



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:53 pm BST

PDB ID : 5HQP  
Title : Crystal structure of the ERp44-peroxiredoxin 4 complex  
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Deposited on : 2016-01-22  
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

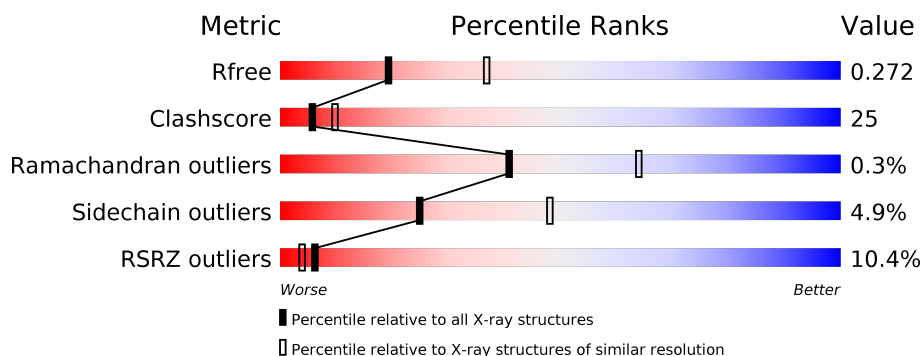
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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.

Mol	Chain	Length	Quality of chain
1	A	246	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>57%</span> <span>15%</span> <span>•</span> <span>26%</span> </div> </div>
1	B	246	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>52%</span> <span>18%</span> <span>•</span> <span>29%</span> </div> </div>
2	C	382	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>45%</span> <span>36%</span> <span>• •</span> <span>15%</span> </div> </div>
2	D	382	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">17%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>21%</span> <span>29%</span> <span>•</span> <span>47%</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7219 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 Peroxiredoxin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1450	937	241	270	2			
1	B	175	Total	C	N	O	S	0	0	0
			1409	912	235	260	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP Q13162
A	27	ARG	-	expression tag	UNP Q13162
A	28	GLY	-	expression tag	UNP Q13162
A	29	SER	-	expression tag	UNP Q13162
A	30	HIS	-	expression tag	UNP Q13162
A	31	HIS	-	expression tag	UNP Q13162
A	32	HIS	-	expression tag	UNP Q13162
A	33	HIS	-	expression tag	UNP Q13162
A	34	HIS	-	expression tag	UNP Q13162
A	35	HIS	-	expression tag	UNP Q13162
A	36	GLY	-	expression tag	UNP Q13162
A	37	SER	-	expression tag	UNP Q13162
A	51	SER	CYS	engineered mutation	UNP Q13162
A	124	SER	CYS	engineered mutation	UNP Q13162
A	155	GLU	THR	engineered mutation	UNP Q13162
B	26	MET	-	expression tag	UNP Q13162
B	27	ARG	-	expression tag	UNP Q13162
B	28	GLY	-	expression tag	UNP Q13162
B	29	SER	-	expression tag	UNP Q13162
B	30	HIS	-	expression tag	UNP Q13162
B	31	HIS	-	expression tag	UNP Q13162
B	32	HIS	-	expression tag	UNP Q13162
B	33	HIS	-	expression tag	UNP Q13162
B	34	HIS	-	expression tag	UNP Q13162
B	35	HIS	-	expression tag	UNP Q13162

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLY	-	expression tag	UNP Q13162
B	37	SER	-	expression tag	UNP Q13162
B	51	SER	CYS	engineered mutation	UNP Q13162
B	124	SER	CYS	engineered mutation	UNP Q13162
B	155	GLU	THR	engineered mutation	UNP Q13162

