



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:28 PM UTC

PDB ID : 5SV7 / pdb_00005sv7
Title : The Crystal structure of a chaperone
Authors : Wang, P.; Li, J.; Sha, B.
Deposited on : 2016-08-04
Resolution : 3.21 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

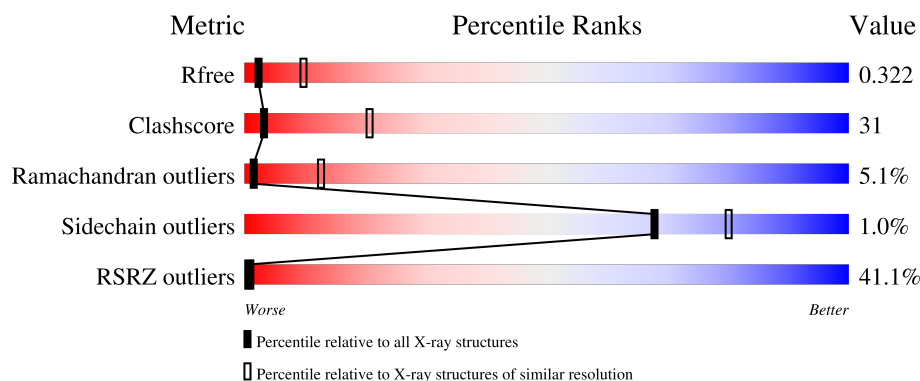
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	326	27% 29% 29% 38%
1	B	326	28% 29% 37% 31%
1	C	326	24% 29% 32% 37%
1	D	326	28% 26% 34% 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6602 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 Eukaryotic translation initiation factor 2-alpha kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1584	1010	269	298	7			
1	B	224	Total	C	N	O	S	0	0	0
			1751	1122	293	329	7			
1	C	206	Total	C	N	O	S	0	0	0
			1608	1031	271	299	7			
1	D	209	Total	C	N	O	S	0	0	0
			1630	1040	273	310	7			

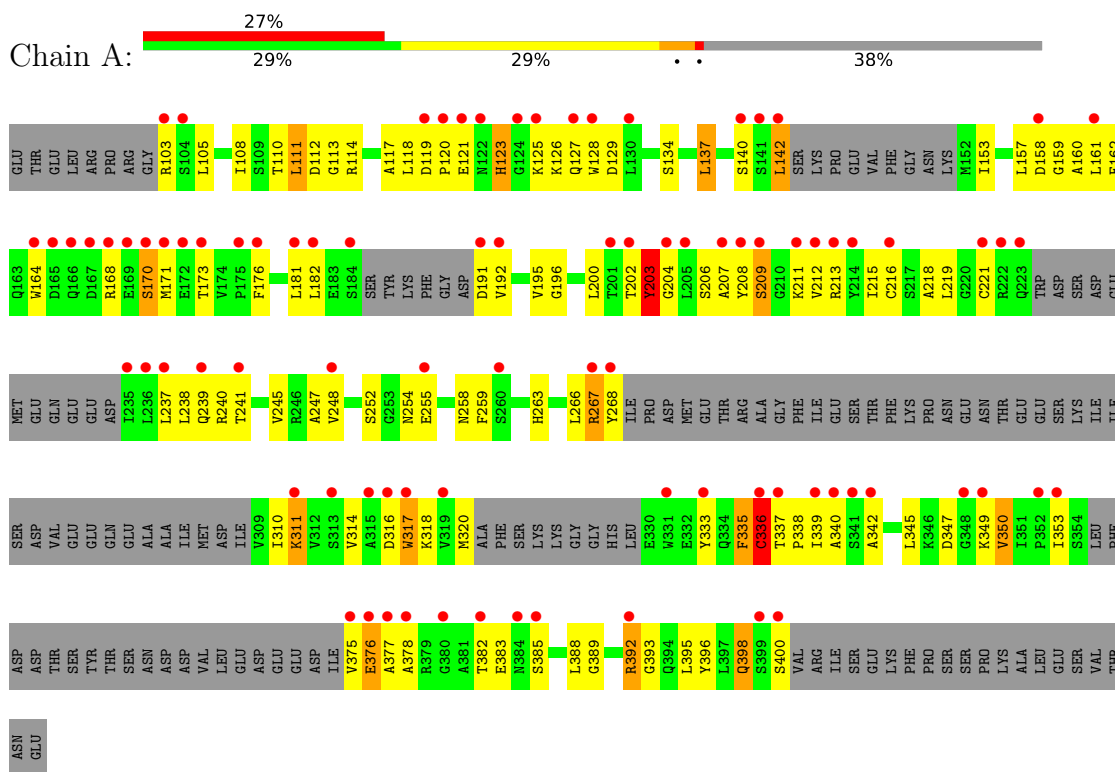
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	3	Total	O	0	0
			3	3		
2	C	6	Total	O	0	0
			6	6		
2	D	11	Total	O	0	0
			11	11		

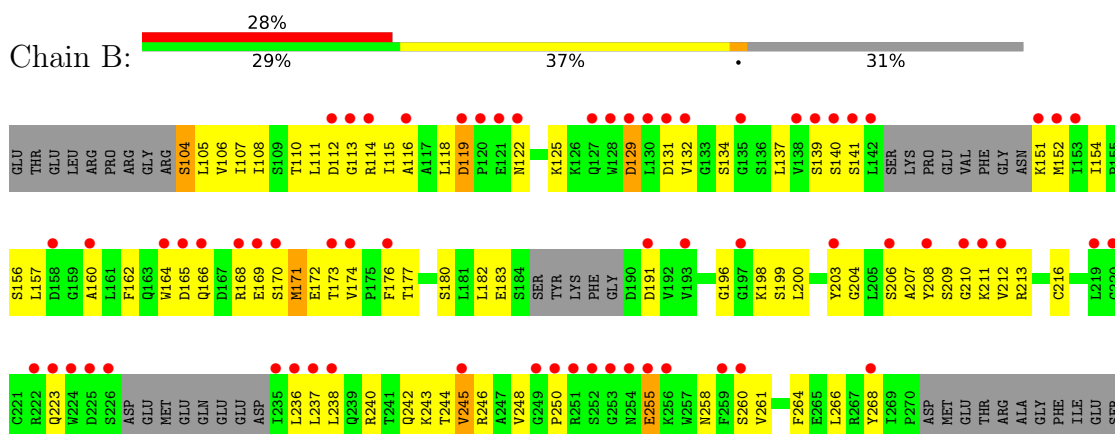
3 Residue-property plots

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.

