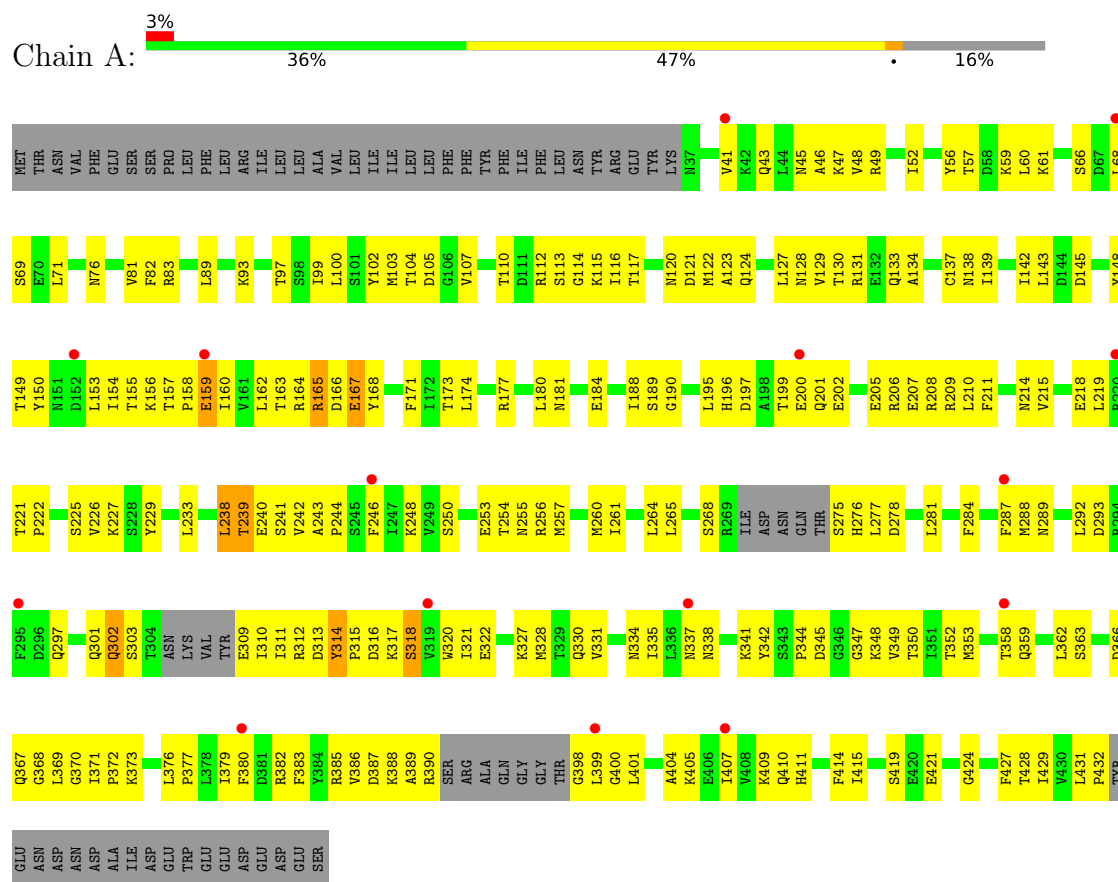
- Molecule 1 is a protein called Putative histidine kinase CovS; VicK-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3045	1905	523	608	9			
1	B	395	Total	C	N	O	S	0	0	0
			3188	1999	545	635	9			

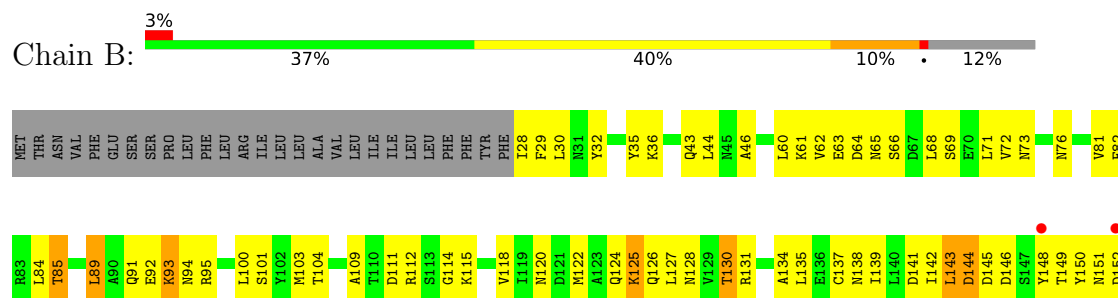
3 Residue-property plots

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: Putative histidine kinase CovS; VicK-like protein



- Molecule 1: Putative histidine kinase CovS; VicK-like protein



ASN	S365	V289	E218	L153
ASP	G370	Y290	L219	I154
ASN	I371	L291	P222	T155
ALA	P372	L292	L223	K156
ILE	K373	Q299	T224	T157
ASP	K374	Q302	K227	P158
GLU	D375	SER	S228	E159
TRP	L376	THR	Y229	I160
GLU	P377	ASN	L230	V161
GLU	L378	ASN	L231	L162
ASP	I379	LYS	A232	T163
GLU	F383	VAL	L233	R164
ASP	Y384	TYR	D234	R165
GLU	R385	E309	D235	D166
SER	V386	I310	G236	Y168
	D387	I311	A237	D169
	K388	R312	L238	E170
	A389	D313	T239	F171
	R390	Y314		I172
	SER	P315		I173
	ARG	D316	V242	L174
	ALA	K317	A243	R175
	GLN	S318	P244	I176
	GLY	V319	S245	R177
	GLY	W320	F246	F178
		I321	V249	A179
		I323	S250	L180
				N181
				R182
				G186
			T254	F187
		K327	N255	I188
		N328	R256	I192
		T329	M257	
		Q330	M258	
		V331	R259	
		I332	W260	
			I261	
	Q410	I335		L195
	H411	L336		H196
	K412		L264	D197
	G413		L265	A198
	F414	I340		T199
	I415	K341		E200
	W416		R269	
	A417	P344	I270	Q201
		D345	D271	E202
	E420	G346	N272	K203
	E421	G347	Q273	E204
	G422	K348	T274	E205
	E423	V349	S275	R206
			H276	E207
		T352		R208
	T426	M353	V279	R209
	F427		E280	L210
	T428		L281	F211
	I429	T356	T282	V212
	V430	D357		S213
	L431		T285	N214
	P432	I361	A286	V215
	Y433	L362	F287	S216
	E434	S363	M288	H217

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.12Å 153.12Å 125.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.62 – 3.30 36.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.62-3.30) 99.5 (36.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.230 , 0.270 (Not available) , 0.289	Depositor DCC
R_{free} test set	1451 reflections (5.62%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 131.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6233	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.35	0/3082	0.79	3/4164 (0.1%)
1	B	0.36	0/3230	0.78	2/4366 (0.0%)
All	All	0.35	0/6312	0.78	5/8530 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ILE	N-CA-C	6.19	116.78	107.75
1	B	157	THR	CA-C-N	5.99	126.49	120.14
1	B	157	THR	C-N-CA	5.99	126.49	120.14
1	A	159	GLU	N-CA-C	5.56	118.32	110.14
1	A	358	THR	N-CA-C	-5.46	106.47	113.02

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	3045	0	3049	234	0
1	B	3188	0	3183	234	0
All	All	6233	0	6232	446	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 36.