- Molecule 2 is a protein called Endoplasmic reticulum resident protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	323	Total	C	N	O	S	0	0	0
			2657	1692	452	499	14			
2	D	204	Total	C	N	O	S	0	0	0
			1676	1056	289	321	10			

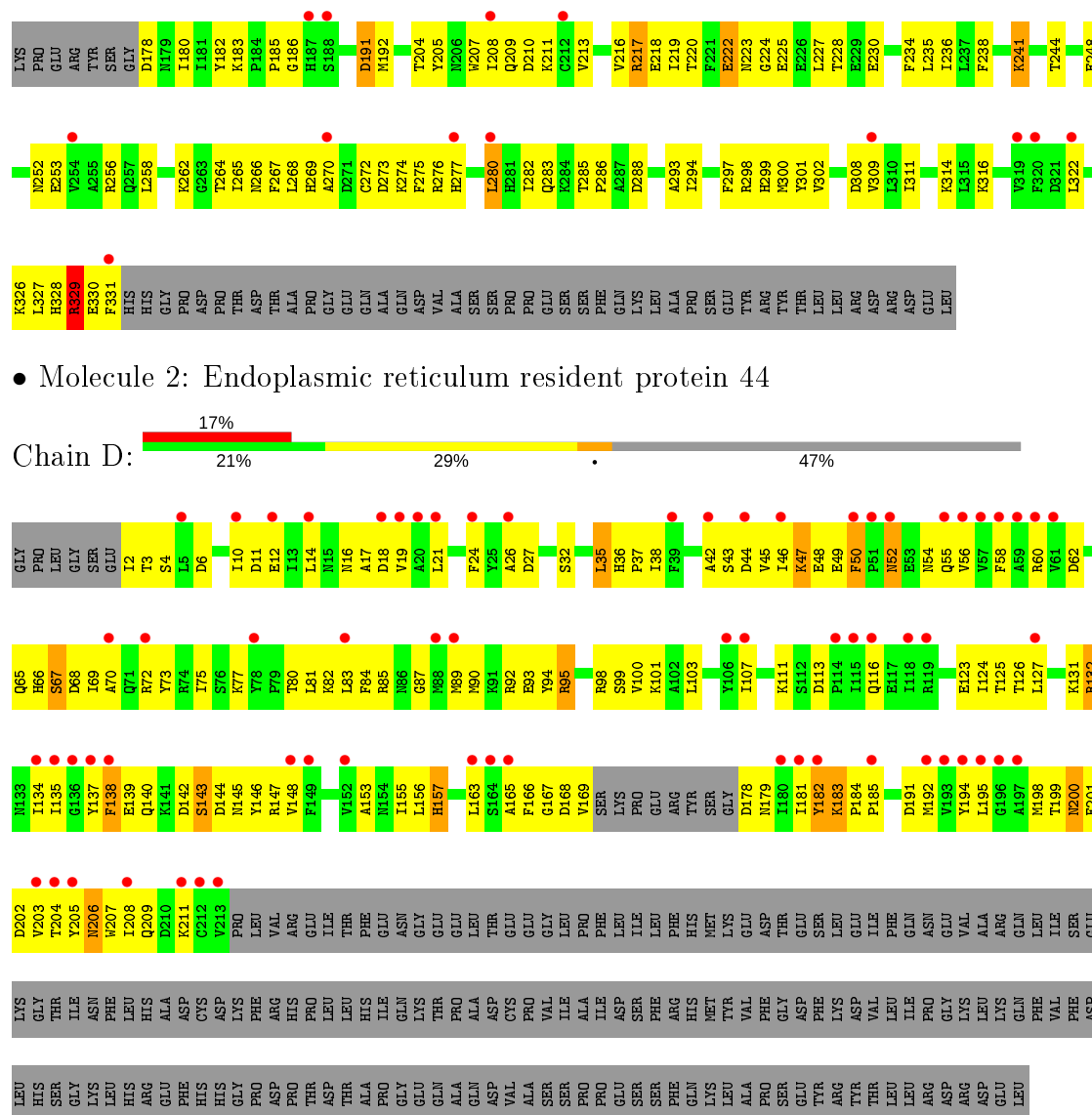
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q9BS26
C	-3	PRO	-	expression tag	UNP Q9BS26
C	-2	LEU	-	expression tag	UNP Q9BS26
C	-1	GLY	-	expression tag	UNP Q9BS26
C	0	SER	-	expression tag	UNP Q9BS26
D	-4	GLY	-	expression tag	UNP Q9BS26
D	-3	PRO	-	expression tag	UNP Q9BS26
D	-2	LEU	-	expression tag	UNP Q9BS26
D	-1	GLY	-	expression tag	UNP Q9BS26
D	0	SER	-	expression tag	UNP Q9BS26

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	8	Total	O	0	0
			8	8		
3	C	8	Total	O	0	0
			8	8		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.29Å 198.98Å 225.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.60 99.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.60) 93.0 (99.49-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.235 , 0.272 0.235 , 0.272	Depositor DCC
$R_{free}$ test set	2377 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.33	0/1487	0.59	0/2018
1	B	0.37	0/1445	0.66	0/1960
2	C	0.51	6/2717 (0.2%)	0.68	4/3670 (0.1%)
2	D	0.54	0/1710	0.86	6/2311 (0.3%)
All	All	0.46	6/7359 (0.1%)	0.71	10/9959 (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	3
2	C	0	2
2	D	0	2
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	ARG	NE-CZ	-8.90	1.21	1.33
2	C	95	ARG	CZ-NH1	-7.86	1.22	1.33
2	C	95	ARG	CZ-NH2	-6.21	1.25	1.33
2	C	95	ARG	CD-NE	-5.75	1.36	1.46
2	C	329	ARG	CZ-NH2	-5.51	1.25	1.33
2	C	329	ARG	NE-CZ	-5.18	1.26	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	60	ARG	NE-CZ-NH1	-8.86	115.87	120.30
2	C	50	PHE	C-N-CD	-8.20	102.56	120.60
2	D	50	PHE	C-N-CD	-6.48	106.35	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	132	ARG	NE-CZ-NH1	-6.14	117.23	120.30
2	C	50	PHE	N-CA-C	-6.04	94.70	111.00
2	C	50	PHE	C-N-CA	6.01	147.24	122.00
2	C	280	LEU	CA-CB-CG	5.72	128.45	115.30
2	D	143	SER	CA-CB-OG	-5.13	97.36	111.20
2	D	35	LEU	CA-CB-CG	5.12	127.09	115.30
2	D	103	LEU	CB-CG-CD2	-5.09	102.35	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Peptide
1	A	251	PRO	Peptide
1	A	252	GLY	Peptide
2	C	127	LEU	Peptide
2	C	128	ASP	Peptide
2	D	113	ASP	Peptide
2	D	200	ASN	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	1450	0	1434	26	0
1	B	1409	0	1395	38	0
2	C	2657	0	2577	139	1
2	D	1676	0	1611	166	1
3	A	11	0	0	0	0
3	B	8	0	0	3	0
3	C	8	0	0	1	0
All	All	7219	0	7017	361	1

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 25.