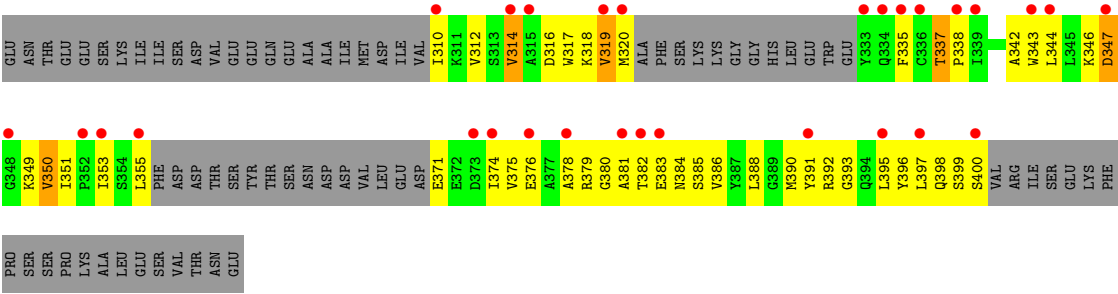
- Molecule 1: Eukaryotic translation initiation factor 2-alpha kinase 3



- Molecule 1: Eukaryotic translation initiation factor 2-alpha kinase 3







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	163.91Å 163.91Å 63.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.85 – 3.21 37.85 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.85-3.21) 98.2 (37.85-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.271 , 0.322 0.271 , 0.322	Depositor DCC
R_{free} test set	1578 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.034 for h,-h-k,-l 0.006 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6602	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	0.52	1/1610 (0.1%)	0.93	1/2172 (0.0%)
1	B	0.52	0/1784	0.80	0/2409
1	C	0.61	0/1636	1.06	3/2209 (0.1%)
1	D	0.58	0/1657	1.01	3/2237 (0.1%)
All	All	0.56	1/6687 (0.0%)	0.95	7/9027 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
1	C	0	1
1	D	0	4
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	TYR	CA-C	5.62	1.59	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	249	GLY	CA-C-N	8.40	129.51	120.11
1	D	249	GLY	C-N-CA	8.40	129.51	120.11
1	D	217	SER	N-CA-C	6.57	120.34	109.96
1	C	255	GLU	CA-C-N	6.30	133.04	121.70
1	C	255	GLU	C-N-CA	6.30	133.04	121.70
1	A	336	CYS	N-CA-C	-5.98	98.34	108.26
1	C	310	ILE	CB-CG1-CD1	5.27	124.86	113.80

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	HIS	Peptide
1	A	203	TYR	Peptide
1	A	267	ARG	Peptide
1	A	335	PHE	Peptide
1	A	336	CYS	Peptide
1	A	398	GLN	Peptide
1	B	104	SER	Peptide
1	B	313	SER	Peptide
1	C	256	LYS	Peptide
1	D	215	ILE	Peptide
1	D	216	CYS	Peptide
1	D	267	ARG	Peptide
1	D	319	VAL	Peptide

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	1584	0	1586	95	0
1	B	1751	0	1749	112	0
1	C	1608	0	1615	109	0
1	D	1630	0	1629	115	0
2	A	9	0	0	1	0
2	B	3	0	0	0	0
2	C	6	0	0	1	0
2	D	11	0	0	0	0
All	All	6602	0	6579	405	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 31.

