



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 5HQP / pdb_00005hqp
Title : Crystal structure of the ERp44-peroxiredoxin 4 complex
Authors : Yang, K.; Li, D.F.; Wang, X.; Wang, C.C.
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

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

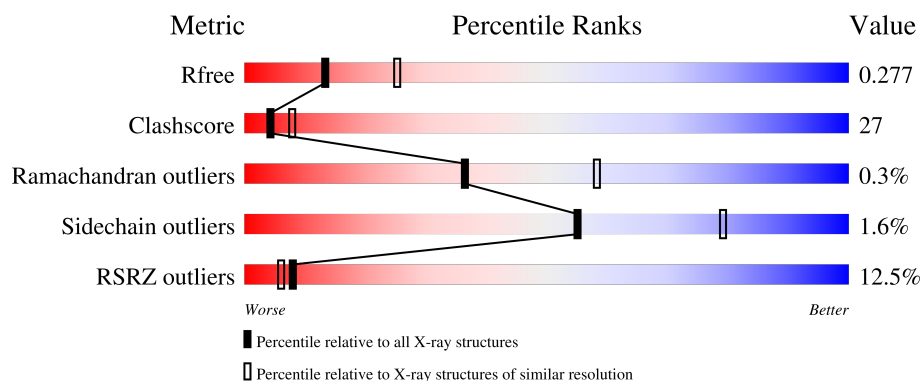
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	246	4% 56% 17% 26%
1	B	246	3% 52% 19% 29%
2	C	382	12% 44% 38% 15%
2	D	382	12% 22% 30% 47%

2 Entry composition [i](#)

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

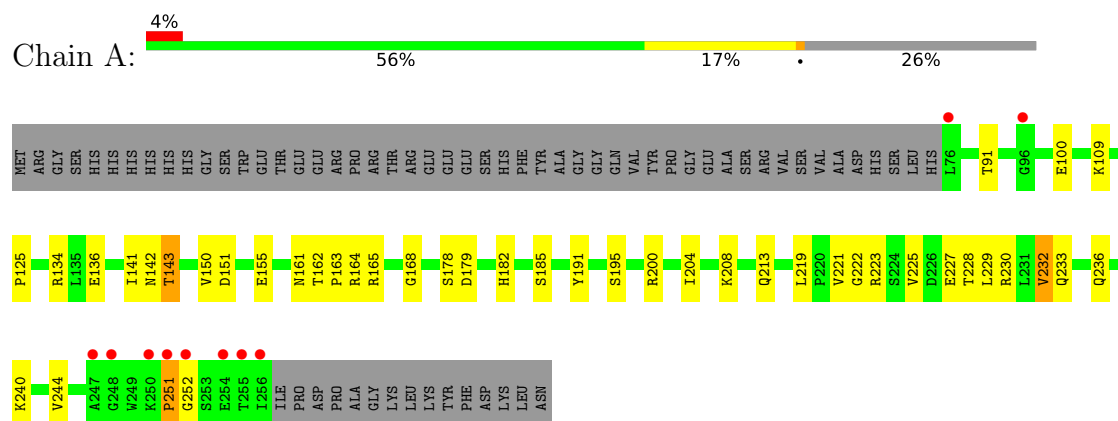
- Molecule 3 is water.

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		

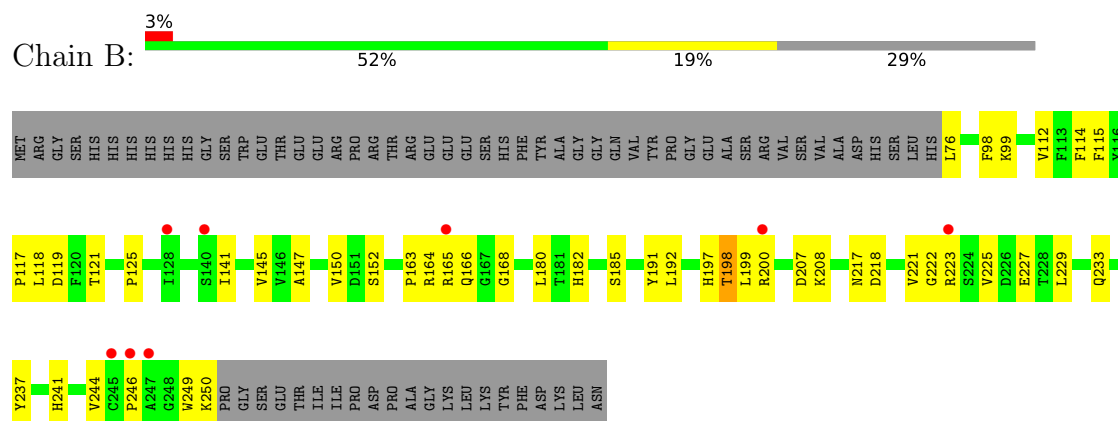
3 Residue-property plots [i](#)

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.