All (361) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:220:THR:HG23	2:C:222:GLU:OE2	1.09	1.22
2:D:44:ASP:OD1	2:D:47:LYS:NZ	1.71	1.20
2:C:220:THR:CG2	2:C:222:GLU:OE2	1.96	1.12
2:D:82:LYS:HZ3	2:D:89:MET:CE	1.64	1.09
2:D:44:ASP:N	2:D:47:LYS:HZ3	1.55	1.04
2:C:205:TYR:O	2:C:209:GLN:HB3	1.58	1.03
2:D:132:ARG:NH1	2:D:183:LYS:O	1.92	1.02
2:C:220:THR:HA	2:C:275:PHE:HZ	1.28	0.97
2:D:44:ASP:CA	2:D:47:LYS:HZ3	1.81	0.93
2:C:85:ARG:HH12	2:C:110:GLN:HE21	1.09	0.93
2:D:58:PHE:HE1	2:D:107:ILE:HD13	1.37	0.90
1:A:200:ARG:HB3	1:A:223:ARG:HH21	1.34	0.89
2:C:144:ASP:OD1	2:C:147:ARG:NH1	2.05	0.89
2:C:217:ARG:HG3	2:C:218:GLU:H	1.35	0.89
2:D:132:ARG:NH1	2:D:184:PRO:HA	1.88	0.88
2:D:82:LYS:HZ3	2:D:89:MET:HE2	1.37	0.88
1:B:76:LEU:N	3:B:301:HOH:O	2.05	0.88
2:C:183:LYS:NZ	2:C:186:GLY:O	2.08	0.87
2:D:132:ARG:NH1	2:D:184:PRO:CA	2.38	0.87
2:D:2:ILE:HD11	2:D:47:LYS:HE3	1.56	0.86
2:D:32:SER:HA	2:D:35:LEU:HD22	1.55	0.85
2:C:220:THR:HA	2:C:275:PHE:CZ	2.11	0.85
2:D:92:ARG:HH21	2:D:95:ARG:H	1.23	0.84
2:C:138:PHE:HA	2:C:178:ASP:OD1	1.76	0.84
2:D:73:TYR:HE2	2:D:84:PHE:CE1	1.96	0.84
2:D:82:LYS:NZ	2:D:89:MET:HE2	1.93	0.84
2:C:219:ILE:HD11	2:C:224:GLY:HA2	1.61	0.82
2:D:82:LYS:NZ	2:D:89:MET:CE	2.42	0.82
2:D:52:ASN:ND2	2:D:55:GLN:N	2.29	0.81
2:C:209:GLN:HE22	2:C:262:LYS:HZ1	1.28	0.81
1:A:91:THR:HG22	1:A:100:GLU:OE2	1.79	0.81
2:C:142:ASP:OD1	2:C:147:ARG:NH2	2.14	0.80
2:D:206:ASN:ND2	2:D:209:GLN:OE1	2.14	0.80
2:D:12:GLU:O	2:D:16:ASN:ND2	2.14	0.80
2:C:258:LEU:HD21	2:C:316:LYS:HA	1.64	0.79
2:D:58:PHE:CE1	2:D:107:ILE:HD13	2.17	0.78
2:D:138:PHE:HD2	2:D:139:GLU:N	1.82	0.77
2:D:44:ASP:HA	2:D:47:LYS:HZ3	1.48	0.77
2:D:82:LYS:HZ3	2:D:89:MET:HE3	1.49	0.77
2:D:132:ARG:CZ	2:D:184:PRO:C	2.53	0.77
2:D:138:PHE:HD2	2:D:139:GLU:H	1.33	0.77
2:D:132:ARG:HH12	2:D:183:LYS:C	1.89	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:TYR:HE2	2:D:84:PHE:HE1	1.30	0.76
1:B:163:PRO:HG2	1:B:166:GLN:HG3	1.66	0.75
1:A:143:THR:HG21	1:A:232:VAL:HG21	1.67	0.75
2:D:44:ASP:HA	2:D:47:LYS:NZ	2.01	0.75
2:D:52:ASN:HD21	2:D:55:GLN:H	1.32	0.75
2:D:131:LYS:O	2:D:132:ARG:NE	2.20	0.74
2:C:209:GLN:HE22	2:C:262:LYS:NZ	1.84	0.74
2:C:134:ILE:HD11	2:C:180:ILE:HD13	1.68	0.74
2:D:69:ILE:HA	2:D:72:ARG:HG3	1.68	0.74
2:C:216:VAL:HG12	2:C:267:PHE:CB	2.18	0.73
2:D:135:ILE:HB	2:D:181:ILE:HG23	1.71	0.72
2:C:191:ASP:N	2:C:191:ASP:OD1	2.23	0.72
2:C:273:ASP:OD1	2:C:274:LYS:HD2	1.89	0.72
2:D:46:ILE:HA	2:D:49:GLU:HB2	1.72	0.72
2:C:216:VAL:HG12	2:C:267:PHE:HB2	1.72	0.71
2:C:22:VAL:HG12	2:C:59:ALA:HB3	1.72	0.70
2:C:68:ASP:OD1	2:C:68:ASP:N	2.24	0.70
2:D:138:PHE:O	2:D:166:PHE:HA	1.91	0.70
2:D:191:ASP:HA	2:D:192:MET:HB2	1.73	0.70
2:D:132:ARG:NH1	2:D:184:PRO:C	2.45	0.70
2:D:52:ASN:ND2	2:D:55:GLN:H	1.89	0.70
2:D:132:ARG:NH2	2:D:184:PRO:O	2.25	0.69
2:D:44:ASP:CA	2:D:47:LYS:NZ	2.54	0.69
2:D:73:TYR:HB2	2:D:75:ILE:HD11	1.73	0.69
2:D:138:PHE:CD2	2:D:139:GLU:N	2.60	0.69
2:C:216:VAL:HA	2:C:267:PHE:O	1.92	0.69
2:D:132:ARG:NH2	2:D:185:PRO:HA	2.08	0.69
2:C:51:PRO:HB2	2:C:53:GLU:H	1.59	0.67
2:D:52:ASN:ND2	2:D:55:GLN:HB2	2.09	0.67
2:D:6:ASP:O	2:D:10:ILE:HG23	1.94	0.67
2:C:209:GLN:HE22	2:C:213:VAL:HG13	1.60	0.67
2:C:301:TYR:HE1	2:C:328:HIS:ND1	1.92	0.67