All (405) 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:345:LEU:HG	1:A:349:LYS:HG3	1.38	1.05
1:B:104:SER:HB3	1:B:346:LYS:HA	1.53	0.89
1:A:157:LEU:HD11	1:A:398:GLN:HG2	1.57	0.87
1:A:203:TYR:O	1:A:238:LEU:N	2.09	0.86
1:C:120:PRO:HD2	1:C:123:HIS:HB2	1.58	0.85
1:B:115:ILE:N	1:B:131:ASP:OD2	2.10	0.84
1:C:192:VAL:N	2:C:501:HOH:O	2.11	0.84
1:C:318:LYS:NZ	1:C:332:GLU:OE2	2.10	0.82
1:A:202:THR:HG22	1:A:239:GLN:HG3	1.62	0.81
1:C:193:VAL:HG13	1:C:248:VAL:HG23	1.62	0.81
1:A:255:GLU:OE2	1:A:258:ASN:ND2	2.11	0.81
1:A:119:ASP:OD2	1:A:127:GLN:NE2	2.14	0.79
1:A:121:GLU:O	1:A:123:HIS:ND1	2.16	0.78
1:D:312:VAL:HG22	1:D:319:VAL:HG13	1.66	0.78
1:C:236:LEU:HD11	1:C:266:LEU:HD13	1.66	0.77
1:D:383:GLU:OE1	1:D:383:GLU:N	2.16	0.77
1:A:125:LYS:HE2	1:A:127:GLN:HE22	1.47	0.76
1:A:392:ARG:N	1:A:393:GLY:HA3	2.03	0.74
1:B:314:VAL:O	1:B:316:ASP:N	2.20	0.74
1:C:268:TYR:CE1	1:C:345:LEU:HD11	2.22	0.74
1:A:142:LEU:HD21	1:A:153:ILE:HB	1.70	0.73
1:D:154:ILE:HD13	1:D:395:LEU:HD22	1.71	0.72
1:A:248:VAL:HA	1:A:255:GLU:HA	1.72	0.72
1:A:123:HIS:HB3	1:A:125:LYS:H	1.55	0.72
1:C:118:LEU:HD11	1:C:319:VAL:HG11	1.71	0.72
1:C:204:GLY:O	1:C:213:ARG:N	2.17	0.72
1:A:112:ASP:OD2	1:A:114:ARG:NH1	2.21	0.71
1:D:177:THR:HB	1:D:180:SER:HB2	1.71	0.71
1:A:320:MET:O	2:A:501:HOH:O	2.09	0.71
1:B:375:VAL:HG12	1:B:379:ARG:HH12	1.55	0.71
1:B:375:VAL:HG12	1:B:379:ARG:NH1	2.06	0.70
1:C:115:ILE:HD11	1:C:128:TRP:CZ3	2.27	0.70
1:A:316:ASP:O	1:A:318:LYS:N	2.24	0.70
1:B:105:LEU:O	1:B:345:LEU:N	2.25	0.70
1:C:126:LYS:HE3	1:C:129:ASP:OD2	1.92	0.70
1:A:375:VAL:O	1:A:377:ALA:N	2.25	0.69
1:C:153:ILE:HD11	1:C:174:VAL:HG11	1.72	0.69
1:B:162:PHE:CD1	1:B:173:THR:HG22	2.29	0.68
1:C:391:TYR:CD1	1:C:392:ARG:HA	2.29	0.68
1:D:381:ALA:HA	1:D:384:ASN:HB2	1.76	0.68
1:C:374:ILE:HG12	1:C:375:VAL:H	1.58	0.67
1:B:376:GLU:HA	1:B:379:ARG:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ALA:HB3	1:D:353:ILE:HG21	1.76	0.67
1:B:209:SER:O	1:B:211:LYS:HB2	1.95	0.66
1:D:386:VAL:HG22	1:D:399:SER:HB2	1.77	0.66
1:B:236:LEU:HD12	1:B:268:TYR:HB2	1.76	0.66
1:B:248:VAL:HG12	1:B:255:GLU:HA	1.77	0.66
1:D:114:ARG:HH22	1:D:129:ASP:HB2	1.60	0.66
1:A:164:TRP:CZ3	1:C:378:ALA:HB2	2.31	0.66
1:A:388:LEU:HD23	1:A:395:LEU:HD22	1.78	0.66
1:C:310:ILE:O	1:C:311:LYS:HG2	1.96	0.66
1:B:140:SER:HB3	1:B:394:GLN:CD	2.21	0.65
1:B:206:SER:HB3	1:B:211:LYS:HB3	1.78	0.65
1:C:318:LYS:HB3	1:C:334:GLN:HA	1.78	0.65
1:D:217:SER:OG	1:D:218:ALA:N	2.30	0.65
1:B:204:GLY:HA2	1:B:237:LEU:HA	1.79	0.64
1:D:128:TRP:HB3	1:D:210:GLY:H	1.62	0.64
1:D:371:GLU:O	1:D:374:ILE:HG12	1.98	0.64
1:C:310:ILE:HG12	1:C:344:LEU:HD22	1.78	0.64
1:D:114:ARG:NH2	1:D:129:ASP:HB2	2.12	0.64
1:A:349:LYS:HG2	1:A:350:VAL:HG13	1.79	0.64
1:B:344:LEU:N	1:B:351:ILE:O	2.30	0.64
1:D:105:LEU:HD21	1:D:208:TYR:HD1	1.61	0.64
1:C:110:THR:HG23	1:C:112:ASP:OD1	1.98	0.63
1:B:114:ARG:HG2	1:B:131:ASP:HB2	1.79	0.63
1:D:141:SER:HB3	1:D:258:ASN:H	1.64	0.63
1:C:105:LEU:HD11	1:C:117:ALA:HB1	1.80	0.63
1:D:140:SER:O	1:D:140:SER:OG	2.14	0.63
1:A:267:ARG:HD3	1:A:350:VAL:HG21	1.80	0.63
1:B:374:ILE:HA	1:B:377:ALA:HB3	1.81	0.63
1:B:325:LYS:O	1:B:327:GLY:N	2.32	0.62
1:A:245:VAL:HG12	1:A:259:PHE:HB2	1.79	0.62
1:B:240:ARG:NH1	1:B:242:GLN:OE1	2.33	0.62
1:D:157:LEU:O	1:D:158:ASP:HB3	1.98	0.62
1:D:174:VAL:HG13	1:D:176:PHE:H	1.65	0.62
1:C:255:GLU:HA	1:C:256:LYS:HB2	1.80	0.62
1:A:125:LYS:HE2	1:A:127:GLN:NE2	2.15	0.62
1:C:247:ALA:O	1:C:256:LYS:HB2	2.00	0.62
1:A:237:LEU:HG	1:A:267:ARG:O	2.00	0.62
1:B:388:LEU:HD12	1:D:382:THR:HG21	1.81	0.62
1:C:316:ASP:O	1:C:318:LYS:N	2.33	0.61
1:A:392:ARG:HD3	1:A:392:ARG:H	1.64	0.61
1:D:126:LYS:O	1:D:127:GLN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ALA:HA	1:B:129:ASP:OD1	2.01	0.61
1:C:249:GLY:N	1:C:254:ASN:O	2.32	0.60
1:D:216:CYS:SG	1:D:217:SER:N	2.73	0.60
1:B:162:PHE:HD1	1:B:173:THR:HG22	1.66	0.60
1:A:206:SER:HA	1:A:213:ARG:HH12	1.68	0.59
1:B:110:THR:HA	1:B:340:ALA:H	1.66	0.59
1:A:252:SER:HB3	1:A:254:ASN:HD21	1.67	0.59
1:C:115:ILE:HD11	1:C:128:TRP:CH2	2.37	0.59
1:B:390:MET:HE3	1:B:395:LEU:HD13	1.85	0.59
1:D:114:ARG:NE	1:D:131:ASP:OD2	2.28	0.59
1:C:388:LEU:HD21	1:C:395:LEU:HD23	1.83	0.59
1:D:314:VAL:HB	1:D:355:LEU:HB2	1.85	0.59
1:B:168:ARG:HD2	1:B:170:SER:OG	2.03	0.59
1:D:111:LEU:HD21	1:D:138:VAL:HG12	1.86	0.58
1:C:248:VAL:HG11	1:D:221:CYS:SG	2.42	0.58
1:A:206:SER:O	1:A:208:TYR:N	2.37	0.58
1:C:391:TYR:O	1:C:394:GLN:HG2	2.03	0.58
1:B:108:ILE:N	1:B:116:ALA:O	2.34	0.58
1:C:139:SER:HA	1:C:394:GLN:HE21	1.69	0.58