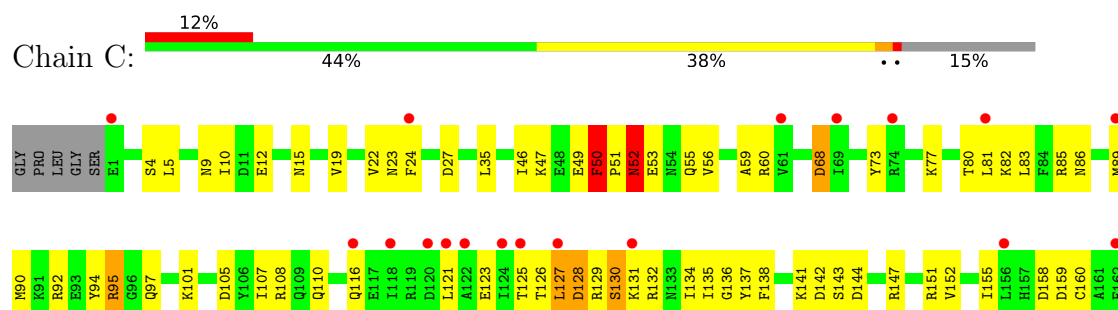
• Molecule 1: Peroxiredoxin-4

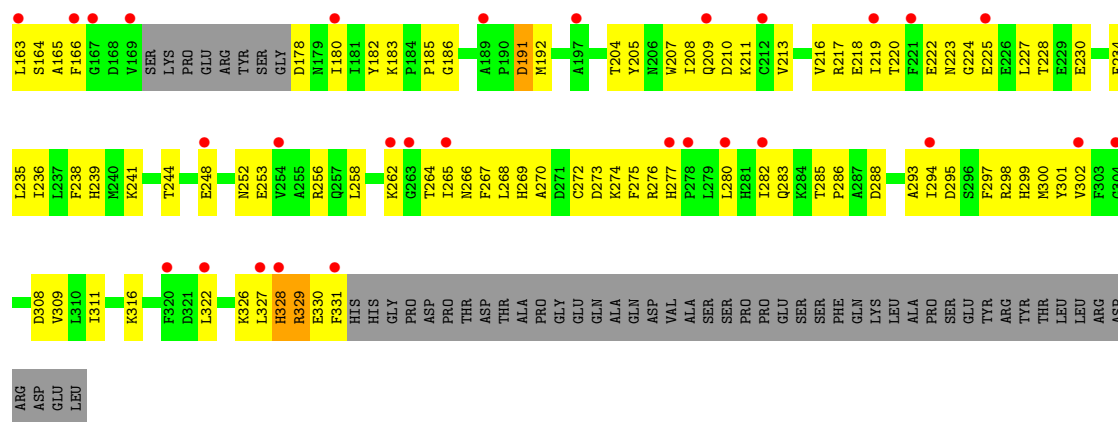


• Molecule 1: Peroxiredoxin-4

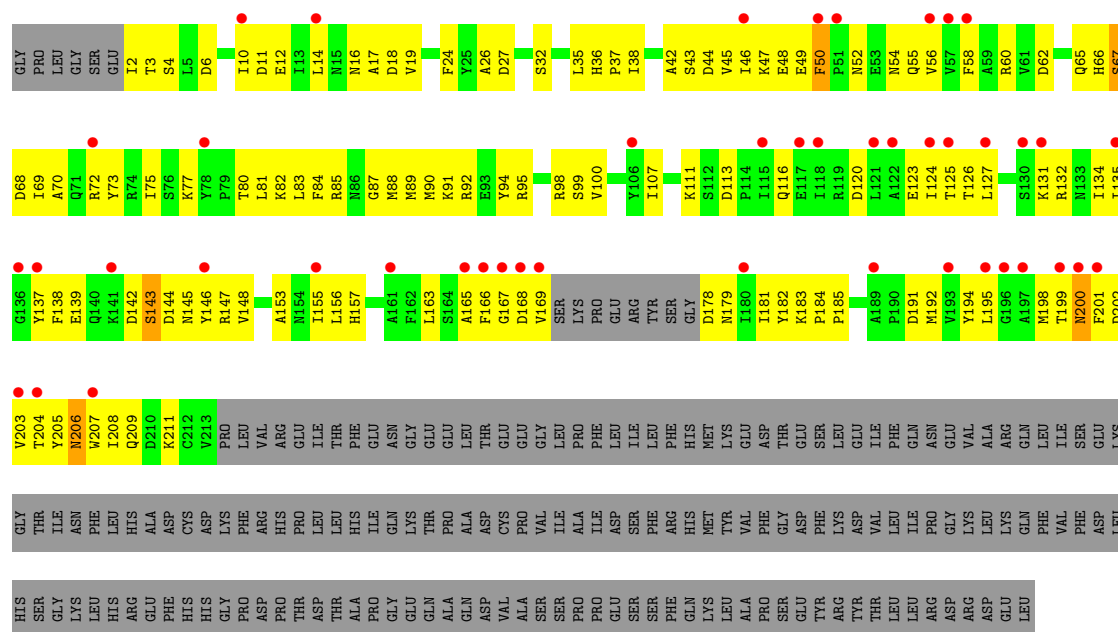
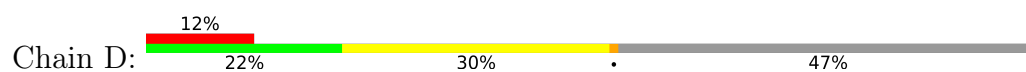


• Molecule 2: Endoplasmic reticulum resident protein 44





● Molecule 2: Endoplasmic reticulum resident protein 44



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.29Å 198.98Å 225.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.60 49.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.60) 93.0 (49.74-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.235 , 0.272 0.241 , 0.277	Depositor DCC
R_{free} test set	2377 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.24	0/1487	0.59	2/2018 (0.1%)
1	B	0.27	0/1445	0.63	0/1960
2	C	0.52	8/2717 (0.3%)	0.76	7/3670 (0.2%)
2	D	0.51	0/1710	0.92	5/2311 (0.2%)
All	All	0.43	8/7359 (0.1%)	0.75	14/9959 (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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	95	ARG	NE-CZ	-10.52	1.21	1.33
2	C	95	ARG	CZ-NH1	-7.09	1.22	1.32
2	C	95	ARG	CD-NE	-6.84	1.36	1.46
2	C	95	ARG	CZ-NH2	-6.51	1.25	1.33