All (446) 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)
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.28	0.94
1:B:142:ILE:HG22	1:B:143:LEU:H	1.32	0.94
1:A:148:TYR:HD2	1:A:149:THR:H	1.16	0.92
1:B:127:LEU:HA	1:B:165:ARG:HD3	1.53	0.89
1:A:121:ASP:HA	1:A:124:GLN:HE21	1.38	0.86
1:A:311:ILE:HG22	1:A:349:VAL:HB	1.58	0.85
1:B:158:PRO:HB3	1:B:177:ARG:HA	1.58	0.85
1:B:433:TYR:CG	1:B:434:GLU:N	2.42	0.84
1:B:32:TYR:HE2	1:B:36:LYS:HG2	1.42	0.83
1:B:239:THR:HA	1:B:243:ALA:HB2	1.59	0.83
1:A:184:GLU:CD	1:A:184:GLU:H	1.85	0.82
1:A:219:LEU:HD11	1:A:261:ILE:HD11	1.59	0.82
1:A:209:ARG:HG2	1:A:209:ARG:NH1	1.91	0.81
1:A:162:LEU:HD11	1:A:173:THR:HG22	1.62	0.81
1:A:314:TYR:HB3	1:A:352:THR:HA	1.62	0.81
1:A:371:ILE:HG13	1:A:372:PRO:HA	1.64	0.80
1:A:314:TYR:HD1	1:A:314:TYR:O	1.63	0.79
1:A:110:THR:HG22	1:A:116:ILE:HA	1.65	0.78
1:B:281:LEU:HD11	1:B:320:TRP:HB3	1.66	0.78
1:B:149:THR:O	1:B:153:LEU:HD23	1.84	0.77
1:B:167:GLU:OE2	1:B:167:GLU:N	2.18	0.77
1:B:280:GLU:O	1:B:282:THR:HG22	1.85	0.77
1:B:388:LYS:HA	1:B:389:ALA:HB3	1.64	0.77
1:A:148:TYR:HD2	1:A:149:THR:N	1.83	0.76
1:B:374:LYS:HD2	1:B:374:LYS:N	2.00	0.76
1:A:257:MET:HE3	1:B:223:LEU:HD11	1.67	0.75
1:B:173:THR:H	1:B:199:THR:HG22	1.51	0.75
1:B:385:ARG:HD3	1:B:388:LYS:HD2	1.67	0.75
1:B:181:ASN:HB2	1:B:192:ILE:HG13	1.70	0.74
1:A:171:PHE:H	1:A:171:PHE:HD2	1.34	0.74
1:A:344:PRO:HD2	1:A:367:GLN:HB3	1.69	0.73
1:A:209:ARG:HH11	1:A:209:ARG:CG	2.00	0.73
1:A:288:MET:HE1	1:A:362:LEU:HD11	1.70	0.73
1:A:382:ARG:HD2	1:A:383:PHE:CE2	2.24	0.72
1:A:177:ARG:NH1	1:B:196:HIS:HE1	1.87	0.72
1:A:229:TYR:CE1	1:A:297:GLN:HG2	2.23	0.72
1:A:371:ILE:HG23	1:A:372:PRO:HA	1.70	0.71
1:A:292:LEU:HD22	1:A:311:ILE:HD12	1.73	0.71
1:B:125:LYS:HD2	1:B:125:LYS:N	2.04	0.71
1:A:316:ASP:O	1:A:317:LYS:HE3	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:HD12	1:B:348:LYS:HG2	1.73	0.70
1:A:314:TYR:O	1:A:314:TYR:CD1	2.44	0.70
1:A:369:LEU:HB3	1:A:421:GLU:HG3	1.71	0.70
1:B:385:ARG:HG2	1:B:388:LYS:HZ3	1.56	0.70
1:B:81:VAL:O	1:B:85:THR:HG23	1.92	0.69
1:B:208:ARG:NH2	1:B:271:ASP:OD2	2.26	0.68
1:B:412:LYS:O	1:B:412:LYS:HD3	1.94	0.68
1:A:229:TYR:O	1:A:233:LEU:HB3	1.92	0.68
1:B:264:LEU:HD12	1:B:399:LEU:HD11	1.76	0.68
1:A:281:LEU:HD23	1:A:322:GLU:HG3	1.75	0.68
1:A:334:ASN:O	1:A:337:ASN:HB2	1.94	0.68
1:A:128:ASN:HB2	1:A:165:ARG:O	1.94	0.68
1:B:388:LYS:HD3	1:B:390:ARG:HG2	1.76	0.68
1:A:255:ASN:OD1	1:B:227:LYS:NZ	2.28	0.67
1:B:101:SER:HA	1:B:120:ASN:HB2	1.77	0.67
1:A:386:VAL:HG13	1:B:272:ASN:ND2	2.10	0.67
1:A:314:TYR:N	1:A:315:PRO:HD2	2.09	0.67
1:A:229:TYR:CD1	1:A:297:GLN:HG2	2.29	0.66
1:A:277:LEU:HD12	1:A:410:GLN:HB3	1.77	0.66
1:A:371:ILE:HG23	1:A:372:PRO:CA	2.25	0.66
1:A:281:LEU:HD11	1:A:320:TRP:HB3	1.77	0.66
1:B:182:ARG:NH1	1:B:186:GLY:O	2.29	0.66
1:A:100:LEU:HA	1:A:103:MET:HE2	1.78	0.66
1:B:127:LEU:HA	1:B:165:ARG:CD	2.26	0.66
1:A:110:THR:O	1:A:190:GLY:HA3	1.96	0.66
1:B:224:THR:HA	1:B:227:LYS:HG2	1.76	0.66
1:B:314:TYR:H	1:B:315:PRO:HD2	1.60	0.65
1:B:403:ILE:HD12	1:B:403:ILE:H	1.61	0.65
1:B:153:LEU:HD13	1:B:180:LEU:HD21	1.77	0.65
1:B:115:LYS:HA	1:B:138:ASN:HA	1.77	0.65