1:D:267:ARG:HG2	1:D:268:TYR:H	1.68	0.58
1:A:385:SER:HB2	1:A:400:SER:HB2	1.85	0.57
1:C:164:TRP:HB3	1:C:171:MET:SD	2.44	0.57
1:B:344:LEU:HD11	1:B:346:LYS:HG2	1.85	0.57
1:B:191:ASP:O	1:B:250:PRO:HD3	2.05	0.57
1:A:158:ASP:HB2	1:A:160:ALA:H	1.70	0.57
1:A:195:VAL:HG13	1:B:200:LEU:O	2.05	0.57
1:B:165:ASP:HB3	1:B:168:ARG:HB3	1.86	0.57
1:D:111:LEU:HD23	1:D:111:LEU:O	2.04	0.57
1:D:215:ILE:HG23	1:D:216:CYS:HB3	1.86	0.57
1:B:236:LEU:HD21	1:B:266:LEU:HD11	1.87	0.56
1:B:388:LEU:HD12	1:D:382:THR:CG2	2.36	0.56
1:D:241:THR:HB	1:D:263:HIS:HB3	1.88	0.56
1:D:376:GLU:O	1:D:380:GLY:N	2.37	0.56
1:B:132:VAL:HG11	1:B:203:TYR:CZ	2.40	0.56
1:B:391:TYR:O	1:B:394:GLN:N	2.37	0.56
1:C:337:THR:OG1	1:C:338:PRO:HD3	2.05	0.56
1:A:209:SER:HB2	1:A:211:LYS:HE3	1.87	0.56
1:C:205:LEU:HB3	1:C:212:VAL:HA	1.87	0.56
1:C:244:THR:CG2	1:D:218:ALA:HB1	2.36	0.56
1:A:388:LEU:CD1	1:C:382:THR:HG21	2.36	0.56
1:B:154:ILE:HD12	1:B:171:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HB2	1:B:353:ILE:HD11	1.88	0.56
1:D:375:VAL:O	1:D:379:ARG:N	2.33	0.56
1:A:162:PHE:CE2	1:A:173:THR:HG22	2.41	0.56
1:A:317:TRP:H	1:A:317:TRP:CD1	2.24	0.56
1:A:171:MET:HB3	1:C:385:SER:OG	2.07	0.55
1:B:207:ALA:HA	1:B:208:TYR:C	2.31	0.55
1:D:105:LEU:HD23	1:D:105:LEU:H	1.70	0.55
1:C:400:SER:N	1:C:401:VAL:HB	2.21	0.55
1:B:174:VAL:HG22	1:B:176:PHE:HD1	1.71	0.55
1:B:111:LEU:HD11	1:B:396:TYR:CZ	2.42	0.54
1:C:177:THR:C	1:C:179:GLU:H	2.16	0.54
1:D:158:ASP:O	1:D:243:LYS:NZ	2.31	0.54
1:A:314:VAL:O	1:A:317:TRP:HD1	1.90	0.54
1:D:346:LYS:O	1:D:347:ASP:C	2.49	0.54
1:B:122:ASN:O	1:B:125:LYS:HG3	2.07	0.54
1:D:390:MET:HE3	1:D:393:GLY:H	1.73	0.54
1:B:140:SER:HB3	1:B:394:GLN:NE2	2.23	0.54
1:B:322:PHE:HE1	1:B:329:LEU:HD23	1.73	0.54
1:B:165:ASP:O	1:B:169:GLU:N	2.41	0.53
1:B:168:ARG:HB3	1:B:170:SER:HB2	1.90	0.53
1:D:204:GLY:O	1:D:205:LEU:HD12	2.08	0.53
1:C:310:ILE:HG12	1:C:344:LEU:CD2	2.38	0.53
1:A:110:THR:OG1	1:A:112:ASP:OD1	2.24	0.53
1:A:337:THR:HB	1:A:338:PRO:CD	2.39	0.53
1:A:310:ILE:HG22	1:A:353:ILE:HD13	1.89	0.53
1:B:390:MET:HG3	1:B:394:GLN:O	2.09	0.53
1:D:111:LEU:HA	1:D:137:LEU:HD22	1.90	0.53
1:D:140:SER:O	1:D:142:LEU:N	2.41	0.53
1:C:158:ASP:H	1:C:159:GLY:HA2	1.74	0.53
1:B:319:VAL:HG12	1:B:335:PHE:HE2	1.74	0.52
1:C:139:SER:HA	1:C:394:GLN:NE2	2.25	0.52
1:A:113:GLY:HA2	1:A:137:LEU:HD23	1.91	0.52
1:B:106:VAL:HG13	1:B:118:LEU:HB2	1.91	0.52
1:C:105:LEU:H	1:C:345:LEU:HB3	1.74	0.52
1:D:105:LEU:HD21	1:D:208:TYR:CD1	2.44	0.52
1:D:346:LYS:O	1:D:349:LYS:HG2	2.08	0.52
1:B:237:LEU:H	1:B:237:LEU:HD23	1.73	0.52
1:B:334:GLN:NE2	1:B:335:PHE:O	2.43	0.52
1:C:195:VAL:HG11	1:D:216:CYS:O	2.10	0.52
1:C:396:TYR:O	1:C:397:LEU:HD12	2.10	0.52
1:D:140:SER:HB2	1:D:259:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:THR:HG23	1:D:218:ALA:HB1	1.92	0.52
1:A:123:HIS:CD2	1:A:125:LYS:HD3	2.44	0.51
1:B:151:LYS:HD2	1:B:166:GLN:HB3	1.92	0.51
1:D:267:ARG:HH21	1:D:269:ILE:HD11	1.75	0.51
1:A:238:LEU:CD1	1:A:266:LEU:HD23	2.40	0.51
1:C:122:ASN:OD1	1:C:123:HIS:N	2.43	0.51
1:C:221:CYS:SG	1:D:248:VAL:HG11	2.51	0.51
1:C:158:ASP:N	1:C:159:GLY:HA2	2.24	0.51
1:D:161:LEU:HB2	1:D:174:VAL:HG11	1.93	0.51
1:B:211:LYS:O	1:B:213:ARG:N	2.44	0.51
1:C:119:ASP:HA	1:C:124:GLY:H	1.76	0.51
1:C:153:ILE:HA	1:C:162:PHE:O	2.11	0.51
1:D:344:LEU:HB2	1:D:351:ILE:HG23	1.91	0.51
1:C:113:GLY:HA3	1:C:135:GLY:O	2.11	0.51
1:B:198:LYS:HG3	1:B:199:SER:N	2.26	0.50
1:C:141:SER:HA	1:C:142:LEU:C	2.36	0.50
1:C:255:GLU:CD	1:C:255:GLU:N	2.69	0.50
1:A:252:SER:HB3	1:A:254:ASN:ND2	2.26	0.50
1:A:268:TYR:HB2	1:A:349:LYS:HD2	1.93	0.50
1:C:312:VAL:HG23	1:C:339:ILE:HD11	1.92	0.50
1:C:236:LEU:HA	1:C:268:TYR:HB2	1.94	0.50
1:A:267:ARG:HG3	1:A:268:TYR:N	2.27	0.50
1:A:382:THR:O	1:A:385:SER:OG	2.30	0.50
1:A:383:GLU:HG2	1:C:383:GLU:HB3	1.94	0.50
1:C:268:TYR:OH	1:C:348:GLY:HA2	2.10	0.50
1:C:374:ILE:HG12	1:C:375:VAL:N	2.25	0.50
1:D:212:VAL:HG21	1:D:215:ILE:HD12	1.93	0.50
1:B:322:PHE:CE1	1:B:329:LEU:HD23	2.47	0.50
1:C:206:SER:O	1:C:208:TYR:N	2.45	0.50
1:C:236:LEU:HD11	1:C:266:LEU:CD1	2.40	0.50
1:A:204:GLY:O	1:A:212:VAL:HA	2.11	0.49
1:D:385:SER:O	1:D:399:SER:HA	2.12	0.49
1:A:238:LEU:HD13	1:A:266:LEU:HD23	1.94	0.49
1:C:266:LEU:C	1:C:267:ARG:HD2	2.37	0.49
1:D:380:GLY:HA2	1:D:383:GLU:OE2	2.12	0.49
1:A:219:LEU:HA	1:B:246:ARG:NH2	2.28	0.49
1:D:112:ASP:HB3	1:D:337:THR:HG21	1.94	0.49
1:B:152:MET:O	1:B:152:MET:HG3	2.12	0.49
1:B:111:LEU:HD21	1:B:157:LEU:HD11	1.94	0.49
1:D:396:TYR:HE1	1:D:398:GLN:HG3	1.78	0.49
1:A:203:TYR:CD2	1:A:215:ILE:HG22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:TRP:HA	1:B:352:PRO:HA	1.95	0.48