2:C:85:ARG:HH12	2:C:110:GLN:NE2	1.90	0.67
2:D:3:THR:HG22	2:D:4:SER:H	1.60	0.67
1:A:213:GLN:HE22	1:B:217:ASN:HD22	1.44	0.66
2:D:132:ARG:HH12	2:D:184:PRO:CA	2.08	0.66
2:D:132:ARG:HA	2:D:132:ARG:NE	2.10	0.66
2:D:32:SER:O	2:D:35:LEU:HD23	1.95	0.66
2:C:301:TYR:HE1	2:C:328:HIS:HD1	1.43	0.66
2:C:227:LEU:HA	2:C:230:GLU:HG3	1.78	0.65
2:C:235:LEU:HD13	2:C:294:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:PHE:HE1	2:D:107:ILE:CD1	2.07	0.65
2:C:123:GLU:OE1	2:C:125:THR:OG1	2.15	0.65
2:C:135:ILE:HD12	2:C:163:LEU:C	2.16	0.65
2:D:123:GLU:O	2:D:127:LEU:HG	1.97	0.65
1:A:229:LEU:O	1:A:233:GLN:HG3	1.97	0.64
2:C:73:TYR:HB3	2:C:89:MET:HE1	1.79	0.64
2:C:135:ILE:HD13	2:C:163:LEU:HB2	1.79	0.64
2:D:44:ASP:N	2:D:47:LYS:NZ	2.40	0.64
2:C:282:ILE:HG12	2:C:302:VAL:CG1	2.29	0.63
2:D:92:ARG:HE	2:D:95:ARG:HD3	1.64	0.63
2:C:330:GLU:HB3	2:C:331:PHE:C	2.19	0.63
2:C:224:GLY:O	2:C:228:THR:HG23	1.99	0.63
2:D:169:VAL:O	2:D:178:ASP:N	2.31	0.62
1:B:164:ARG:HG2	1:B:165:ARG:HH12	1.64	0.62
2:C:282:ILE:HG13	2:C:283:GLN:H	1.65	0.62
2:D:10:ILE:HG13	2:D:11:ASP:N	2.14	0.62
2:C:12:GLU:N	2:C:12:GLU:OE1	2.29	0.62
2:C:276:ARG:HG2	2:C:280:LEU:CD2	2.30	0.62
2:C:241:LYS:HD3	2:C:241:LYS:H	1.64	0.62
2:C:49:GLU:OE1	2:C:108:ARG:HD3	2.00	0.61
2:D:156:LEU:HD21	2:D:209:GLN:HA	1.82	0.61
2:D:52:ASN:CG	2:D:55:GLN:HB2	2.21	0.61
2:C:217:ARG:HG3	2:C:218:GLU:N	2.11	0.61
2:C:222:GLU:CD	2:C:223:ASN:H	2.04	0.61
2:C:327:LEU:HD22	2:C:329:ARG:HD2	1.82	0.61
2:C:5:LEU:HD22	2:C:10:ILE:HA	1.82	0.61
2:C:298:ARG:HD3	2:C:299:HIS:CE1	2.36	0.61
2:D:26:ALA:O	2:D:32:SER:OG	2.18	0.61
1:A:141:ILE:HG13	1:A:143:THR:HG23	1.82	0.61
2:C:50:PHE:HD1	2:C:55:GLN:OE1	1.82	0.60
2:C:276:ARG:O	2:C:280:LEU:N	2.32	0.60
2:D:142:ASP:O	2:D:147:ARG:NH1	2.35	0.60
2:D:116:GLN:HB2	2:D:163:LEU:HG	1.84	0.60
2:C:220:THR:CA	2:C:275:PHE:HZ	2.10	0.60
2:D:73:TYR:CE2	2:D:84:PHE:HE1	2.17	0.59
2:D:38:ILE:HG23	2:D:100:VAL:HG13	1.83	0.59
2:C:209:GLN:HE22	2:C:213:VAL:CG1	2.14	0.59
2:D:50:PHE:HB3	2:D:52:ASN:HB3	1.82	0.59
2:D:138:PHE:CE1	2:D:143:SER:OG	2.53	0.59
2:D:135:ILE:HD11	2:D:183:LYS:HG2	1.84	0.59
2:C:209:GLN:NE2	2:C:262:LYS:NZ	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:HIS:HA	2:C:280:LEU:HB2	1.85	0.58
2:D:111:LYS:HA	2:D:111:LYS:HE3	1.84	0.58
2:C:236:ILE:HA	2:C:268:LEU:O	2.03	0.58
2:D:81:LEU:HD12	2:D:94:TYR:HD1	1.69	0.58
1:B:119:ASP:OD1	1:B:121:THR:HG22	2.03	0.58
2:D:132:ARG:HA	2:D:132:ARG:CZ	2.33	0.58
1:B:168:GLY:O	3:B:302:HOH:O	2.17	0.58
2:C:293:ALA:HA	2:C:301:TYR:O	2.03	0.57
2:C:85:ARG:NH1	2:C:110:GLN:HB3	2.19	0.57
2:D:181:ILE:HD11	2:D:191:ASP:OD2	2.05	0.57
2:D:179:ASN:HA	2:D:198:MET:HE1	1.87	0.57
2:D:70:ALA:HA	2:D:75:ILE:HD13	1.87	0.57
2:C:216:VAL:HG12	2:C:267:PHE:HB3	1.86	0.57
1:A:134:ARG:HD3	1:A:225:VAL:HG21	1.86	0.57
1:A:251:PRO:HB3	1:B:164:ARG:HH11	1.69	0.56
2:C:205:TYR:O	2:C:209:GLN:CB	2.46	0.56
2:C:301:TYR:CE1	2:C:328:HIS:ND1	2.74	0.56
2:D:73:TYR:O	2:D:89:MET:HE1	2.05	0.56
2:D:43:SER:O	2:D:47:LYS:HD3	2.05	0.56
1:A:200:ARG:HB3	1:A:223:ARG:NH2	2.13	0.56
2:D:182:TYR:CE2	2:D:211:LYS:HB3	2.41	0.55
2:C:209:GLN:NE2	2:C:213:VAL:CG1	2.69	0.55
2:D:137:TYR:CE2	2:D:181:ILE:HG21	2.42	0.55
2:D:82:LYS:HZ3	2:D:89:MET:CG	2.19	0.55