2	C	329	ARG	NE-CZ	-6.12	1.26	1.33
2	C	329	ARG	CZ-NH2	-5.82	1.25	1.33
2	C	328	HIS	CE1-NE2	-5.51	1.27	1.32
2	C	329	ARG	CD-NE	-5.43	1.38	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	50	PHE	CA-C-N	8.43	147.24	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	50	PHE	C-N-CA	8.43	147.24	127.00
2	C	50	PHE	C-N-CD	-8.20	102.56	120.60
2	D	143	SER	CA-CB-OG	-6.87	97.36	111.10
2	C	50	PHE	N-CA-C	-6.84	94.70	109.81
2	D	50	PHE	CA-C-N	6.51	142.64	127.00
2	D	50	PHE	C-N-CA	6.51	142.64	127.00
2	D	50	PHE	C-N-CD	-6.48	106.35	120.60
2	C	52	ASN	CA-C-N	5.88	132.77	121.54
2	C	52	ASN	C-N-CA	5.88	132.77	121.54
2	D	60	ARG	NE-CZ-NH1	-5.63	115.87	121.50
2	C	128	ASP	N-CA-C	5.55	118.44	109.79
1	A	221	VAL	CA-C-N	-5.23	115.41	122.63
1	A	221	VAL	C-N-CA	-5.23	115.41	122.63

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 [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	1450	0	1434	28	0
1	B	1409	0	1395	38	0
2	C	2657	0	2577	149	1
2	D	1676	0	1611	177	1
3	A	11	0	0	0	0
3	B	8	0	0	3	0
3	C	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7219	0	7017	384	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 27.