1:D:129:ASP:N	1:D:129:ASP:OD1	2.46	0.48
1:B:317:TRP:CZ2	1:B:338:PRO:HG3	2.47	0.48
1:D:132:VAL:HG22	1:D:133:GLY:N	2.28	0.48
1:D:154:ILE:HD12	1:D:171:MET:HE1	1.95	0.48
1:D:344:LEU:O	1:D:350:VAL:HA	2.12	0.48
1:C:181:LEU:HD13	1:C:245:VAL:HG21	1.95	0.48
1:D:191:ASP:OD1	1:D:192:VAL:N	2.46	0.48
1:C:237:LEU:HD12	1:C:267:ARG:H	1.78	0.48
1:A:255:GLU:CD	1:A:258:ASN:HD22	2.22	0.48
1:D:337:THR:HG23	1:D:338:PRO:HD2	1.94	0.48
1:D:342:ALA:C	1:D:343:TRP:CG	2.92	0.48
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.57	0.48
1:B:312:VAL:HG22	1:B:319:VAL:HG23	1.96	0.48
1:D:105:LEU:HD12	1:D:117:ALA:HB1	1.96	0.48
1:A:237:LEU:HD12	1:A:237:LEU:O	2.14	0.48
1:B:122:ASN:O	1:B:125:LYS:HE2	2.14	0.47
1:B:236:LEU:HD13	1:B:345:LEU:HD21	1.96	0.47
1:B:344:LEU:HD22	1:B:345:LEU:H	1.79	0.47
1:B:379:ARG:NH2	1:D:388:LEU:O	2.47	0.47
1:A:192:VAL:HG21	1:A:247:ALA:HB1	1.97	0.47
1:B:151:LYS:HE2	1:B:166:GLN:N	2.29	0.47
1:D:310:ILE:HG13	1:D:320:MET:C	2.39	0.47
1:B:208:TYR:HA	1:B:209:SER:HA	1.59	0.47
1:B:310:ILE:HG23	1:B:353:ILE:HG12	1.96	0.47
1:D:153:ILE:HD13	1:D:163:GLN:HA	1.95	0.47
1:C:114:ARG:NH1	1:C:131:ASP:HB3	2.29	0.47
1:D:182:LEU:HD21	1:D:196:GLY:HA3	1.96	0.47
1:D:388:LEU:HD11	1:D:395:LEU:HD21	1.97	0.47
1:A:200:LEU:HD23	1:B:182:LEU:HD22	1.96	0.47
1:D:391:TYR:CD1	1:D:392:ARG:HG2	2.49	0.47
1:A:202:THR:HG22	1:A:239:GLN:CG	2.39	0.47
1:A:337:THR:HB	1:A:338:PRO:HD2	1.96	0.47
1:D:266:LEU:HB3	1:D:350:VAL:HG11	1.97	0.47
1:D:316:ASP:HB3	1:D:318:LYS:HE2	1.96	0.47
1:A:158:ASP:N	1:A:159:GLY:HA2	2.30	0.47
1:B:387:TYR:HE2	1:B:396:TYR:OH	1.97	0.47
1:C:179:GLU:OE2	1:C:243:LYS:NZ	2.43	0.47
1:D:119:ASP:OD1	1:D:122:ASN:HB3	2.15	0.47
1:D:193:VAL:HG22	1:D:248:VAL:HG23	1.97	0.47
1:D:115:ILE:HB	1:D:130:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:SER:OG	1:A:142:LEU:HB2	2.15	0.47
1:A:168:ARG:HB2	1:A:170:SER:HB2	1.97	0.46
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.53	0.46
1:B:107:ILE:HG13	1:B:266:LEU:HD21	1.96	0.46
1:C:177:THR:O	1:C:179:GLU:N	2.49	0.46
1:D:161:LEU:O	1:D:174:VAL:HG12	2.15	0.46
1:C:310:ILE:O	1:C:310:ILE:HD12	2.15	0.46
1:A:382:THR:HG23	1:C:171:MET:HE3	1.97	0.46
1:C:398:GLN:HB3	1:C:401:VAL:HG21	1.96	0.46
1:A:191:ASP:OD1	1:A:191:ASP:N	2.49	0.46
1:A:349:LYS:HG2	1:A:350:VAL:HG22	1.98	0.46
1:C:240:ARG:HB2	1:C:264:PHE:CE1	2.51	0.46
1:D:215:ILE:HB	1:D:224:TRP:HZ3	1.80	0.46
1:A:254:ASN:HB3	1:B:223:GLN:OE1	2.16	0.46
1:A:314:VAL:O	1:A:317:TRP:CD1	2.69	0.46
1:B:243:LYS:HB2	1:B:261:VAL:HG22	1.98	0.46
1:B:245:VAL:HG13	1:B:245:VAL:O	2.16	0.46
1:D:174:VAL:HG22	1:D:175:PRO:HD2	1.97	0.46
1:C:177:THR:C	1:C:179:GLU:N	2.72	0.45
1:A:375:VAL:HG23	1:A:376:GLU:N	2.31	0.45
1:B:209:SER:OG	1:B:210:GLY:N	2.49	0.45
1:B:314:VAL:HG22	1:B:355:LEU:HB2	1.98	0.45
1:C:118:LEU:HA	1:C:126:LYS:HA	1.97	0.45
1:D:376:GLU:HA	1:D:379:ARG:HB2	1.97	0.45
1:A:388:LEU:HD11	1:C:382:THR:HG21	1.97	0.45
1:D:177:THR:H	1:D:180:SER:HB3	1.82	0.45
1:D:240:ARG:HD2	1:D:263:HIS:O	2.16	0.45
1:A:389:GLY:HA3	1:A:396:TYR:CZ	2.52	0.45
1:B:388:LEU:HG	1:B:397:LEU:HB3	1.98	0.45
1:A:117:ALA:HB2	1:A:128:TRP:CE2	2.51	0.45
1:B:139:SER:HB2	1:B:260:SER:OG	2.15	0.45
1:C:153:ILE:HG13	1:C:162:PHE:O	2.16	0.45
1:C:159:GLY:O	1:C:178:VAL:HG23	2.17	0.45
1:C:310:ILE:HG21	1:C:344:LEU:HD22	1.98	0.45
1:B:238:LEU:HD11	1:B:264:PHE:HB3	1.99	0.45
1:C:156:SER:C	1:C:158:ASP:H	2.24	0.45
1:C:248:VAL:HG12	1:C:255:GLU:HB3	1.98	0.45
1:C:252:SER:O	1:C:254:ASN:N	2.46	0.45
1:D:111:LEU:HD22	1:D:391:TYR:CG	2.51	0.45
1:B:132:VAL:HG11	1:B:203:TYR:CE1	2.52	0.45
1:A:105:LEU:HD22	1:A:117:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG11	1:B:216:CYS:O	2.17	0.45
1:B:182:LEU:HD21	1:B:196:GLY:HA3	1.98	0.45
1:B:116:ALA:HA	1:B:129:ASP:CG	2.42	0.44
1:B:335:PHE:CD2	1:B:339:ILE:HD11	2.52	0.44
1:C:243:LYS:HE2	1:C:243:LYS:HB3	1.66	0.44
1:C:237:LEU:O	1:C:266:LEU:HA	2.17	0.44
1:D:141:SER:HB3	1:D:257:TRP:HA	1.98	0.44
1:D:215:ILE:HG12	1:D:216:CYS:HB3	1.98	0.44
1:A:336:CYS:SG	1:A:337:THR:HA	2.58	0.44
1:A:103:ARG:HA	1:A:103:ARG:HD3	1.88	0.44
1:B:344:LEU:HD13	1:B:346:LYS:H	1.82	0.44
1:D:154:ILE:O	1:D:162:PHE:N	2.46	0.44
1:B:160:ALA:HB2	1:B:177:THR:HG22	1.99	0.44
1:C:132:VAL:HG11	1:C:203:TYR:CE2	2.52	0.44
1:D:124:GLY:O	1:D:125:LYS:C	2.61	0.44
1:D:247:ALA:HB2	1:D:257:TRP:CZ2	2.53	0.44
1:B:119:ASP:CG	1:B:122:ASN:HB3	2.43	0.43
1:B:156:SER:HA	1:B:397:LEU:O	2.18	0.43
1:B:314:VAL:HG22	1:B:355:LEU:HD12	2.00	0.43
1:C:130:LEU:HD21	1:C:238:LEU:HD22	2.00	0.43