1:A:100:LEU:HD23	1:A:103:MET:HE1	1.79	0.65
1:A:218:GLU:HB3	1:A:260:MET:HE2	1.78	0.65
1:A:250:SER:O	1:A:254:THR:HG23	1.96	0.65
1:A:41:VAL:O	1:A:45:ASN:HB2	1.96	0.65
1:B:44:LEU:HD11	1:B:72:VAL:HG22	1.79	0.65
1:A:277:LEU:HD23	1:A:278:ASP:H	1.62	0.65
1:A:316:ASP:CG	1:A:317:LYS:H	2.05	0.65
1:B:269:ARG:HB3	1:B:275:SER:HB2	1.78	0.64
1:B:142:ILE:HG22	1:B:143:LEU:N	2.10	0.64
1:A:314:TYR:N	1:A:315:PRO:CD	2.60	0.64
1:A:338:ASN:HB3	1:A:399:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLY:HA2	1:B:423:GLU:C	2.21	0.64
1:B:156:LYS:HD2	1:B:156:LYS:O	1.98	0.64
1:A:163:THR:HB	1:A:165:ARG:CG	2.28	0.63
1:A:371:ILE:HD13	1:A:419:SER:O	1.98	0.63
1:B:281:LEU:HD23	1:B:322:GLU:HG2	1.80	0.63
1:B:122:MET:HE3	1:B:126:GLN:HE21	1.63	0.63
1:B:243:ALA:HB3	1:B:244:PRO:HD3	1.81	0.63
1:B:299:GLN:HE22	1:B:309:GLU:HG3	1.62	0.62
1:A:71:LEU:HD21	1:B:44:LEU:HD23	1.81	0.62
1:B:32:TYR:CE2	1:B:36:LYS:HG2	2.30	0.62
1:A:208:ARG:HB2	1:B:212:VAL:HG11	1.81	0.62
1:A:49:ARG:HD2	1:A:52:ILE:HD12	1.80	0.62
1:A:211:PHE:O	1:A:215:VAL:HG22	1.99	0.62
1:A:421:GLU:N	1:A:421:GLU:OE1	2.32	0.62
1:B:163:THR:O	1:B:172:ILE:HG22	1.99	0.61
1:B:232:ALA:O	1:B:237:ALA:HB3	2.01	0.61
1:B:356:THR:HG23	1:B:361:ILE:HD11	1.80	0.61
1:A:338:ASN:HB3	1:A:399:LEU:HD22	1.81	0.61
1:B:44:LEU:CD1	1:B:72:VAL:HG22	2.31	0.61
1:A:338:ASN:HA	1:A:341:LYS:HB3	1.82	0.61
1:A:114:GLY:HA3	1:A:139:ILE:HD11	1.81	0.61
1:A:148:TYR:CD2	1:A:149:THR:N	2.69	0.61
1:B:422:GLY:HA2	1:B:423:GLU:O	2.01	0.61
1:B:61:LYS:HD3	1:B:61:LYS:O	2.00	0.60
1:B:168:TYR:CG	1:B:169:ASP:N	2.65	0.60
1:A:143:LEU:HB3	1:A:145:ASP:OD2	2.01	0.60
1:B:327:LYS:O	1:B:330:GLN:HB2	2.01	0.60
1:A:102:TYR:HE2	1:B:182:ARG:HB2	1.66	0.60
1:B:32:TYR:C	1:B:32:TYR:HD2	2.10	0.60
1:A:89:LEU:HD12	1:B:89:LEU:HB3	1.83	0.59
1:B:62:VAL:HG12	1:B:64:ASP:H	1.68	0.59
1:B:288:MET:SD	1:B:353:MET:HE1	2.42	0.59
1:A:164:ARG:C	1:A:166:ASP:H	2.09	0.59
1:B:287:PHE:CZ	1:B:291:ILE:HD11	2.37	0.59
1:B:341:LYS:HZ3	1:B:388:LYS:HD3	1.67	0.59
1:A:107:VAL:H	1:A:120:ASN:ND2	1.99	0.59
1:B:217:HIS:C	1:B:217:HIS:CD2	2.80	0.59
1:B:66:SER:O	1:B:69:SER:HB3	2.03	0.59
1:B:373:LYS:H	1:B:373:LYS:HD2	1.68	0.58
1:A:48:VAL:O	1:A:52:ILE:HG13	2.02	0.58
1:B:371:ILE:HD13	1:B:379:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TYR:C	1:B:32:TYR:CD2	2.81	0.58
1:B:142:ILE:HB	1:B:145:ASP:OD2	2.03	0.58
1:A:288:MET:HG3	1:A:292:LEU:HD12	1.85	0.58
1:A:196:HIS:HD2	1:B:175:ARG:HH12	1.51	0.58
1:B:320:TRP:N	1:B:434:GLU:HG2	2.19	0.58
1:A:93:LYS:O	1:A:97:THR:HG22	2.04	0.57
1:B:197:ASP:OD1	1:B:199:THR:HG23	2.03	0.57
1:B:383:PHE:CZ	1:B:399:LEU:HD21	2.38	0.57
1:A:150:TYR:O	1:A:154:ILE:HG13	2.04	0.57
1:B:73:ASN:HA	1:B:76:ASN:HB2	1.87	0.57
1:A:128:ASN:CG	1:A:128:ASN:O	2.48	0.57
1:A:238:LEU:O	1:A:239:THR:C	2.47	0.57
1:A:243:ALA:N	1:A:244:PRO:HD2	2.19	0.57
1:B:219:LEU:O	1:B:222:PRO:HD2	2.05	0.57
1:A:327:LYS:HB3	1:A:407:ILE:HD13	1.87	0.57
1:B:131:ARG:O	1:B:135:LEU:HG	2.04	0.57
1:A:124:GLN:OE1	1:A:131:ARG:N	2.38	0.57
1:B:32:TYR:HD2	1:B:32:TYR:O	1.88	0.57
1:B:163:THR:HG21	1:B:165:ARG:CZ	2.35	0.56
1:B:210:LEU:O	1:B:210:LEU:HG	2.02	0.56
1:A:127:LEU:HA	1:A:165:ARG:HD3	1.86	0.56
1:A:335:ILE:HG23	1:A:427:PHE:CD2	2.39	0.56