1:B:197:HIS:HE1	1:B:218:ASP:OD1	1.89	0.55
2:C:225:GLU:OE2	2:C:225:GLU:N	2.37	0.55
2:C:253:GLU:HG2	2:C:309:VAL:HG22	1.88	0.55
2:C:209:GLN:NE2	2:C:213:VAL:HG13	2.22	0.54
2:C:234:PHE:HB3	2:C:236:ILE:HD11	1.89	0.54
2:D:69:ILE:HG13	2:D:72:ARG:NH2	2.23	0.54
2:D:72:ARG:HB2	2:D:73:TYR:HD1	1.73	0.54
2:C:275:PHE:N	2:C:275:PHE:HD2	2.06	0.54
2:D:69:ILE:HG13	2:D:72:ARG:HH21	1.73	0.54
1:B:125:PRO:HG3	3:B:302:HOH:O	2.08	0.54
2:C:191:ASP:HA	2:C:192:MET:HB2	1.90	0.53
2:C:228:THR:HG22	2:C:297:PHE:CE1	2.43	0.53
2:D:183:LYS:HE2	2:D:191:ASP:OD2	2.08	0.53
2:D:14:LEU:HD23	2:D:87:GLY:HA2	1.89	0.53
2:D:139:GLU:OE2	2:D:167:GLY:HA2	2.08	0.53
2:D:132:ARG:CZ	2:D:185:PRO:N	2.70	0.53
2:D:92:ARG:NH2	2:D:95:ARG:H	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:LYS:HD2	2:C:89:MET:CE	2.39	0.53
2:C:213:VAL:HG13	2:C:262:LYS:HZ1	1.74	0.53
2:D:58:PHE:HZ	2:D:107:ILE:HG21	1.74	0.53
2:C:116:GLN:HB2	2:C:163:LEU:HD23	1.91	0.53
2:D:138:PHE:HE1	2:D:143:SER:HG	1.49	0.53
2:C:85:ARG:NH1	2:C:110:GLN:HE21	1.93	0.52
2:C:228:THR:HG22	2:C:297:PHE:HE1	1.74	0.52
2:D:18:ASP:O	2:D:85:ARG:HA	2.08	0.52
2:D:45:VAL:HG12	2:D:46:ILE:HD12	1.90	0.52
2:D:132:ARG:NH2	2:D:184:PRO:C	2.63	0.52
2:D:19:VAL:HG21	2:D:56:VAL:HG12	1.92	0.52
2:D:134:ILE:HG13	2:D:208:ILE:HG23	1.92	0.52
2:C:4:SER:HA	2:C:60:ARG:HG2	1.91	0.52
2:C:136:GLY:HA2	2:C:180:ILE:HG22	1.91	0.52
2:D:211:LYS:N	2:D:211:LYS:HD2	2.25	0.52
2:D:62:ASP:O	2:D:66:HIS:HB2	2.10	0.52
2:D:83:LEU:C	2:D:84:PHE:HD2	2.13	0.51
2:C:276:ARG:HG2	2:C:280:LEU:HD21	1.93	0.51
2:D:145:ASN:OD1	2:D:199:THR:HG22	2.11	0.51
2:C:275:PHE:CD2	2:C:275:PHE:N	2.78	0.51
2:D:195:LEU:HD12	2:D:195:LEU:O	2.11	0.51
2:D:211:LYS:H	2:D:211:LYS:HD2	1.75	0.51
2:D:42:ALA:HB2	2:D:100:VAL:HA	1.92	0.51
1:B:115:PHE:HB3	1:B:198:THR:HG21	1.93	0.51
1:A:244:VAL:HG21	2:C:77:LYS:HD2	1.93	0.50
2:C:241:LYS:NZ	2:C:273:ASP:OD2	2.36	0.50
1:B:121:THR:HG21	1:B:197:HIS:NE2	2.27	0.50
1:A:251:PRO:HB3	1:B:164:ARG:NH1	2.27	0.50
2:C:294:ILE:O	2:C:300:MET:HA	2.12	0.50
2:D:52:ASN:ND2	2:D:55:GLN:CB	2.74	0.50
1:B:249:TRP:N	1:B:249:TRP:CD1	2.78	0.50
2:C:151:ARG:O	2:C:155:ILE:HD12	2.12	0.50
2:C:282:ILE:HG13	2:C:283:GLN:N	2.25	0.50
2:D:45:VAL:O	2:D:48:GLU:HG3	2.12	0.50
2:D:73:TYR:HB2	2:D:75:ILE:CD1	2.41	0.50
1:B:117:PRO:HG2	1:B:200:ARG:CZ	2.42	0.50
2:C:135:ILE:HD12	2:C:163:LEU:O	2.11	0.50
2:D:19:VAL:CG2	2:D:56:VAL:HG12	2.41	0.49
2:C:326:LYS:HD3	2:C:327:LEU:HG	1.95	0.49
2:C:135:ILE:CD1	2:C:163:LEU:C	2.80	0.49
2:D:135:ILE:CD1	2:D:183:LYS:HG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:SER:HB3	1:B:180:LEU:HD21	1.95	0.49
2:C:135:ILE:HD13	2:C:163:LEU:CB	2.43	0.49
2:C:218:GLU:HA	2:C:269:HIS:O	2.11	0.49
2:D:137:TYR:HD1	2:D:165:ALA:HB3	1.77	0.49
2:D:132:ARG:HH11	2:D:182:TYR:HE1	1.60	0.49
2:C:282:ILE:CG1	2:C:283:GLN:H	2.25	0.49
2:C:35:LEU:HD21	2:C:81:LEU:HD21	1.94	0.49
2:D:191:ASP:HA	2:D:192:MET:CB	2.41	0.49
2:C:15:ASN:HA	2:C:86:ASN:O	2.12	0.49
1:B:244:VAL:HB	2:D:77:LYS:HB3	1.94	0.49
1:A:204:ILE:HB	1:A:213:GLN:HB3	1.94	0.49
2:C:272:CYS:SG	2:C:286:PRO:HA	2.53	0.48
1:B:164:ARG:HG2	1:B:165:ARG:NH1	2.28	0.48
2:D:68:ASP:HB2	2:D:72:ARG:HH12	1.79	0.48
2:C:244:THR:O	2:C:248:GLU:HG2	2.14	0.48
2:C:51:PRO:HB2	2:C:53:GLU:N	2.28	0.48