1:C:161:LEU:HD23	1:C:177:THR:HA	1.99	0.43
1:A:195:VAL:HG12	1:A:196:GLY:N	2.32	0.43
1:C:159:GLY:O	1:C:161:LEU:HD22	2.18	0.43
1:D:268:TYR:CD1	1:D:268:TYR:N	2.86	0.43
1:A:176:PHE:HB3	1:A:181:LEU:HD13	2.00	0.43
1:A:241:THR:HB	1:A:263:HIS:CE1	2.54	0.43
1:A:118:LEU:HD22	1:A:333:TYR:CE2	2.54	0.43
1:A:119:ASP:HB3	1:A:123:HIS:HB2	1.99	0.43
1:B:170:SER:O	1:B:172:GLU:N	2.52	0.43
1:C:115:ILE:HG12	1:C:238:LEU:HD21	2.00	0.43
1:D:243:LYS:O	1:D:260:SER:HA	2.18	0.43
1:D:249:GLY:HA2	1:D:250:PRO:HD3	1.72	0.43
1:A:157:LEU:CD1	1:A:398:GLN:HG2	2.38	0.43
1:A:162:PHE:HE2	1:A:173:THR:HG22	1.83	0.43
1:D:152:MET:HE2	1:D:152:MET:HB3	1.67	0.43
1:A:218:ALA:HB2	1:B:196:GLY:O	2.18	0.43
1:B:354:SER:OG	1:B:356:PHE:O	2.22	0.43
1:C:199:SER:O	1:C:200:LEU:HD12	2.19	0.43
1:B:164:TRP:CH2	1:D:378:ALA:HB2	2.53	0.43
1:B:319:VAL:HG12	1:B:335:PHE:CE2	2.53	0.43
1:B:386:VAL:HG22	1:B:399:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:HD23	1:C:118:LEU:H	1.84	0.43
1:C:252:SER:C	1:C:254:ASN:H	2.26	0.43
1:D:238:LEU:HD13	1:D:266:LEU:CD2	2.48	0.43
1:B:170:SER:C	1:B:172:GLU:HG2	2.44	0.42
1:D:130:LEU:HD12	1:D:131:ASP:H	1.83	0.42
1:A:126:LYS:HD3	1:A:129:ASP:HB2	2.01	0.42
1:D:105:LEU:CD2	1:D:208:TYR:HD1	2.28	0.42
1:D:154:ILE:HD13	1:D:395:LEU:CD2	2.42	0.42
1:D:241:THR:O	1:D:262:GLY:HA2	2.19	0.42
1:A:216:CYS:HA	1:A:221:CYS:HA	2.01	0.42
1:B:207:ALA:HB2	1:B:210:GLY:C	2.44	0.42
1:B:399:SER:OG	1:B:400:SER:N	2.52	0.42
1:C:313:SER:O	1:C:316:ASP:N	2.49	0.42
1:B:180:SER:O	1:B:183:GLU:HG2	2.19	0.42
1:C:250:PRO:HB3	1:D:267:ARG:NH2	2.34	0.42
1:A:108:ILE:HD13	1:A:342:ALA:HB1	2.01	0.42
1:A:134:SER:HB2	1:A:240:ARG:CZ	2.50	0.42
1:B:177:THR:H	1:B:180:SER:HB3	1.84	0.42
1:C:111:LEU:HA	1:C:137:LEU:HB2	2.02	0.42
1:C:237:LEU:HD12	1:C:237:LEU:O	2.19	0.42
1:D:242:GLN:NE2	1:D:260:SER:HB3	2.34	0.42
1:D:317:TRP:CG	1:D:338:PRO:HA	2.54	0.42
1:B:108:ILE:HD11	1:B:116:ALA:HB3	2.00	0.42
1:B:132:VAL:HG11	1:B:203:TYR:OH	2.20	0.42
1:C:203:TYR:CD1	1:C:203:TYR:N	2.88	0.42
1:C:268:TYR:CD1	1:C:345:LEU:HD11	2.52	0.42
1:D:215:ILE:HG23	1:D:216:CYS:SG	2.60	0.42
1:A:310:ILE:O	1:A:311:LYS:C	2.62	0.42
1:B:244:THR:HG22	1:B:260:SER:HB3	2.02	0.42
1:C:107:ILE:C	1:C:108:ILE:HD12	2.45	0.42
1:C:153:ILE:HG23	1:C:153:ILE:O	2.20	0.42
1:B:165:ASP:H	1:B:170:SER:HB3	1.84	0.41
1:C:118:LEU:HD11	1:C:319:VAL:CG1	2.46	0.41
1:D:111:LEU:HB2	1:D:338:PRO:O	2.19	0.41
1:D:203:TYR:CD1	1:D:203:TYR:N	2.88	0.41
1:A:153:ILE:HA	1:A:162:PHE:O	2.21	0.41
1:B:207:ALA:HA	1:B:209:SER:CA	2.50	0.41
1:B:391:TYR:CZ	1:B:392:ARG:HB2	2.56	0.41
1:C:126:LYS:O	1:C:126:LYS:HG3	2.20	0.41
1:D:161:LEU:HB2	1:D:174:VAL:CG1	2.49	0.41
1:D:269:ILE:HA	1:D:270:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HA	1:B:258:ASN:HB3	2.03	0.41
1:B:308:ILE:HA	1:B:322:PHE:O	2.21	0.41
1:B:379:ARG:O	1:B:382:THR:OG1	2.37	0.41
1:C:223:GLN:CB	1:C:224:TRP:HA	2.51	0.41
1:B:172:GLU:OE1	1:D:400:SER:HB2	2.20	0.41
1:B:131:ASP:HB3	1:B:132:VAL:H	1.62	0.41
1:B:343:TRP:CE3	1:B:352:PRO:HB3	2.56	0.41
1:C:181:LEU:HA	1:C:184:SER:O	2.21	0.41
1:C:200:LEU:HD22	1:D:182:LEU:HD22	2.02	0.41
1:C:254:ASN:HA	1:C:255:GLU:OE1	2.20	0.41
1:D:126:LYS:O	1:D:127:GLN:CB	2.68	0.41
1:D:130:LEU:HD12	1:D:131:ASP:N	2.36	0.41
1:D:171:MET:HE3	1:D:397:LEU:HD11	2.01	0.41
1:D:208:TYR:HA	1:D:209:SER:HA	1.74	0.41
1:D:317:TRP:NE1	1:D:338:PRO:HB3	2.36	0.41
1:C:337:THR:HG21	1:C:391:TYR:CE1	2.56	0.41
1:C:392:ARG:N	1:C:393:GLY:HA3	2.35	0.41
1:D:237:LEU:N	1:D:267:ARG:O	2.37	0.41
1:D:238:LEU:HD13	1:D:266:LEU:HD23	2.03	0.41
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.81	0.40
1:A:310:ILE:O	1:A:310:ILE:CG2	2.68	0.40
1:B:112:ASP:OD1	1:B:113:GLY:N	2.54	0.40
1:B:118:LEU:O	1:B:119:ASP:HB2	2.21	0.40
1:D:106:VAL:O	1:D:117:ALA:HA	2.21	0.40
1:D:266:LEU:HD12	1:D:343:TRP:CG	2.56	0.40
1:A:111:LEU:HD22	1:A:340:ALA:HB2	2.02	0.40
1:A:117:ALA:HB3	1:A:128:TRP:H	1.85	0.40
1:A:378:ALA:C	1:C:388:LEU:HD13	2.47	0.40
1:C:133:GLY:HA2	1:C:135:GLY:N	2.36	0.40
1:A:335:PHE:HB2	1:A:339:ILE:HD11	2.04	0.40
1:C:177:THR:O	1:C:181:LEU:HG	2.22	0.40
1:C:161:LEU:O	1:C:174:VAL:HG22	2.22	0.40
1:C:134:SER:O	1:C:135:GLY:C	2.64	0.40
1:C:244:THR:HG21	1:D:218:ALA:HB1	2.02	0.40
1:D:110:THR:HG21	1:D:335:PHE:CE1	2.56	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	189/326 (58%)	156 (82%)	24 (13%)	9 (5%)	2	14
1	B	212/326 (65%)	169 (80%)	33 (16%)	10 (5%)	2	14
1	C	192/326 (59%)	161 (84%)	20 (10%)	11 (6%)	1	11
1	D	195/326 (60%)	150 (77%)	35 (18%)	10 (5%)	1	13
All	All	788/1304 (60%)	636 (81%)	112 (14%)	40 (5%)	1	13