1:B:379:ILE:HD11	1:B:417:ALA:HB2	1.87	0.56
1:B:407:ILE:O	1:B:410:GLN:HB2	2.06	0.56
1:A:238:LEU:O	1:A:240:GLU:N	2.38	0.56
1:A:376:LEU:O	1:A:379:ILE:HG12	2.05	0.56
1:B:227:LYS:O	1:B:231:GLU:HB2	2.06	0.56
1:B:115:LYS:NZ	1:B:135:LEU:O	2.36	0.56
1:B:385:ARG:NE	1:B:390:ARG:HH22	2.04	0.56
1:B:314:TYR:N	1:B:315:PRO:HD2	2.21	0.56
1:A:60:LEU:HD12	1:A:76:ASN:OD1	2.06	0.56
1:A:202:GLU:O	1:A:206:ARG:HG2	2.06	0.56
1:A:102:TYR:CE2	1:B:182:ARG:HB2	2.41	0.55
1:A:181:ASN:HB3	1:A:189:SER:HB2	1.87	0.55
1:A:314:TYR:HB3	1:A:352:THR:CA	2.35	0.55
1:B:168:TYR:CD1	1:B:169:ASP:N	2.75	0.55
1:A:210:LEU:HA	1:A:386:VAL:HG21	1.89	0.55
1:B:250:SER:O	1:B:254:THR:HG23	2.06	0.55
1:B:256:ARG:HH21	1:B:260:MET:HE1	1.71	0.55
1:A:110:THR:HA	1:A:117:THR:HG23	1.88	0.55
1:A:164:ARG:C	1:A:166:ASP:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:CG2	1:B:143:LEU:H	2.15	0.55
1:A:89:LEU:CD1	1:B:89:LEU:HB3	2.37	0.55
1:A:163:THR:HB	1:A:165:ARG:HG2	1.89	0.54
1:A:214:ASN:HB3	1:A:264:LEU:HD13	1.89	0.54
1:A:180:LEU:N	1:A:180:LEU:HD22	2.22	0.54
1:A:113:SER:O	1:A:149:THR:HG21	2.06	0.54
1:A:242:VAL:C	1:A:244:PRO:HD2	2.32	0.54
1:A:244:PRO:HA	1:B:238:LEU:HD21	1.90	0.54
1:A:380:PHE:CD1	1:A:405:LYS:HD2	2.42	0.54
1:B:203:LYS:HA	1:B:206:ARG:HH12	1.73	0.54
1:A:331:VAL:HG13	1:A:404:ALA:HB1	1.89	0.53
1:B:347:GLY:O	1:B:348:LYS:HB2	2.07	0.53
1:A:155:THR:O	1:A:156:LYS:C	2.51	0.53
1:A:312:ARG:O	1:A:312:ARG:HG2	2.08	0.53
1:B:415:ILE:HA	1:B:428:THR:O	2.09	0.53
1:A:284:PHE:HE2	1:A:362:LEU:HD12	1.72	0.53
1:B:388:LYS:HA	1:B:389:ALA:CB	2.32	0.53
1:B:29:PHE:C	1:B:29:PHE:CD2	2.87	0.53
1:A:369:LEU:HD13	1:A:421:GLU:HG3	1.91	0.53
1:B:158:PRO:CB	1:B:177:ARG:HA	2.36	0.52
1:B:299:GLN:NE2	1:B:309:GLU:HG3	2.24	0.52
1:A:277:LEU:HD21	1:A:411:HIS:HE1	1.73	0.52
1:B:156:LYS:HD2	1:B:156:LYS:C	2.35	0.52
1:A:284:PHE:CE2	1:A:362:LEU:HD12	2.44	0.52
1:B:153:LEU:HD13	1:B:180:LEU:CD2	2.39	0.52
1:B:414:PHE:CD1	1:B:415:ILE:N	2.73	0.52
1:B:433:TYR:CD1	1:B:434:GLU:N	2.78	0.52
1:A:288:MET:O	1:A:292:LEU:HB2	2.10	0.52
1:A:173:THR:HG21	1:A:202:GLU:HG3	1.91	0.52
1:B:195:LEU:HD12	1:B:195:LEU:N	2.24	0.52
1:B:92:GLU:HA	1:B:95:ARG:NH1	2.24	0.52
1:B:203:LYS:HA	1:B:206:ARG:NH1	2.24	0.52
1:A:359:GLN:HG3	1:A:432:PRO:C	2.36	0.51
1:A:371:ILE:HD11	1:A:373:LYS:NZ	2.25	0.51
1:B:93:LYS:HE3	1:B:94:ASN:OD1	2.10	0.51
1:A:107:VAL:H	1:A:120:ASN:HD21	1.58	0.51
1:A:415:ILE:HG23	1:A:415:ILE:O	2.09	0.51
1:B:291:ILE:HD13	1:B:329:THR:HG23	1.92	0.51
1:B:356:THR:HG23	1:B:361:ILE:CD1	2.40	0.51
1:A:390:ARG:HD3	1:B:269:ARG:HH12	1.75	0.51
1:B:242:VAL:HB	1:B:246:PHE:CE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ILE:O	1:A:312:ARG:NH2	2.43	0.51
1:B:272:ASN:C	1:B:273:GLN:HG2	2.36	0.51
1:B:282:THR:CG2	1:B:323:ILE:HG12	2.40	0.51
1:B:188:ILE:N	1:B:188:ILE:HD12	2.26	0.51
1:A:257:MET:O	1:A:261:ILE:HG12	2.10	0.51
1:A:164:ARG:NH1	1:A:171:PHE:HB3	2.25	0.51
1:A:275:SER:C	1:A:276:HIS:CG	2.89	0.51
1:A:315:PRO:HG3	1:A:353:MET:HE2	1.93	0.51
1:B:62:VAL:HG13	1:B:69:SER:OG	2.10	0.51
1:B:219:LEU:C	1:B:222:PRO:HD2	2.36	0.51
1:B:420:GLU:C	1:B:422:GLY:H	2.16	0.51
1:A:301:GLN:HA	1:A:302:GLN:HB2	1.94	0.50