1:B:225:VAL:O	1:B:229:LEU:HD12	2.14	0.48
2:C:134:ILE:HD13	2:C:208:ILE:HG23	1.96	0.48
2:D:42:ALA:HB2	2:D:100:VAL:HG12	1.96	0.48
2:D:73:TYR:HE2	2:D:84:PHE:CZ	2.30	0.47
2:C:126:THR:O	2:C:127:LEU:HD13	2.14	0.47
2:C:130:SER:HB2	2:C:131:LYS:H	1.50	0.47
2:C:264:THR:O	2:C:265:ILE:HD13	2.14	0.47
2:C:222:GLU:OE1	2:C:223:ASN:HB3	2.14	0.47
1:B:165:ARG:O	2:C:27:ASP:HB3	2.14	0.47
2:D:184:PRO:HD3	2:D:191:ASP:OD1	2.13	0.47
2:C:22:VAL:HG23	2:C:24:PHE:CE1	2.49	0.47
2:C:47:LYS:HD2	2:C:51:PRO:HB3	1.96	0.47
1:A:125:PRO:HG3	1:A:164:ARG:HG2	1.96	0.47
2:D:138:PHE:CD1	2:D:146:TYR:HB2	2.49	0.47
2:D:116:GLN:H	2:D:163:LEU:HA	1.80	0.47
2:D:32:SER:O	2:D:35:LEU:CD2	2.62	0.46
2:D:73:TYR:CE2	2:D:84:PHE:CE1	2.88	0.46
2:D:82:LYS:NZ	2:D:89:MET:HE3	2.19	0.46
2:C:222:GLU:CD	2:C:223:ASN:N	2.68	0.46
2:D:111:LYS:CE	2:D:111:LYS:HA	2.45	0.46
2:D:194:TYR:HB2	2:D:207:TRP:CE2	2.50	0.46
1:B:185:SER:HB3	1:B:191:TYR:HB2	1.95	0.46
2:D:82:LYS:HB3	2:D:82:LYS:HE3	1.62	0.46
1:A:109:LYS:HG2	1:A:142:ASN:HD21	1.81	0.46
1:A:151:ASP:HB3	1:A:155:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:ILE:CD1	2:C:164:SER:N	2.78	0.46
2:C:252:ASN:O	2:C:256:ARG:HG3	2.16	0.46
2:C:285:THR:HG22	2:C:288:ASP:OD2	2.16	0.46
1:B:112:VAL:CG1	1:B:145:VAL:HG22	2.46	0.46
1:B:141:ILE:HD11	1:B:229:LEU:HD23	1.97	0.46
2:C:266:ASN:HB2	3:C:401:HOH:O	2.14	0.46
2:C:238:PHE:CD1	2:C:270:ALA:HB3	2.49	0.46
2:D:36:HIS:HB2	2:D:37:PRO:HD3	1.97	0.46
2:D:66:HIS:O	2:D:69:ILE:N	2.47	0.46
1:A:228:THR:O	1:A:232:VAL:HG12	2.16	0.46
2:C:152:VAL:HG22	2:C:205:TYR:HB2	1.98	0.46
2:C:207:TRP:O	2:C:210:ASP:HB3	2.16	0.46
1:A:165:ARG:O	2:D:27:ASP:HB3	2.16	0.46
1:B:241:HIS:HB3	1:B:244:VAL:CG2	2.46	0.45
2:D:138:PHE:CE1	2:D:146:TYR:HB2	2.52	0.45
2:D:85:ARG:HH22	2:D:111:LYS:NZ	2.14	0.45
2:D:32:SER:CA	2:D:35:LEU:HD22	2.38	0.45
2:C:294:ILE:HG21	2:C:322:LEU:HD22	1.98	0.45
2:D:198:MET:HA	2:D:204:THR:HG21	1.98	0.45
2:D:17:ALA:HA	2:D:54:ASN:OD1	2.16	0.45
1:B:164:ARG:CG	1:B:165:ARG:NH1	2.80	0.45
2:D:132:ARG:CZ	2:D:185:PRO:HA	2.46	0.45
2:D:52:ASN:HB2	2:D:55:GLN:HG3	1.98	0.45
1:A:200:ARG:CB	1:A:223:ARG:HH21	2.18	0.45
2:C:46:ILE:HG21	2:C:107:ILE:HG21	1.99	0.45
2:C:204:THR:O	2:C:208:ILE:HG13	2.17	0.45
2:D:127:LEU:O	2:D:131:LYS:HD2	2.16	0.45
2:D:132:ARG:HH12	2:D:184:PRO:N	2.15	0.45
2:D:124:ILE:HD12	2:D:125:THR:H	1.82	0.45
2:D:144:ASP:O	2:D:148:VAL:HG23	2.17	0.44
2:D:66:HIS:O	2:D:68:ASP:N	2.50	0.44
2:D:82:LYS:NZ	2:D:89:MET:CG	2.80	0.44
1:A:162:THR:HB	1:A:168:GLY:HA3	1.99	0.44
2:D:42:ALA:N	2:D:100:VAL:HG12	2.32	0.44
2:C:234:PHE:O	2:C:294:ILE:HA	2.17	0.44
2:C:101:LYS:NZ	2:C:105:ASP:OD1	2.38	0.44
2:D:183:LYS:HA	2:D:184:PRO:HD3	1.72	0.44
2:C:85:ARG:HH12	2:C:110:GLN:HB3	1.82	0.44
1:A:236:GLN:O	1:A:240:LYS:HG3	2.17	0.44
2:C:131:LYS:NZ	2:C:159:ASP:C	2.71	0.44
2:C:132:ARG:HG2	2:C:182:TYR:OH	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ILE:HG22	2:C:160:CYS:SG	2.58	0.44
2:D:132:ARG:HH21	2:D:185:PRO:HA	1.83	0.44
2:D:194:TYR:HB2	2:D:207:TRP:CZ2	2.53	0.44
2:D:38:ILE:HG21	2:D:99:SER:HA	1.99	0.44
2:D:200:ASN:OD1	2:D:203:VAL:CG1	2.66	0.43
1:B:207:ASP:OD1	1:B:208:LYS:HG3	2.16	0.43
1:B:114:PHE:O	1:B:147:ALA:HA	2.19	0.43
2:C:92:ARG:NH2	2:C:158:ASP:OD2	2.50	0.43