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)
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:44:ASP:N	2:D:47:LYS:HZ2	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:D:82:LYS:HZ3	2:D:89:MET:CE	1.72	1.01
2:C:220:THR:HA	2:C:275:PHE:HZ	1.28	0.97
2:D:44:ASP:CA	2:D:47:LYS:HZ2	1.81	0.93
2:C:209:GLN:HE22	2:C:262:LYS:HZ1	1.15	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
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:C:219:ILE:HD11	2:C:224:GLY:HA2	1.61	0.82
2:D:132:ARG:CZ	2:D:184:PRO:C	2.53	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:D:132:ARG:HH12	2:D:183:LYS:C	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:LYS:HZ3	2:D:89:MET:HE3	1.48	0.78
2:D:44:ASP:HA	2:D:47:LYS:HZ2	1.48	0.77
2:D:138:PHE:HD2	2:D:139:GLU:N	1.82	0.77
2:D:138:PHE:HD2	2:D:139:GLU:H	1.33	0.77
2:D:73:TYR:HE2	2:D:84:PHE:HE1	1.30	0.76
2:D:82:LYS:NZ	2:D:89:MET:HE2	2.00	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:132:ARG:NH1	2:D:184:PRO:C	2.45	0.74
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:73:TYR:HB3	2:C:89:MET:HE1	1.70	0.74
2:C:216:VAL:HG12	2:C:267:PHE:CB	2.18	0.73
2:D:85:ARG:H	2:D:90:MET:HE3	1.53	0.72
2:D:135:ILE:HB	2:D:181:ILE:HG23	1.71	0.72
2:C:191:ASP:OD1	2:C:191:ASP:N	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:C:135:ILE:HD12	2:C:163:LEU:C	2.16	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:330:GLU:HB3	2:C:331:PHE:C	2.19	0.68
2:C:51:PRO:HB2	2:C:53:GLU:H	1.59	0.67
2:D:6:ASP:O	2:D:10:ILE:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ASN:ND2	2:D:55:GLN:HB2	2.09	0.67
2:D:207:TRP:CD1	2:D:211:LYS:HZ3	2.13	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:209:GLN:NE2	2:C:262:LYS:HZ1	1.90	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:207:TRP:CG	2:D:211:LYS:HZ3	2.13	0.66
2:D:132:ARG:NE	2:D:132:ARG:HA	2.10	0.66
2:D:32:SER:O	2:D:35:LEU:HD23	1.95	0.66
2:C:82:LYS:HD2	2:C:89:MET:HE2	1.78	0.66
2:D:52:ASN:CG	2:D:55:GLN:HB2	2.21	0.66
2:C:222:GLU:CD	2:C:223:ASN:H	2.04	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
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:D:82:LYS:HZ3	2:D:89:MET:HE2	1.53	0.65
2:D:82:LYS:NZ	2:D:89:MET:HE3	2.11	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:D:82:LYS:HZ3	2:D:89:MET:CG	2.10	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: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:OE1	2:C:12:GLU:N	2.29	0.62
2:C:276:ARG:HG2	2:C:280:LEU:CD2	2.30	0.62
2:C:241:LYS:H	2:C:241:LYS:HD3	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:179:ASN:HA	2:D:198:MET:HE1	1.81	0.61
2:C:5:LEU:HD22	2:C:10:ILE:HA	1.82	0.61
2:C:327:LEU:HD22	2:C:329:ARG:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:217:ARG:HG3	2:C:218:GLU:N	2.11	0.59
2:C:220:THR:HG23	2:C:222:GLU:CD	2.15	0.59
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:135:ILE:HD11	2:D:183:LYS:HG2	1.84	0.59
2:D:138:PHE:CE1	2:D:143:SER:OG	2.53	0.59
2:C:277:HIS:HA	2:C:280:LEU:HB2	1.85	0.58
2:D:111:LYS:HE3	2:D:111:LYS:HA	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:CZ	2:D:132:ARG:HA	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:C:209:GLN:NE2	2:C:262:LYS:NZ	2.51	0.57