1:A:162:LEU:CD1	1:A:173:THR:HG22	2.39	0.50
1:A:380:PHE:HB3	1:A:405:LYS:HD3	1.93	0.50
1:A:388:LYS:HG2	1:A:389:ALA:H	1.76	0.50
1:A:47:LYS:HD3	1:A:60:LEU:HD11	1.92	0.50
1:A:68:LEU:HD12	1:A:69:SER:N	2.27	0.50
1:B:112:ARG:H	1:B:112:ARG:NH1	2.09	0.50
1:B:148:TYR:O	1:B:152:ASP:HB2	2.11	0.50
1:B:376:LEU:HD11	1:B:417:ALA:O	2.11	0.50
1:A:157:THR:OG1	1:A:159:GLU:HG3	2.11	0.50
1:A:205:GLU:OE1	1:B:208:ARG:NH1	2.44	0.50
1:B:399:LEU:O	1:B:401:LEU:N	2.45	0.50
1:A:348:LYS:HD2	1:A:348:LYS:N	2.26	0.50
1:B:168:TYR:C	1:B:170:GLU:H	2.19	0.50
1:A:292:LEU:CD2	1:A:311:ILE:HD12	2.42	0.50
1:A:317:LYS:O	1:A:318:SER:HB3	2.12	0.50
1:A:129:VAL:HG13	1:A:130:THR:O	2.12	0.49
1:A:207:GLU:HB3	1:A:268:SER:HB3	1.93	0.49
1:B:173:THR:H	1:B:199:THR:CG2	2.22	0.49
1:A:316:ASP:CG	1:A:317:LYS:N	2.70	0.49
1:B:130:THR:O	1:B:131:ARG:C	2.55	0.49
1:B:143:LEU:O	1:B:144:ASP:C	2.55	0.49
1:B:352:THR:HG23	1:B:363:SER:OG	2.13	0.49
1:B:319:VAL:C	1:B:434:GLU:HG2	2.38	0.49
1:A:102:TYR:CD1	1:A:102:TYR:N	2.80	0.49
1:B:155:THR:O	1:B:157:THR:N	2.46	0.49
1:B:162:LEU:O	1:B:162:LEU:HD22	2.13	0.49
1:B:310:ILE:HB	1:B:348:LYS:HA	1.94	0.49
1:B:412:LYS:HD3	1:B:412:LYS:C	2.38	0.49
1:A:197:ASP:OD1	1:A:199:THR:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:CE	1:A:362:LEU:HD11	2.41	0.48
1:B:379:ILE:HD11	1:B:417:ALA:CB	2.43	0.48
1:B:173:THR:HG23	1:B:199:THR:HA	1.94	0.48
1:A:369:LEU:HB3	1:A:421:GLU:CG	2.42	0.48
1:B:151:ASN:OD1	1:B:151:ASN:C	2.55	0.48
1:B:173:THR:HG23	1:B:199:THR:HG22	1.95	0.48
1:A:155:THR:OG1	1:A:157:THR:HG22	2.14	0.48
1:B:92:GLU:HG2	1:B:95:ARG:HH12	1.77	0.48
1:B:341:LYS:HZ3	1:B:390:ARG:HG2	1.79	0.48
1:B:357:ASP:OD2	1:B:357:ASP:N	2.46	0.48
1:A:221:THR:N	1:A:222:PRO:HD2	2.29	0.48
1:A:301:GLN:HA	1:A:302:GLN:CB	2.43	0.48
1:A:331:VAL:HG22	1:A:404:ALA:HA	1.95	0.48
1:B:43:GLN:O	1:B:46:ALA:HB3	2.14	0.48
1:B:208:ARG:O	1:B:211:PHE:HB3	2.14	0.48
1:A:239:THR:HG22	1:A:241:SER:OG	2.14	0.48
1:B:154:ILE:HG13	1:B:155:THR:N	2.29	0.48
1:A:341:LYS:NZ	1:A:398:GLY:O	2.47	0.48
1:B:155:THR:C	1:B:157:THR:N	2.70	0.48
1:A:335:ILE:CD1	1:A:429:ILE:HD11	2.44	0.47
1:A:371:ILE:CG2	1:A:372:PRO:HA	2.39	0.47
1:A:233:LEU:O	1:A:233:LEU:HG	2.14	0.47
1:A:313:ASP:C	1:A:315:PRO:HD2	2.39	0.47
1:B:164:ARG:O	1:B:166:ASP:N	2.47	0.47
1:B:180:LEU:HD22	1:B:180:LEU:HA	1.63	0.47
1:B:341:LYS:NZ	1:B:390:ARG:HG2	2.29	0.47
1:A:312:ARG:HD2	1:A:350:THR:HG23	1.96	0.47
1:B:388:LYS:HB3	1:B:390:ARG:HG3	1.97	0.47
1:A:99:ILE:HD11	1:B:109:ALA:HB2	1.97	0.47
1:B:155:THR:O	1:B:156:LYS:HG3	2.14	0.47
1:A:105:ASP:OD1	1:A:105:ASP:N	2.46	0.47
1:B:403:ILE:HD12	1:B:403:ILE:N	2.28	0.47
1:A:177:ARG:NH1	1:B:196:HIS:CE1	2.75	0.47
1:B:222:PRO:HB2	1:B:257:MET:SD	2.55	0.47
1:B:234:ASP:C	1:B:236:GLY:N	2.73	0.47
1:A:315:PRO:HB3	1:A:353:MET:HE3	1.97	0.47
1:A:371:ILE:HG22	1:A:421:GLU:OE2	2.14	0.47
1:B:68:LEU:HD22	1:B:68:LEU:HA	1.75	0.47
1:A:102:TYR:N	1:A:102:TYR:HD1	2.13	0.47
1:A:265:LEU:HD11	1:B:216:SER:OG	2.16	0.47
1:B:134:ALA:O	1:B:137:CYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ASP:OD2	1:A:278:ASP:C	2.58	0.46
1:A:197:ASP:OD1	1:A:197:ASP:C	2.58	0.46
1:B:361:ILE:N	1:B:361:ILE:HD12	2.30	0.46
1:A:68:LEU:HD12	1:A:68:LEU:C	2.41	0.46
