



# Full wwPDB X-ray Structure Validation Report i

Sep 24, 2023 – 01:15 AM EDT

PDB ID : 5SV7  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

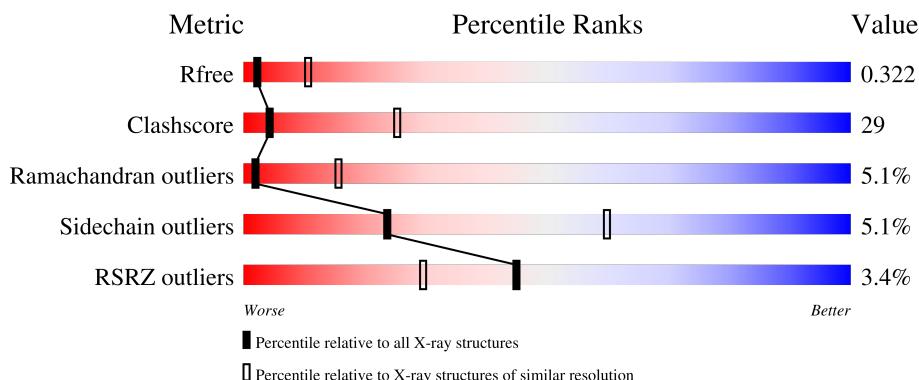
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

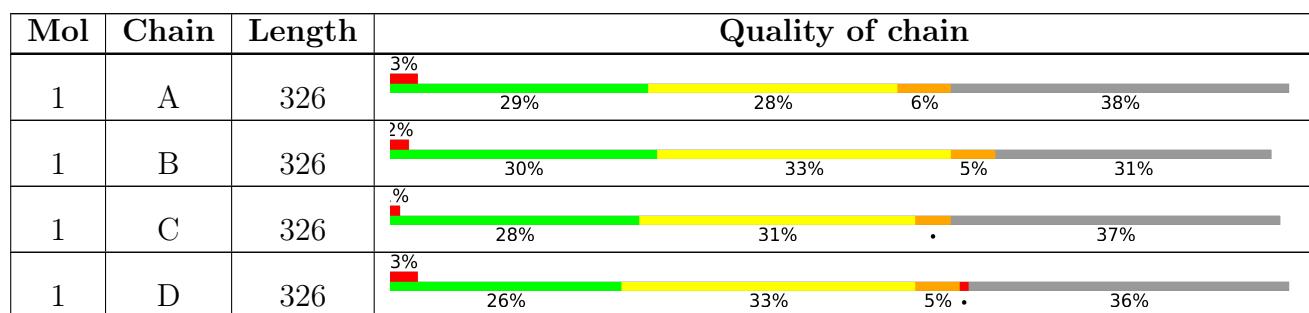
The reported resolution of this entry is 3.21 Å.

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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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  $\geq 3$ , 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.



## 2 Entry composition [\(i\)](#)

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 1584	N 1010	O 269	S 298	7	0	0
1	B	224	Total	C 1751	N 1122	O 293	S 329	7	0	0
1	C	206	Total	C 1608	N 1031	O 271	S 299	7	0	0
1	D	209	Total	C 1630	N 1040	O 273	S 310	7	0	0

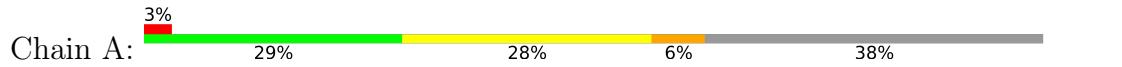
- Molecule 2 is water.

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

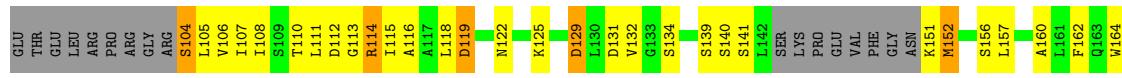
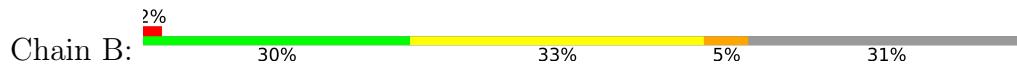
### 3 Residue-property plots [\(i\)](#)

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.