2:C:182:TYR:CZ	2:C:211:LYS:HB3	2.54	0.43
1:A:185:SER:HB3	1:A:191:TYR:HB2	2.00	0.43
2:C:137:TYR:CD1	2:C:165:ALA:HB3	2.54	0.43
2:C:51:PRO:C	2:C:53:GLU:N	2.70	0.43
1:B:150:VAL:CG2	1:B:182:HIS:CD2	3.01	0.43
1:B:192:LEU:HD21	1:B:199:LEU:HD11	2.01	0.43
1:B:237:TYR:CZ	1:B:246:PRO:HG3	2.54	0.43
2:D:83:LEU:O	2:D:90:MET:HG2	2.19	0.43
1:B:229:LEU:O	1:B:233:GLN:HG3	2.18	0.43
2:D:123:GLU:HA	2:D:126:THR:OG1	2.19	0.42
2:C:129:ARG:HA	2:C:185:PRO:C	2.39	0.42
2:D:201:PHE:N	2:D:201:PHE:CD2	2.86	0.42
2:D:24:PHE:HB2	2:D:80:THR:OG1	2.19	0.42
2:D:65:GLN:HG2	2:D:66:HIS:CE1	2.54	0.42
2:D:90:MET:SD	2:D:155:ILE:HG13	2.59	0.42
2:D:75:ILE:N	2:D:75:ILE:HD12	2.34	0.42
2:C:298:ARG:CD	2:C:299:HIS:CE1	3.03	0.42
2:D:77:LYS:O	2:D:80:THR:HG23	2.20	0.42
2:D:134:ILE:HG13	2:D:208:ILE:CG2	2.49	0.42
2:D:153:ALA:O	2:D:157:HIS:HB3	2.20	0.42
2:D:132:ARG:CZ	2:D:185:PRO:CA	2.98	0.42
2:C:209:GLN:NE2	2:C:262:LYS:HZ2	2.16	0.42
2:C:46:ILE:HG21	2:C:56:VAL:HG11	2.02	0.42
2:D:10:ILE:O	2:D:14:LEU:HB3	2.19	0.42
2:C:51:PRO:HB2	2:C:53:GLU:HA	2.02	0.42
1:B:227:GLU:HG3	1:B:227:GLU:O	2.20	0.41
1:A:136:GLU:HB3	2:C:277:HIS:HD2	1.85	0.41
2:C:308:ASP:O	2:C:311:ILE:HD12	2.20	0.41
1:B:241:HIS:HB3	1:B:244:VAL:HG21	2.02	0.41
2:D:183:LYS:HD2	2:D:183:LYS:HA	1.78	0.41
1:B:222:GLY:HA2	1:B:223:ARG:NH2	2.34	0.41
1:B:250:LYS:O	1:B:250:LYS:NZ	2.46	0.41
2:D:19:VAL:HG23	2:D:56:VAL:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:PHE:HE1	2:D:143:SER:OG	1.95	0.41
1:B:115:PHE:HB3	1:B:198:THR:CG2	2.50	0.41
2:C:301:TYR:CE1	2:C:328:HIS:CE1	3.08	0.41
2:D:144:ASP:N	2:D:144:ASP:OD1	2.54	0.41
1:A:161:ASN:O	1:A:163:PRO:HD3	2.21	0.41
1:B:98:PHE:O	1:B:99:LYS:HD3	2.21	0.41
2:C:276:ARG:C	2:C:280:LEU:HD23	2.41	0.41
2:C:301:TYR:OH	2:C:328:HIS:CE1	2.74	0.41
2:D:202:ASP:HA	2:D:205:TYR:HB3	2.01	0.41
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.82	0.41
2:C:136:GLY:CA	2:C:180:ILE:HG22	2.50	0.41
1:B:237:TYR:CE1	1:B:246:PRO:HG3	2.56	0.41
2:C:121:LEU:HA	2:C:121:LEU:HD22	1.85	0.41
2:C:77:LYS:O	2:C:80:THR:HG23	2.21	0.41
2:C:19:VAL:HG13	2:C:83:LEU:HD11	2.02	0.41
2:D:67:SER:O	2:D:70:ALA:N	2.52	0.41
2:D:66:HIS:C	2:D:68:ASP:N	2.74	0.41
2:D:68:ASP:OD1	2:D:72:ARG:NH2	2.48	0.41
1:A:150:VAL:CG2	1:A:182:HIS:CD2	3.03	0.40
2:D:124:ILE:HD12	2:D:125:THR:N	2.36	0.40
2:D:83:LEU:O	2:D:84:PHE:HD2	2.04	0.40
1:B:118:LEU:HA	1:B:118:LEU:HD23	1.91	0.40
2:C:141:LYS:HD3	2:C:141:LYS:HA	1.83	0.40
2:C:23:ASN:HA	2:C:81:LEU:HD23	2.03	0.40
2:D:10:ILE:O	2:D:14:LEU:CB	2.69	0.40
2:D:148:VAL:HG21	2:D:199:THR:O	2.22	0.40
2:D:198:MET:HA	2:D:204:THR:CG2	2.51	0.40
2:D:98:ARG:HH11	2:D:98:ARG:HD2	1.77	0.40
1:A:150:VAL:HG23	1:A:179:ASP:O	2.21	0.40
2:C:219:ILE:CD1	2:C:224:GLY:HA2	2.41	0.40
2:C:234:PHE:O	2:C:294:ILE:HG23	2.21	0.40
2:D:73:TYR:CE2	2:D:84:PHE:CZ	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:ARG:NH2	2:D:168:ASP:O[5_455]	2.19	0.01

## 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	179/246 (73%)	172 (96%)	7 (4%)	0	100	100
1	B	173/246 (70%)	166 (96%)	7 (4%)	0	100	100
2	C	319/382 (84%)	297 (93%)	20 (6%)	2 (1%)	25	47
2	D	200/382 (52%)	179 (90%)	20 (10%)	1 (0%)	29	52
All	All	871/1256 (69%)	814 (94%)	54 (6%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	50	PHE