2:D:181:ILE:HD11	2:D:191:ASP:OD2	2.05	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
2:D:132:ARG:NH2	2:D:184:PRO:C	2.63	0.56
1:A:251:PRO:HB3	1:B:164:ARG:HH11	1.69	0.56
2:D:83:LEU:C	2:D:84:PHE:HD2	2.13	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: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:C:94:TYR:OH	2:C:97:GLN:O	2.19	0.55
2:D:73:TYR:O	2:D:89:MET:HE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:TYR:CE2	2:D:181:ILE:HG21	2.42	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:C:135:ILE:CD1	2:C:163:LEU:C	2.80	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
2:C:131:LYS:HZ1	2:C:159:ASP:C	2.15	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:14:LEU:HD23	2:D:87:GLY:HA2	1.89	0.53
2:D:183:LYS:HE2	2:D:191:ASP:OD2	2.08	0.53
2:D:139:GLU:OE2	2:D:167:GLY:HA2	2.08	0.53
2:D:92:ARG:NH2	2:D:95:ARG:H	2.00	0.53
2:D:132:ARG:CZ	2:D:185:PRO:N	2.70	0.53
2:C:82:LYS:HD2	2:C:89:MET:CE	2.39	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: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:62:ASP:O	2:D:66:HIS:HB2	2.10	0.52
2:D:211:LYS:HD2	2:D:211:LYS:N	2.25	0.52
2:C:222:GLU:CD	2:C:223:ASN:N	2.68	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:N	2:C:275:PHE:CD2	2.78	0.51
2:D:195:LEU:O	2:D:195:LEU:HD12	2.11	0.51
2:D:211:LYS:HD2	2:D:211:LYS:H	1.75	0.51
2:D:42:ALA:HB2	2:D:100:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:135:ILE:CD1	2:D:183:LYS:HG2	2.42	0.49
1:B:152:SER:HB3	1:B:180:LEU:HD21	1.95	0.49
2:C:135:ILE:HD12	2:C:163:LEU:O	2.11	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:132:ARG:HH11	2:D:182:TYR:HE1	1.60	0.49
2:D:137:TYR:HD1	2:D:165:ALA:HB3	1.77	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
1:B:244:VAL:HB	2:D:77:LYS:HB3	1.94	0.49
2:C:15:ASN:HA	2:C:86:ASN:O	2.12	0.49
1:A:204:ILE:HB	1:A:213:GLN:HB3	1.94	0.49
2:C:131:LYS:NZ	2:C:159:ASP:C	2.71	0.48
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:51:PRO:HB2	2:C:53:GLU:N	2.28	0.48
2:C:244:THR:O	2:C:248:GLU:HG2	2.14	0.48
1:B:225:VAL:O	1:B:229:LEU:HD12	2.14	0.48
2:C:51:PRO:C	2:C:53:GLU:N	2.70	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:D:82:LYS:HZ2	2:D:89:MET:HE2	1.79	0.47
2:C:85:ARG:HG3	2:C:90:MET:HE3	1.96	0.47
2:C:126:THR:O	2:C:127:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ARG:HA	2:C:185:PRO:C	2.39	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
1:A:125:PRO:HG3	1:A:164:ARG:HG2	1.96	0.47
2:C:47:LYS:HD2	2:C:51:PRO:HB3	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:111:LYS:HA	2:D:111:LYS:CE	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
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
1:A:165:ARG:O	2:D:27:ASP:HB3	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:B:241:HIS:HB3	1:B:244:VAL:CG2	2.46	0.45
2:D:82:LYS:HZ3	2:D:89:MET:HG3	1.79	0.45
2:D:138:PHE:CE1	2:D:146:TYR:HB2	2.52	0.45
2:D:32:SER:CA	2:D:35:LEU:HD22	2.38	0.45
2:D:85:ARG:HH22	2:D:111:LYS:NZ	2.14	0.45
2:C:276:ARG:C	2:C:280:LEU:HD23	2.41	0.45
2:C:295:ASP:OD2	2:C:300:MET:HE2	2.16	0.45
2:D:66:HIS:C	2:D:68:ASP:N	2.74	0.45