1:B:163:THR:CG2	1:B:165:ARG:HG3	2.45	0.46
1:B:279:VAL:HG12	1:B:323:ILE:C	2.40	0.46
1:B:400:GLY:N	1:B:403:ILE:HD13	2.30	0.46
1:A:163:THR:HB	1:A:165:ARG:HG3	1.96	0.46
1:B:142:ILE:HB	1:B:145:ASP:CG	2.40	0.46
1:B:234:ASP:C	1:B:236:GLY:H	2.22	0.46
1:A:200:GLU:HG2	1:A:201:GLN:N	2.31	0.45
1:A:281:LEU:HD22	1:A:321:ILE:C	2.41	0.45
1:A:352:THR:HG23	1:A:363:SER:HG	1.81	0.45
1:A:368:GLY:C	1:A:369:LEU:HD23	2.40	0.45
1:B:422:GLY:CA	1:B:423:GLU:C	2.89	0.45
1:A:142:ILE:O	1:A:142:ILE:HG22	2.16	0.45
1:A:371:ILE:HG22	1:A:421:GLU:CD	2.41	0.45
1:A:371:ILE:CG1	1:A:372:PRO:HA	2.39	0.45
1:B:224:THR:HA	1:B:227:LYS:CG	2.45	0.45
1:B:233:LEU:HD11	1:B:246:PHE:HB3	1.96	0.45
1:A:371:ILE:HG23	1:A:372:PRO:N	2.31	0.45
1:B:229:TYR:CE1	1:B:249:VAL:HG11	2.51	0.45
1:B:315:PRO:HD3	1:B:353:MET:HG2	1.98	0.45
1:B:151:ASN:HA	1:B:154:ILE:HG12	1.98	0.45
1:A:226:VAL:HG21	1:A:254:THR:HG22	1.98	0.45
1:B:63:GLU:O	1:B:64:ASP:C	2.59	0.45
1:B:216:SER:O	1:B:217:HIS:C	2.59	0.45
1:B:388:LYS:CA	1:B:389:ALA:HB3	2.40	0.45
1:A:115:LYS:HG3	1:A:137:CYS:O	2.17	0.45
1:A:162:LEU:HA	1:A:162:LEU:HD13	1.64	0.45
1:A:380:PHE:CD1	1:A:405:LYS:HB2	2.52	0.45
1:B:175:ARG:HD2	1:B:196:HIS:HB3	1.99	0.45
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.73	0.44
1:B:375:ASP:OD1	1:B:375:ASP:N	2.50	0.44
1:A:386:VAL:HG12	1:A:387:ASP:OD1	2.18	0.44
1:A:81:VAL:CG1	1:A:82:PHE:N	2.80	0.44
1:A:61:LYS:HB2	1:A:61:LYS:NZ	2.32	0.44
1:A:207:GLU:O	1:A:210:LEU:HB3	2.17	0.44
1:A:409:LYS:NZ	1:A:414:PHE:HA	2.32	0.44
1:A:105:ASP:OD2	1:A:196:HIS:HD2	2.01	0.44
1:A:209:ARG:HG2	1:B:272:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HB3	1:A:129:VAL:O	2.18	0.44
1:B:104:THR:O	1:B:122:MET:HG2	2.17	0.44
1:B:288:MET:HE1	1:B:332:ILE:HG21	1.99	0.44
1:B:335:ILE:CG2	1:B:364:ILE:HD12	2.47	0.44
1:A:68:LEU:C	1:A:68:LEU:CD1	2.91	0.44
1:A:196:HIS:CD2	1:B:175:ARG:HH12	2.32	0.44
1:A:400:GLY:O	1:A:401:LEU:HD12	2.18	0.44
1:B:109:ALA:HB3	1:B:118:VAL:HB	1.99	0.44
1:B:365:SER:HA	1:B:426:THR:HB	2.00	0.44
1:A:130:THR:OG1	1:A:133:GLN:HG3	2.18	0.44
1:A:153:LEU:HD22	1:A:188:ILE:HG21	2.00	0.44
1:A:348:LYS:O	1:A:366:ASP:HA	2.17	0.44
1:B:214:ASN:O	1:B:218:GLU:HB2	2.18	0.44
1:A:159:GLU:C	1:A:159:GLU:OE1	2.61	0.44
1:A:257:MET:CE	1:B:223:LEU:HD11	2.45	0.44
1:A:164:ARG:O	1:A:166:ASP:N	2.51	0.43
1:A:218:GLU:CD	1:A:385:ARG:HH22	2.20	0.43
1:B:91:GLN:O	1:B:95:ARG:HG3	2.18	0.43
1:B:231:GLU:O	1:B:235:ASP:HB2	2.18	0.43
1:A:56:TYR:CE1	1:A:83:ARG:HD3	2.53	0.43
1:A:120:ASN:O	1:A:124:GLN:HG3	2.18	0.43
1:B:62:VAL:HG12	1:B:64:ASP:N	2.31	0.43
1:B:420:GLU:C	1:B:422:GLY:N	2.76	0.43
1:B:28:ILE:N	1:B:30:LEU:HD12	2.32	0.43
1:B:163:THR:HG22	1:B:165:ARG:HG3	2.01	0.43
1:A:121:ASP:O	1:A:124:GLN:HB2	2.18	0.43
1:A:243:ALA:N	1:A:244:PRO:CD	2.82	0.43
1:B:214:ASN:HB3	1:B:383:PHE:CD1	2.54	0.43
1:A:150:TYR:CD1	1:A:154:ILE:HD11	2.54	0.43
1:B:153:LEU:CD1	1:B:180:LEU:HD21	2.46	0.43
1:B:288:MET:HE3	1:B:292:LEU:HG	2.01	0.43
1:A:289:ASN:O	1:A:293:ASP:CG	2.62	0.43
1:B:64:ASP:HA	1:B:65:ASN:HA	1.47	0.43
1:B:145:ASP:O	1:B:146:ASP:HB2	2.19	0.43
1:B:285:THR:OG1	1:B:315:PRO:HB2	2.19	0.43
1:A:210:LEU:HA	1:A:386:VAL:CG2	2.48	0.43