2	D	67	SER
2	C	52	ASN

### 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	158/213 (74%)	151 (96%)	7 (4%)	28	53
1	B	153/213 (72%)	149 (97%)	4 (3%)	46	72
2	C	293/343 (85%)	277 (94%)	16 (6%)	21	43
2	D	184/343 (54%)	172 (94%)	12 (6%)	17	34
All	All	788/1112 (71%)	749 (95%)	39 (5%)	25	48

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	143	THR
1	A	195	SER
1	A	208	LYS
1	A	213	GLN
1	A	232	VAL
1	A	254	GLU
1	B	165	ARG
1	B	198	THR
1	B	221	VAL
1	B	223	ARG
2	C	48	GLU
2	C	68	ASP
2	C	88	MET
2	C	95	ARG
2	C	101	LYS
2	C	119	ARG
2	C	130	SER
2	C	131	LYS
2	C	143	SER
2	C	166	PHE
2	C	191	ASP
2	C	217	ARG
2	C	222	GLU
2	C	241	LYS
2	C	314	LYS
2	C	329	ARG
2	D	21	LEU
2	D	47	LYS
2	D	52	ASN
2	D	93	GLU
2	D	95	ARG
2	D	101	LYS
2	D	138	PHE
2	D	140	GLN
2	D	157	HIS
2	D	182	TYR
2	D	183	LYS
2	D	206	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	182	HIS
1	A	213	GLN
1	B	161	ASN
1	B	197	HIS
1	B	236	GLN
2	C	16	ASN
2	C	55	GLN
2	C	110	GLN
2	C	140	GLN
2	C	209	GLN
2	D	110	GLN
2	D	154	ASN
2	D	206	ASN

### 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 carbohydrates 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, 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	181/246 (73%)	0.45	3 (1%) 70 66	57, 80, 114, 141	0
1	B	175/246 (71%)	0.57	1 (0%) 89 88	56, 76, 108, 124	0
2	C	323/382 (84%)	0.61	22 (6%) 17 12	59, 106, 170, 211	0
2	D	204/382 (53%)	1.54	66 (32%) 0 0	106, 171, 215, 228	0
All	All	883/1256 (70%)	0.79	92 (10%) 6 4	56, 99, 190, 228	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	VAL	11.4
2	D	56	VAL	9.7
2	D	165	ALA	8.0
2	D	195	LEU	7.3
2	D	19	VAL	7.2
2	D	203	VAL	7.0
2	D	14	LEU	6.5
2	D	137	TYR	6.3
2	C	277	HIS	6.3
2	D	46	ILE	5.4
2	D	20	ALA	5.4
2	D	118	ILE	5.3
2	D	208	ILE	5.1
2	D	18	ASP	5.0
2	D	55	GLN	4.6
2	D	51	PRO	4.4
2	D	181	ILE	4.4
2	D	50	PHE	4.3
2	D	127	LEU	4.2
2	D	106	TYR	4.2
2	D	149	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	116	GLN	4.1
2	D	78	TYR	4.1
2	D	58	PHE	4.1
2	D	72	ARG	4.0
2	D	152	VAL	4.0
2	D	136	GLY	4.0
2	D	196	GLY	3.9
2	C	118	ILE	3.9
2	C	188	SER	3.8
2	D	21	LEU	3.8
2	D	83	LEU	3.7
2	D	134	ILE	3.7
2	D	59	ALA	3.6
2	D	135	ILE	3.6
2	D	204	THR	3.5
2	D	119	ARG	3.5
2	C	331	PHE	3.4
2	D	180	ILE	3.4
2	C	163	LEU	3.4
2	C	187	HIS	3.3
2	D	10	ILE	3.3
2	D	197	ALA	3.2
2	D	42	ALA	3.2
2	D	211	LYS	3.1
2	D	115	ILE	3.1
2	D	138	PHE	3.1
2	C	322	LEU	3.1
2	D	44	ASP	3.1
2	C	254	VAL	3.1
2	D	89	MET	3.0
2	C	208	ILE	3.0
2	D	52	ASN	3.0
2	C	69	ILE	2.9
2	D	192	MET	2.9
2	D	107	ILE	2.9
2	D	60	ARG	2.9
2	C	81	LEU	2.9
1	A	255	THR	2.9
2	D	24	PHE	2.9
2	D	70	ALA	2.9
2	D	194	TYR	2.8
2	D	5	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	88	MET	2.8
2	D	12	GLU	2.7
2	D	213	VAL	2.7
2	C	24	PHE	2.6
1	B	246	PRO	2.5
2	D	114	PRO	2.5
2	D	193	VAL	2.5
1	A	254	GLU	2.4
2	D	163	LEU	2.4
2	D	212	CYS	2.4
2	D	61	VAL	2.3
2	D	164	SER	2.3
2	D	205	TYR	2.3
2	D	148	VAL	2.3
2	D	182	TYR	2.3
2	C	309	VAL	2.3
2	C	319	VAL	2.3
2	C	131	LYS	2.3
2	C	270	ALA	2.2
2	D	26	ALA	2.2
2	D	39	PHE	2.2
2	C	320	PHE	2.1
2	D	185	PRO	2.1
2	C	21	LEU	2.1
2	C	120	ASP	2.1
2	C	212	CYS	2.0
1	A	123	VAL	2.0
2	C	5	LEU	2.0
2	C	280	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.