2:C:294:ILE:HG21	2:C:322:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:ALA:HA	2:D:54:ASN:OD1	2.16	0.45
2:D:198:MET:HA	2:D:204:THR:HG21	1.98	0.45
1:B:164:ARG:CG	1:B:165:ARG:NH1	2.80	0.45
2:C:213:VAL:HG13	2:C:262:LYS:HZ1	1.80	0.45
2:D:52:ASN:HB2	2:D:55:GLN:HG3	1.98	0.45
2:D:132:ARG:CZ	2:D:185:PRO:HA	2.46	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: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
2:D:144:ASP:O	2:D:148:VAL:HG23	2.17	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:123:GLU:C	2:C:125:THR:N	2.75	0.44
2:C:132:ARG:HG2	2:C:182:TYR:OH	2.18	0.44
2:D:67:SER:C	2:D:70:ALA:H	2.25	0.44
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:38:ILE:HG21	2:D:99:SER:HA	1.99	0.44
2:D:194:TYR:HB2	2:D:207:TRP:CZ2	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:GLU:HA	2:D:126:THR:OG1	2.19	0.42
1:A:151:ASP:O	1:A:178:SER:OG	2.30	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:201:PHE:CD2	2:D:201:PHE:N	2.86	0.42
2:D:75:ILE:N	2:D:75:ILE:HD12	2.34	0.42
1:A:227:GLU:CD	1:A:230:ARG:HH21	2.28	0.42
2:D:43:SER:C	2:D:47:LYS:HZ2	2.21	0.42
2:C:239:HIS:C	2:C:272:CYS:HB2	2.44	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:132:ARG:CZ	2:D:185:PRO:CA	2.98	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: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
2:D:82:LYS:CE	2:D:89:MET:HE3	2.50	0.42
1:A:136:GLU:HB3	2:C:277:HIS:HD2	1.85	0.41
1:B:227:GLU:O	1:B:227:GLU:HG3	2.20	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:43:SER:C	2:D:47:LYS:HD3	2.45	0.41
2:D:183:LYS:HA	2:D:183:LYS:HD2	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
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:C:9:ASN:HA	2:C:12:GLU:CD	2.45	0.41
2:D:144:ASP:OD1	2:D:144:ASP:N	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: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:HA	1:A:219:LEU:HD23	1.82	0.41
2:C:52:ASN:CG	2:C:55:GLN:NE2	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:VAL:HG13	2:C:83:LEU:HD11	2.02	0.41
2:C:77:LYS:O	2:C:80:THR:HG23	2.21	0.41
2:C:121:LEU:HD22	2:C:121:LEU:HA	1.85	0.41
2:D:67:SER:O	2:D:70:ALA:N	2.52	0.41
2:D:68:ASP:OD1	2:D:72:ARG:NH2	2.48	0.41
2:D:89:MET:O	2:D:91:LYS:NZ	2.49	0.41
1:A:150:VAL:CG2	1:A:182:HIS:CD2	3.03	0.40
2:D:83:LEU:O	2:D:84:PHE:HD2	2.04	0.40
2:D:124:ILE:HD12	2:D:125:THR:N	2.36	0.40
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.91	0.40
2:C:225:GLU:N	2:C:225:GLU:CD	2.79	0.40
2:C:23:ASN:HA	2:C:81:LEU:HD23	2.03	0.40
2:C:141:LYS:HA	2:C:141:LYS:HD3	1.83	0.40
2:D:10:ILE:O	2:D:14:LEU:CB	2.69	0.40
2:D:98:ARG:HH11	2:D:98:ARG:HD2	1.77	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
1:A:150:VAL:HG23	1:A:179:ASP:O	2.21	0.40
2:C:51:PRO:C	2:C:53:GLU:H	2.30	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
2:D:88:MET:HE3	2:D:89:MET:H	1.86	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 [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	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%)	21	42
2	D	200/382 (52%)	179 (90%)	20 (10%)	1 (0%)	24	46
All	All	871/1256 (69%)	814 (94%)	54 (6%)	3 (0%)	36	58