1:A:260:MET:HE3	1:A:330:GLN:HG2	2.00	0.43
1:B:175:ARG:HD3	1:B:177:ARG:HG3	2.01	0.43
1:B:224:THR:O	1:B:227:LYS:HG3	2.18	0.43
1:B:384:TYR:C	1:B:385:ARG:HG3	2.44	0.43
1:B:223:LEU:HD13	1:B:257:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HB3	1:B:89:LEU:HD13	2.00	0.42
1:A:248:LYS:NZ	1:B:234:ASP:OD2	2.42	0.42
1:A:338:ASN:HB3	1:A:399:LEU:HD23	2.01	0.42
1:A:43:GLN:O	1:A:46:ALA:HB3	2.18	0.42
1:A:120:ASN:ND2	1:A:123:ALA:H	2.17	0.42
1:B:81:VAL:O	1:B:82:PHE:C	2.62	0.42
1:A:366:ASP:O	1:A:424:GLY:HA3	2.19	0.42
1:A:380:PHE:CG	1:A:405:LYS:HD2	2.54	0.42
1:B:111:ASP:HB2	1:B:112:ARG:NH1	2.34	0.42
1:A:105:ASP:OD2	1:A:196:HIS:CD2	2.72	0.42
1:B:290:TYR:C	1:B:290:TYR:CD2	2.97	0.42
1:A:287:PHE:CE1	1:A:328:MET:HB3	2.53	0.42
1:A:376:LEU:HB3	1:A:377:PRO:HD3	2.01	0.42
1:B:32:TYR:O	1:B:35:TYR:HB3	2.20	0.42
1:B:287:PHE:CZ	1:B:291:ILE:CD1	3.02	0.42
1:A:180:LEU:N	1:A:180:LEU:CD2	2.82	0.42
1:A:415:ILE:HA	1:A:428:THR:O	2.19	0.42
1:B:315:PRO:O	1:B:316:ASP:HB2	2.19	0.42
1:B:336:LEU:O	1:B:340:ILE:HD13	2.19	0.42
1:A:162:LEU:HD13	1:A:173:THR:HA	2.01	0.42
1:A:149:THR:HG22	1:A:153:LEU:HD12	2.01	0.42
1:A:233:LEU:HB2	1:A:246:PHE:HD1	1.85	0.42
1:B:142:ILE:HB	1:B:145:ASP:OD1	2.20	0.42
1:A:174:LEU:HD23	1:A:197:ASP:HA	2.01	0.42
1:A:431:LEU:HA	1:A:432:PRO:HD3	1.82	0.42
1:A:341:LYS:HE2	1:A:342:TYR:CE2	2.55	0.42
1:B:202:GLU:OE1	1:B:206:ARG:NH2	2.52	0.42
1:A:225:SER:O	1:A:226:VAL:C	2.63	0.41
1:A:229:TYR:HE1	1:A:297:GLN:HG2	1.82	0.41
1:B:258:MET:HE2	1:B:258:MET:HB2	1.90	0.41
1:B:431:LEU:HA	1:B:432:PRO:HD3	1.94	0.41
1:A:81:VAL:HG12	1:A:82:PHE:N	2.34	0.41
1:A:104:THR:O	1:A:122:MET:HE3	2.20	0.41
1:B:163:THR:HG21	1:B:165:ARG:NE	2.35	0.41
1:A:405:LYS:HG3	1:A:415:ILE:CG2	2.50	0.41
1:B:141:ASP:O	1:B:142:ILE:HD13	2.19	0.41
1:B:217:HIS:C	1:B:217:HIS:HD2	2.27	0.41
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.91	0.41
1:A:195:LEU:N	1:A:195:LEU:HD23	2.35	0.41
1:A:371:ILE:HD11	1:A:373:LYS:HZ2	1.85	0.41
1:B:62:VAL:C	1:B:64:ASP:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLN:NE2	1:B:131:ARG:HG3	2.35	0.41
1:A:47:LYS:HE3	1:A:57:THR:HG23	2.02	0.41
1:A:370:GLY:HA3	1:A:419:SER:OG	2.20	0.41
1:B:415:ILE:C	1:B:416:TRP:CD1	2.99	0.41
1:B:155:THR:C	1:B:156:LYS:HG3	2.45	0.41
1:B:166:ASP:HA	1:B:167:GLU:OE2	2.20	0.41
1:A:155:THR:O	1:A:156:LYS:HG3	2.21	0.41
1:A:309:GLU:HA	1:A:347:GLY:N	2.36	0.41
1:A:368:GLY:O	1:A:369:LEU:HD23	2.20	0.41
1:B:100:LEU:HD23	1:B:103:MET:HE3	2.02	0.41
1:B:126:GLN:O	1:B:165:ARG:HD2	2.20	0.41
1:B:370:GLY:C	1:B:371:ILE:HG13	2.46	0.41
1:A:138:ASN:OD1	1:A:139:ILE:HD12	2.21	0.41
1:A:167:GLU:H	1:A:167:GLU:HG3	1.67	0.41
1:A:276:HIS:O	1:A:327:LYS:NZ	2.30	0.41
1:B:44:LEU:HD12	1:B:60:LEU:HD12	2.03	0.41
1:A:371:ILE:HG13	1:A:372:PRO:CA	2.42	0.40
1:B:114:GLY:C	1:B:138:ASN:ND2	2.79	0.40
1:B:387:ASP:O	1:B:389:ALA:HB3	2.21	0.40
1:A:59:LYS:HG2	1:A:76:ASN:HB3	2.03	0.40
1:A:120:ASN:N	1:A:120:ASN:HD22	2.19	0.40
1:A:253:GLU:OE2	1:A:256:ARG:NH1	2.53	0.40
1:A:314:TYR:CG	1:A:352:THR:HB	2.56	0.40
1:A:112:ARG:H	1:A:112:ARG:HG2	1.62	0.40
1:A:240:GLU:CD	1:A:240:GLU:H	2.29	0.40
1:A:405:LYS:HA	1:A:415:ILE:HG21	2.03	0.40