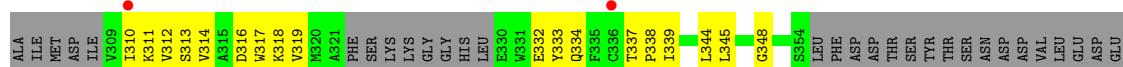
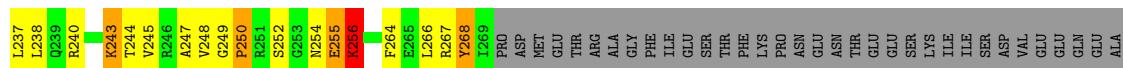
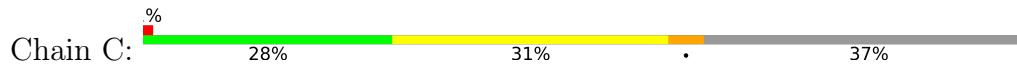
- Molecule 1: Eukaryotic translation initiation factor 2-alpha kinase 3



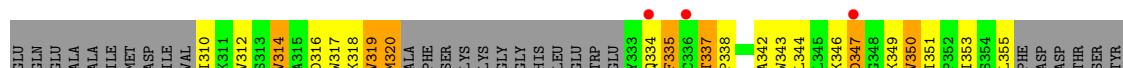
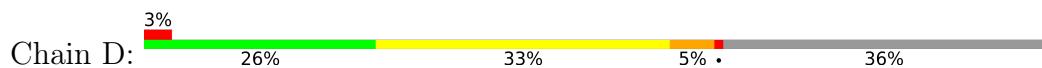
- Molecule 1: Eukaryotic translation initiation factor 2-alpha kinase 3



- 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 i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 98.3 (37.85-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	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 (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.53$ , $< L^2 > = 0.37$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  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	0.56	0/1610	0.86	1/2172 (0.0%)
1	B	0.63	3/1784 (0.2%)	0.78	2/2409 (0.1%)
1	C	0.61	0/1636	0.95	1/2209 (0.0%)
1	D	0.63	1/1657 (0.1%)	0.91	3/2237 (0.1%)
All	All	0.61	4/6687 (0.1%)	0.87	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	GLU	CD-OE1	-8.04	1.16	1.25
1	B	216	CYS	CB-SG	-6.33	1.71	1.82
1	B	332	GLU	CD-OE2	-6.21	1.18	1.25
1	D	131	ASP	CA-CB	5.01	1.65	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	LEU	CA-CB-CG	7.84	133.34	115.30
1	D	200	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	345	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	219	LEU	CA-CB-CG	5.78	128.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	355	LEU	CA-CB-CG	5.44	127.82	115.30
1	D	161	LEU	CA-CB-CG	5.10	127.03	115.30

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 [\(i\)](#)

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	1584	0	1586	89	0
1	B	1751	0	1749	105	0
1	C	1608	0	1615	102	0
1	D	1630	0	1629	112	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	384	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 29.

All (384) 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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:116:ALA:HA	1:B:129:ASP:OD1	2.01	0.61
1:B:140:SER:HB3	1:B:394:GLN:CD	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:171:MET:HB3	1:C:385:SER:OG	2.07	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: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:B:122:ASN:O	1:B:125:LYS:HG3	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ARG:HH21	1:D:269:ILE:HD11	1.75	0.51
1:A:238:LEU:CD1	1:A:266:LEU:HG23	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: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:B:207:ALA:HA	1:B:208:TYR:C	2.31	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: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:D:346:LYS:O	1:D:347:ASP:C	2.49	0.49
1:D:380:GLY:HA2	1:D:383:GLU:OE2	2.12	0.49
1:C:177:THR:C	1:C:179:GLU:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:337:THR:HG23	1:D:338:PRO:HD2	1.94	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: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:216:CYS:HG	1:D:217:SER:H	1.60	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: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
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:C:398:GLN:HB3	1:C:401:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:255:GLU:CD	1:C:255:GLU:N	2.69	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: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:C:266:LEU:C	1:C:267:ARG:HD2	2.37	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:C:141:SER:HA	1:C:142:LEU:C	2.36	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:247:ALA:HB2	1:D:257:TRP:CZ2	2.53	0.44
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:D:342:ALA:C	1:D:343:TRP:CG	2.92	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:A:218:ALA:HB2	1:B:196:GLY:O	2.18	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
1:C:118:LEU:HD23	1:C:118:LEU:H	1.84	0.43
1:D:238:LEU:HD13	1:D:266:LEU:CD2	2.48	0.43
1:D:310:ILE:HG13	1:D:320:MET:C	2.39	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:C	1:C:179:GLU:N	2.72	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:B:244:THR:HG22	1:B:260:SER:HB3	2.02	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:152:MET:HE2	1:D:164:TRP:HE3	1.86	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 [\(i\)](#)