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	TRP
1	A	350	VAL
1	A	376	GLU
1	B	119	ASP
1	B	212	VAL
1	B	315	ALA
1	B	326	GLY
1	D	127	GLN
1	D	216	CYS
1	D	314	VAL
1	A	170	SER
1	A	207	ALA
1	A	209	SER
1	A	311	LYS
1	B	134	SER
1	B	141	SER
1	B	245	VAL
1	B	314	VAL
1	C	207	ALA
1	C	314	VAL
1	D	126	LYS
1	D	141	SER

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Mol	Chain	Res	Type
1	D	350	VAL
1	A	347	ASP
1	D	337	THR
1	D	347	ASP
1	B	255	GLU
1	C	123	HIS
1	C	135	GLY
1	B	171	MET
1	C	157	LEU
1	C	256	LYS
1	C	317	TRP
1	C	391	TYR
1	D	124	GLY
1	C	250	PRO
1	C	178	VAL
1	D	159	GLY
1	A	120	PRO
1	C	119	ASP

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	174/286 (61%)	169 (97%)	5 (3%)	37	67
1	B	192/286 (67%)	190 (99%)	2 (1%)	68	80
1	C	176/286 (62%)	176 (100%)	0	100	100
1	D	180/286 (63%)	180 (100%)	0	100	100
All	All	722/1144 (63%)	715 (99%)	7 (1%)	68	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	A	137	LEU
1	A	142	LEU