1:B:238:LEU:HD12	1:B:239:THR:HG23	2.04	0.40
1:B:272:ASN:HB2	1:B:274:THR:HG23	2.02	0.40
1:B:282:THR:HG23	1:B:323:ILE:HG12	2.04	0.40
1:A:114:GLY:C	1:A:138:ASN:ND2	2.80	0.40
1:A:277:LEU:HD23	1:A:278:ASP:N	2.33	0.40
1:B:205:GLU:O	1:B:209:ARG:HG3	2.20	0.40
1:B:209:ARG:O	1:B:212:VAL:HG22	2.22	0.40
1:B:239:THR:HG22	1:B:243:ALA:HB1	2.03	0.40
1:B:332:ILE:HD11	1:B:362:LEU:HD11	2.04	0.40
1:A:129:VAL:HG11	1:A:134:ALA:HB2	2.03	0.40
1:B:264:LEU:HD12	1:B:399:LEU:CD1	2.50	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	372/450 (83%)	315 (85%)	44 (12%)	13 (4%)	3	18
1	B	389/450 (86%)	322 (83%)	53 (14%)	14 (4%)	2	17
All	All	761/900 (85%)	637 (84%)	97 (13%)	27 (4%)	3	18

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	PRO
1	A	167	GLU
1	A	239	THR
1	B	315	PRO
1	B	400	GLY
1	A	168	TYR
1	A	345	ASP
1	B	156	LYS
1	B	165	ARG
1	B	168	TYR
1	B	347	GLY
1	A	238	LEU
1	B	169	ASP
1	A	66	SER
1	A	165	ARG
1	A	302	GLN
1	B	144	ASP
1	B	216	SER
1	B	345	ASP
1	A	227	LYS
1	A	318	SER
1	B	314	TYR
1	B	316	ASP
1	A	303	SER
1	B	164	ARG

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Mol	Chain	Res	Type
1	B	344	PRO
1	A	314	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	297/413 (72%)	240 (81%)	57 (19%)	1 7

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	LEU
1	B	84	LEU
1	B	85	THR
1	B	89	LEU
1	B	93	LYS
1	B	125	LYS
1	B	128	ASN
1	B	130	THR
1	B	139	ILE
1	B	143	LEU
1	B	150	TYR
1	B	153	LEU
1	B	156	LYS
1	B	157	THR
1	B	159	GLU
1	B	160	ILE
1	B	162	LEU
1	B	164	ARG
1	B	171	PHE
1	B	172	ILE
1	B	173	THR
1	B	175	ARG
1	B	180	LEU
1	B	200	GLU

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Mol	Chain	Res	Type
1	B	204	GLU
1	B	208	ARG
1	B	210	LEU
1	B	223	LEU
1	B	227	LYS
1	B	234	ASP
1	B	235	ASP
1	B	242	VAL
1	B	256	ARG
1	B	261	ILE
1	B	264	LEU
1	B	265	LEU
1	B	273	GLN
1	B	276	HIS
1	B	279	VAL
1	B	282	THR
1	B	285	THR
1	B	291	ILE
1	B	311	ILE
1	B	316	ASP
1	B	330	GLN
1	B	332	ILE
1	B	349	VAL
1	B	357	ASP
1	B	376	LEU
1	B	378	LEU
1	B	397	THR
1	B	399	LEU
1	B	401	LEU
1	B	412	LYS
1	B	416	TRP
1	B	426	THR
1	B	430	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	B	128	ASN
1	B	133	GLN
1	B	196	HIS
1	B	272	ASN

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Mol	Chain	Res	Type
1	B	299	GLN

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

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	380/450 (84%)	0.36	15 (3%) 43 29	95, 152, 216, 254	0
1	B	395/450 (87%)	0.39	14 (3%) 47 31	90, 137, 221, 263	0
All	All	775/900 (86%)	0.37	29 (3%) 45 31	90, 144, 220, 263	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	GLU	4.7
1	A	68	LEU	3.6
1	B	152	ASP	3.6
1	A	152	ASP	3.1
1	A	220	ARG	3.0
1	A	159	GLU	2.8
1	B	397	THR	2.8
1	A	246	PHE	2.8
1	B	317	LYS	2.8
1	B	148	TYR	2.7
1	A	200	GLU	2.7
1	B	153	LEU	2.7
1	A	399	LEU	2.6
1	A	380	PHE	2.5
1	B	200	GLU	2.5
1	A	358	THR	2.3
1	B	178	PHE	2.3
1	B	171	PHE	2.3
1	A	337	ASN	2.3
1	A	319	VAL	2.3
1	A	287	PHE	2.2
1	B	312	ARG	2.2
1	A	41	VAL	2.2
1	B	287	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	295	PHE	2.1
1	B	187	PHE	2.1
1	A	407	ILE	2.0
1	B	353	MET	2.0
1	B	290	TYR	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.