### 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	189/326 (58%)	156 (82%)	24 (13%)	9 (5%)	2 17
1	B	212/326 (65%)	169 (80%)	33 (16%)	10 (5%)	2 17
1	C	192/326 (59%)	161 (84%)	20 (10%)	11 (6%)	1 14
1	D	195/326 (60%)	150 (77%)	35 (18%)	10 (5%)	2 15
All	All	788/1304 (60%)	636 (81%)	112 (14%)	40 (5%)	2 15

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
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 [\(i\)](#)

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%)	165 (95%)	9 (5%)	23 59
1	B	192/286 (67%)	181 (94%)	11 (6%)	20 56
1	C	176/286 (62%)	166 (94%)	10 (6%)	20 56
1	D	180/286 (63%)	173 (96%)	7 (4%)	32 67
All	All	722/1144 (63%)	685 (95%)	37 (5%)	24 60

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	137	LEU
1	A	165	ASP
1	A	208	TYR
1	A	263	HIS
1	A	266	LEU
1	A	333	TYR
1	A	392	ARG
1	A	394	GLN
1	B	114	ARG
1	B	129	ASP
1	B	152	MET
1	B	208	TYR
1	B	211	LYS
1	B	213	ARG
1	B	240	ARG
1	B	246	ARG
1	B	316	ASP
1	B	336	CYS
1	B	391	TYR
1	C	129	ASP
1	C	134	SER
1	C	152	MET
1	C	156	SER

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Mol	Chain	Res	Type
1	C	164	TRP
1	C	243	LYS
1	C	255	GLU
1	C	268	TYR
1	C	333	TYR
1	C	384	ASN
1	D	105	LEU
1	D	131	ASP
1	D	190	ASP
1	D	251	ARG
1	D	320	MET
1	D	334	GLN
1	D	335	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	254	ASN
1	B	394	GLN
1	C	254	ASN
1	C	394	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	203/326 (62%)	0.27	9 (4%)	34	21	27, 41, 65, 83	0
1	B	224/326 (68%)	0.22	6 (2%)	54	39	21, 38, 64, 72	0
1	C	206/326 (63%)	0.12	4 (1%)	66	53	9, 29, 55, 66	0
1	D	209/326 (64%)	0.29	10 (4%)	30	18	16, 31, 61, 73	0
All	All	842/1304 (64%)	0.23	29 (3%)	45	29	9, 36, 62, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	SER	4.5
1	A	336	CYS	3.8
1	D	252	SER	3.6
1	D	172	GLU	3.1
1	A	384	ASN	3.0
1	B	372	GLU	2.9
1	A	213	ARG	2.7
1	A	316	ASP	2.7
1	D	208	TYR	2.6
1	B	170	SER	2.5
1	D	166	GLN	2.5
1	A	184	SER	2.5
1	D	336	CYS	2.4
1	D	347	ASP	2.3
1	B	166	GLN	2.3
1	D	270	PRO	2.3
1	D	251	ARG	2.3
1	B	225	ASP	2.3
1	A	182	LEU	2.2
1	B	251	ARG	2.2
1	A	191	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	165	ASP	2.2
1	A	121	GLU	2.2
1	C	336	CYS	2.2
1	D	334	GLN	2.1
1	C	400	SER	2.1
1	A	309	VAL	2.1
1	B	315	ALA	2.0
1	C	310	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 monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.