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Mol	Chain	Res	Type
1	A	203	TYR
1	A	392	ARG
1	B	129	ASP
1	B	137	LEU

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	127	GLN
1	A	254	ASN
1	B	239	GLN
1	B	254	ASN
1	B	384	ASN
1	B	394	GLN
1	C	254	ASN
1	D	163	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 ⓘ

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	203/326 (62%)	2.09	87 (42%) 0 1	27, 41, 65, 83	0
1	B	224/326 (68%)	1.90	91 (40%) 0 1	21, 38, 64, 72	0
1	C	206/326 (63%)	1.84	77 (37%) 1 1	9, 29, 55, 66	0
1	D	209/326 (64%)	2.03	91 (43%) 0 1	16, 31, 61, 73	0
All	All	842/1304 (64%)	1.96	346 (41%) 0 1	9, 36, 62, 83	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	336	CYS	8.0
1	D	172	GLU	7.7
1	D	209	SER	7.3
1	A	384	ASN	7.0
1	C	310	ILE	6.4
1	A	316	ASP	6.4
1	D	335	PHE	6.4
1	A	176	PHE	6.3
1	A	376	GLU	6.3
1	B	315	ALA	5.9
1	A	121	GLU	5.9
1	C	165	ASP	5.8
1	D	252	SER	5.8
1	A	235	ILE	5.8
1	D	336	CYS	5.7
1	D	208	TYR	5.5
1	C	158	ASP	5.5
1	C	400	SER	5.5
1	C	309	VAL	5.4
1	B	127	GLN	5.4
1	A	213	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	399	SER	5.0
1	C	267	ARG	5.0
1	B	235	ILE	5.0
1	A	140	SER	4.9
1	A	141	SER	4.9
1	B	211	LYS	4.9
1	B	166	GLN	4.7
1	C	391	TYR	4.7
1	D	223	GLN	4.6
1	C	135	GLY	4.6
1	C	141	SER	4.6
1	C	336	CYS	4.6
1	B	170	SER	4.4
1	C	172	GLU	4.4
1	A	202	THR	4.4
1	B	383	GLU	4.3
1	D	216	CYS	4.3
1	A	204	GLY	4.3
1	D	268	TYR	4.2
1	A	142	LEU	4.2
1	A	182	LEU	4.2
1	D	123	HIS	4.1
1	D	255	GLU	4.1
1	C	347	ASP	4.0
1	D	334	GLN	4.0
1	A	313	SER	4.0
1	C	176	PHE	4.0
1	D	131	ASP	4.0
1	D	113	GLY	4.0
1	B	259	PHE	4.0
1	C	268	TYR	3.9
1	D	259	PHE	3.9
1	D	218	ALA	3.8
1	D	373	ASP	3.8
1	B	141	SER	3.8
1	A	175	PRO	3.7
1	D	173	THR	3.7
1	A	170	SER	3.7
1	B	251	ARG	3.7
1	B	212	VAL	3.7
1	A	223	GLN	3.7
1	A	201	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	3.6
1	A	212	VAL	3.6
1	D	333	TYR	3.6
1	C	393	GLY	3.6
1	D	153	ILE	3.6
1	B	121	GLU	3.5
1	D	339	ILE	3.5
1	A	166	GLN	3.5
1	B	372	GLU	3.5
1	A	164	TRP	3.5
1	B	208	TYR	3.5
1	C	221	CYS	3.5
1	C	109	SER	3.5
1	C	134	SER	3.5
1	B	254	ASN	3.4
1	B	210	GLY	3.4
1	A	167	ASP	3.4
1	B	138	VAL	3.4
1	C	374	ILE	3.4
1	D	235	ILE	3.4
1	A	221	CYS	3.4
1	A	341	SER	3.4
1	D	192	VAL	3.4
1	D	395	LEU	3.4
1	C	151	LYS	3.4
1	B	314	VAL	3.4
1	D	165	ASP	3.4
1	B	384	ASN	3.3
1	A	169	GLU	3.3
1	B	400	SER	3.3
1	C	337	THR	3.3
1	B	132	VAL	3.3
1	C	380	GLY	3.3
1	C	381	ALA	3.3
1	A	165	ASP	3.3
1	A	127	GLN	3.3
1	C	314	VAL	3.3
1	B	164	TRP	3.3
1	A	353	ILE	3.3
1	D	381	ALA	3.3
1	D	219	LEU	3.2
1	C	390	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	315	ALA	3.2
1	A	239	GLN	3.2
1	A	119	ASP	3.2
1	C	119	ASP	3.2
1	D	353	ILE	3.2
1	A	184	SER	3.2
1	B	223	GLN	3.2
1	B	378	ALA	3.2
1	C	236	LEU	3.2
1	B	130	LEU	3.1
1	B	249	GLY	3.1
1	C	142	LEU	3.1
1	D	142	LEU	3.1
1	B	128	TRP	3.1
1	B	169	GLU	3.1
1	D	383	GLU	3.1
1	B	336	CYS	3.1
1	C	245	VAL	3.1
1	A	222	ARG	3.1
1	A	267	ARG	3.1
1	C	122	ASN	3.1
1	C	116	ALA	3.1
1	B	224	TRP	3.1
1	D	164	TRP	3.1
1	D	201	THR	3.1
1	C	224	TRP	3.1
1	D	152	MET	3.1
1	D	250	PRO	3.1
1	D	314	VAL	3.0
1	D	269	ILE	3.0
1	D	158	ASP	3.0
1	D	191	ASP	3.0
1	A	216	CYS	3.0
1	D	347	ASP	3.0
1	B	176	PHE	3.0
1	D	374	ILE	3.0
1	D	248	VAL	3.0
1	C	120	PRO	3.0
1	B	139	SER	3.0
1	A	375	VAL	3.0
1	C	132	VAL	3.0
1	C	348	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	173	THR	3.0
1	B	142	LEU	2.9
1	D	251	ARG	2.9
1	B	119	ASP	2.9
1	B	337	THR	2.9
1	C	164	TRP	2.9
1	C	401	VAL	2.9
1	C	384	ASN	2.9
1	B	313	SER	2.9
1	C	341	SER	2.9
1	B	395	LEU	2.9
1	A	241	THR	2.8
1	B	250	PRO	2.8
1	A	122	ASN	2.8
1	B	153	ILE	2.8
1	A	255	GLU	2.8
1	D	114	ARG	2.8
1	D	169	GLU	2.8
1	B	256	LYS	2.8
1	A	339	ILE	2.8
1	A	120	PRO	2.8
1	D	261	VAL	2.8
1	D	397	LEU	2.8
1	D	348	GLY	2.8
1	B	268	TYR	2.8
1	A	377	ALA	2.8
1	A	125	LYS	2.8
1	B	206	SER	2.8
1	C	375	VAL	2.8
1	C	257	TRP	2.8
1	D	166	GLN	2.8
1	D	343	TRP	2.7
1	B	225	ASP	2.7
1	C	385	SER	2.7
1	D	129	ASP	2.7
1	D	237	LEU	2.7
1	B	255	GLU	2.7
1	D	170	SER	2.7
1	B	191	ASP	2.7
1	B	376	GLU	2.7
1	B	160	ALA	2.7
1	D	378	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	LEU	2.7
1	C	192	VAL	2.7
1	B	373	ASP	2.7
1	A	352	PRO	2.6
1	D	106	VAL	2.6
1	D	315	ALA	2.6
1	D	319	VAL	2.6
1	D	391	TYR	2.6
1	D	241	THR	2.6
1	B	391	TYR	2.6
1	D	135	GLY	2.6
1	C	383	GLU	2.6
1	A	319	VAL	2.6
1	C	117	ALA	2.6
1	D	267	ARG	2.6
1	A	268	TYR	2.6
1	D	400	SER	2.6
1	A	236	LEU	2.6
1	D	344	LEU	2.6
1	A	382	THR	2.6
1	C	214	TYR	2.5
1	D	270	PRO	2.5
1	A	130	LEU	2.5
1	A	103	ARG	2.5
1	D	221	CYS	2.5
1	C	127	GLN	2.5
1	D	178	VAL	2.5
1	D	167	ASP	2.5
1	C	118	LEU	2.5
1	C	212	VAL	2.5
1	A	207	ALA	2.5
1	A	342	ALA	2.5
1	A	378	ALA	2.5
1	B	165	ASP	2.5
1	D	154	ILE	2.5
1	B	173	THR	2.5
1	C	269	ILE	2.5
1	D	176	PHE	2.5
1	A	192	VAL	2.5
1	B	377	ALA	2.4
1	B	260	SER	2.4
1	A	171	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	324	LYS	2.4
1	A	317	TRP	2.4
1	A	340	ALA	2.4
1	B	226	SER	2.4
1	B	356	PHE	2.4
1	C	140	SER	2.4
1	C	354	SER	2.4
1	C	138	VAL	2.4
1	C	248	VAL	2.4
1	B	326	GLY	2.4
1	A	260	SER	2.4
1	A	385	SER	2.4
1	A	400	SER	2.4
1	B	135	GLY	2.4
1	B	158	ASP	2.4
1	B	219	LEU	2.4
1	B	237	LEU	2.4
1	B	397	LEU	2.4
1	C	206	SER	2.4
1	D	175	PRO	2.4
1	B	387	TYR	2.3
1	C	121	GLU	2.3
1	B	193	VAL	2.3
1	A	128	TRP	2.3
1	D	382	THR	2.3
1	B	129	ASP	2.3
1	B	236	LEU	2.3
1	A	248	VAL	2.3
1	C	213	ARG	2.3
1	A	173	THR	2.3
1	B	140	SER	2.3
1	C	321	ALA	2.3
1	A	333	TYR	2.3
1	B	319	VAL	2.3
1	C	339	ILE	2.3
1	A	392	ARG	2.3
1	B	168	ARG	2.3
1	D	193	VAL	2.3
1	D	265	GLU	2.3
1	A	124	GLY	2.3
1	A	348	GLY	2.3
1	D	253	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	152	MET	2.3
1	C	171	MET	2.3
1	B	355	LEU	2.3
1	A	209	SER	2.3
1	D	168	ARG	2.3
1	B	131	ASP	2.3
1	C	265	GLU	2.2
1	A	380	GLY	2.2
1	B	338	PRO	2.2
1	A	237	LEU	2.2
1	A	331	TRP	2.2
1	C	382	THR	2.2
1	D	376	GLU	2.2
1	D	310	ILE	2.2
1	A	337	THR	2.2
1	D	127	GLN	2.2
1	B	122	ASN	2.2
1	D	254	ASN	2.2
1	B	220	GLY	2.2
1	C	249	GLY	2.2
1	C	315	ALA	2.2
1	D	338	PRO	2.2
1	B	151	LYS	2.2
1	C	125	LYS	2.2
1	D	211	LYS	2.2
1	D	202	THR	2.2
1	B	252	SER	2.2
1	C	105	LEU	2.2
1	D	157	LEU	2.2
1	B	197	GLY	2.2
1	C	175	PRO	2.2
1	B	114	ARG	2.2
1	C	168	ARG	2.2
1	A	191	ASP	2.2
1	B	238	LEU	2.1
1	D	355	LEU	2.1
1	A	104	SER	2.1
1	D	320	MET	2.1
1	B	342	ALA	2.1
1	D	352	PRO	2.1
1	A	158	ASP	2.1
1	B	174	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	203	TYR	2.1
1	A	211	LYS	2.1
1	C	256	LYS	2.1
1	B	120	PRO	2.1
1	D	180	SER	2.1
1	D	132	VAL	2.1
1	A	311	LYS	2.1
1	C	266	LEU	2.1
1	C	344	LEU	2.1
1	B	222	ARG	2.1
1	D	163	GLN	2.1
1	B	113	GLY	2.1
1	A	161	LEU	2.1
1	B	152	MET	2.1
1	B	245	VAL	2.0
1	D	217	SER	2.0
1	C	107	ILE	2.0
1	D	257	TRP	2.0
1	B	112	ASP	2.0
1	B	396	TYR	2.0
1	D	190	ASP	2.0
1	B	253	GLY	2.0
1	C	169	GLU	2.0
1	A	181	LEU	2.0
1	B	116	ALA	2.0
1	A	208	TYR	2.0
1	A	214	TYR	2.0
1	A	349	LYS	2.0
1	A	168	ARG	2.0
1	A	205	LEU	2.0
1	C	153	ILE	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.