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%)	154 (98%)	4 (2%)	42	69
1	B	153/213 (72%)	151 (99%)	2 (1%)	61	82
2	C	293/343 (85%)	288 (98%)	5 (2%)	53	78
2	D	184/343 (54%)	182 (99%)	2 (1%)	65	84
All	All	788/1112 (71%)	775 (98%)	13 (2%)	55	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	THR
1	A	195	SER
1	A	208	LYS
1	A	232	VAL
1	B	198	THR
1	B	221	VAL
2	C	68	ASP
2	C	130	SER

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Mol	Chain	Res	Type
2	C	143	SER
2	C	166	PHE
2	C	191	ASP
2	D	120	ASP
2	D	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	183	GLN
1	A	213	GLN
1	B	161	ASN
1	B	197	HIS
1	B	233	GLN
2	C	23	ASN
2	C	54	ASN
2	C	55	GLN
2	C	97	GLN
2	C	110	GLN
2	C	140	GLN
2	C	145	ASN
2	C	209	GLN
2	C	277	HIS
2	C	283	GLN
2	C	323	HIS
2	D	154	ASN
2	D	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	181/246 (73%)	0.40	10 (5%) 30 25	57, 80, 114, 141	0
1	B	175/246 (71%)	0.49	8 (4%) 37 32	56, 76, 108, 124	0
2	C	323/382 (84%)	1.06	47 (14%) 6 4	59, 106, 170, 211	0
2	D	204/382 (53%)	1.32	45 (22%) 2 2	106, 171, 215, 228	0
All	All	883/1256 (70%)	0.87	110 (12%) 8 6	56, 99, 190, 228	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	124	ILE	6.7
2	C	169	VAL	6.2
2	C	221	PHE	5.6
2	D	166	PHE	5.2
2	D	169	VAL	5.2
2	D	195	LEU	4.8
2	C	282	ILE	4.3
2	C	166	PHE	4.1
2	C	277	HIS	4.1
1	A	256	ILE	3.9
2	D	196	GLY	3.9
2	D	203	VAL	3.8
2	C	167	GLY	3.7
2	C	124	ILE	3.6
2	C	331	PHE	3.6
1	A	255	THR	3.6
2	C	74	ARG	3.6
1	A	254	GLU	3.6
2	D	57	VAL	3.5
2	D	137	TYR	3.5
2	C	116	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	118	ILE	3.4
1	B	200	ARG	3.3
1	B	246	PRO	3.3
2	D	121	LEU	3.3
2	D	141	LYS	3.2
2	D	127	LEU	3.2
2	D	161	ALA	3.1
2	D	10	ILE	3.1
2	D	56	VAL	3.1
2	C	320	PHE	3.1
2	C	122	ALA	3.0
1	A	251	PRO	3.0
1	B	128	ILE	3.0
2	D	118	ILE	3.0
2	C	327	LEU	3.0
2	C	189	ALA	3.0
2	C	262	LYS	2.9
1	B	245	CYS	2.9
1	A	76	LEU	2.9
2	C	265	ILE	2.9
2	D	167	GLY	2.8
2	D	78	TYR	2.8
1	B	140	SER	2.8
2	D	14	LEU	2.8
2	D	135	ILE	2.7
2	C	163	LEU	2.7
1	B	247	ALA	2.7
2	C	248	GLU	2.7
2	D	50	PHE	2.7
2	D	136	GLY	2.7
2	D	197	ALA	2.7
2	D	201	PHE	2.6
1	B	165	ARG	2.6
1	A	250	LYS	2.6
2	C	225	GLU	2.6
1	A	252	GLY	2.6
2	C	120	ASP	2.5
2	C	263	GLY	2.5
2	C	61	VAL	2.5
2	C	302	VAL	2.5
2	D	193	VAL	2.5
2	D	115	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	278	PRO	2.5
2	C	24	PHE	2.5
2	D	199	THR	2.4
2	C	328	HIS	2.4
2	D	168	ASP	2.4
2	C	254	VAL	2.4
1	A	248	GLY	2.4
2	C	69	ILE	2.3
1	A	96	GLY	2.3
2	D	165	ALA	2.3
2	C	125	THR	2.3
2	C	1	GLU	2.3
2	D	207	TRP	2.3
2	D	58	PHE	2.3
2	D	189	ALA	2.2
2	D	204	THR	2.2
2	C	127	LEU	2.2
2	C	162	PHE	2.2
2	D	131	LYS	2.2
2	C	209	GLN	2.2
2	C	322	LEU	2.2
2	C	219	ILE	2.2
2	D	155	ILE	2.2
2	C	197	ALA	2.2
2	C	81	LEU	2.2
2	D	180	ILE	2.2
2	D	125	THR	2.2
1	B	223	ARG	2.2
2	C	212	CYS	2.2
2	D	72	ARG	2.2
2	D	51	PRO	2.2
2	D	106	TYR	2.2
2	C	121	LEU	2.1
2	C	280	LEU	2.1
2	C	131	LYS	2.1
2	D	122	ALA	2.1
2	D	146	TYR	2.1
2	C	180	ILE	2.1
1	A	247	ALA	2.1
2	C	89	MET	2.1
2	D	200	ASN	2.1
2	C	304	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	117	GLU	2.0
2	D	130	SER	2.0
2	D	46	ILE	2.0
2	C	156	LEU	2.0
2	C	294	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.