



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:47 PM UTC

PDB ID : 5B6M / pdb_00005b6m
Title : Crystal structure of human peroxiredoxin 6 in reduced state
Authors : Kim, K.H.; Lee, W.T.; Kim, E.E.
Deposited on : 2016-05-30
Resolution : 2.50 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

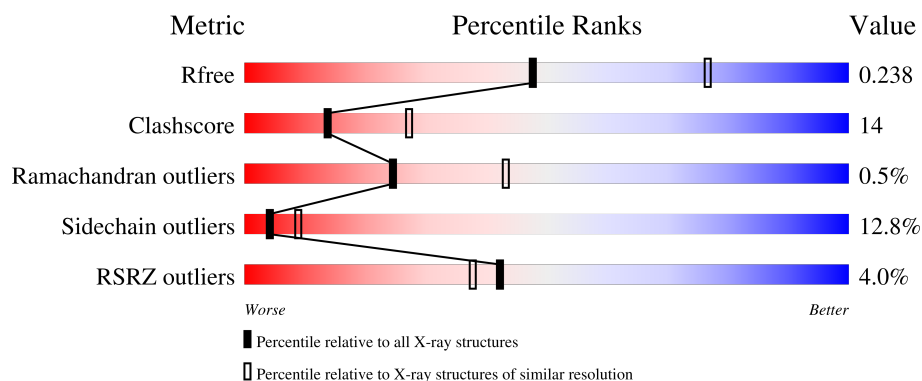
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	224	72% 24% ..
1	B	224	70% 23% 5% ..
1	C	224	4% 62% 29% 5% ..
1	D	224	12% 43% 38% 12% 6%
1	E	224	6% 47% 42% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	224	66% 25% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10485 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	B	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	C	214	Total	C	N	O	S	0	0	0
			1692	1090	284	313	5			
1	D	211	Total	C	N	O	S	0	0	0
			1670	1081	280	305	4			
1	E	221	Total	C	N	O	S	0	0	0
			1747	1127	293	322	5			
1	F	223	Total	C	N	O	S	0	0	0
			1758	1134	295	324	5			

- Molecule 2 is water.

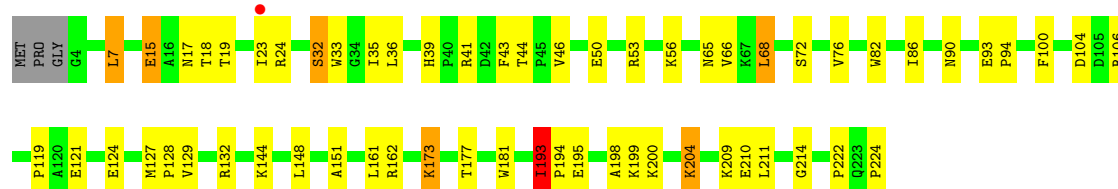
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	31	Total	O	0	0
			31	31		
2	C	18	Total	O	0	0
			18	18		
2	D	10	Total	O	0	0
			10	10		
2	E	20	Total	O	0	0
			20	20		
2	F	22	Total	O	0	0
			22	22		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

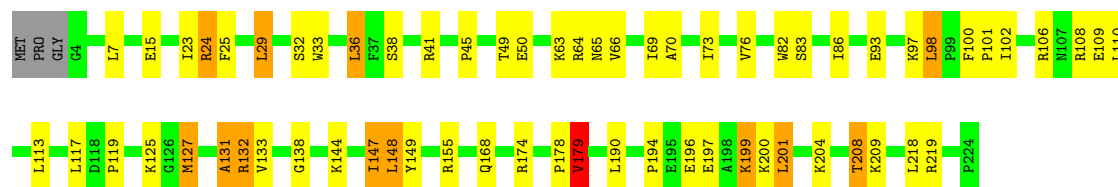
• Molecule 1: Peroxiredoxin-6

Chain A: 



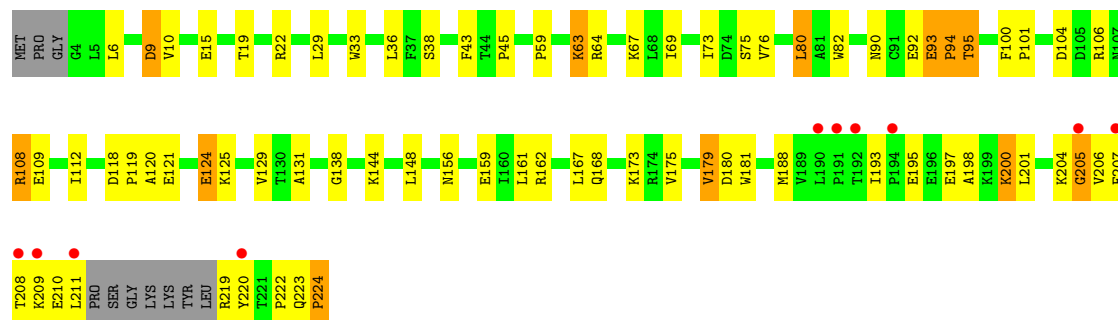
• Molecule 1: Peroxiredoxin-6

Chain B: 



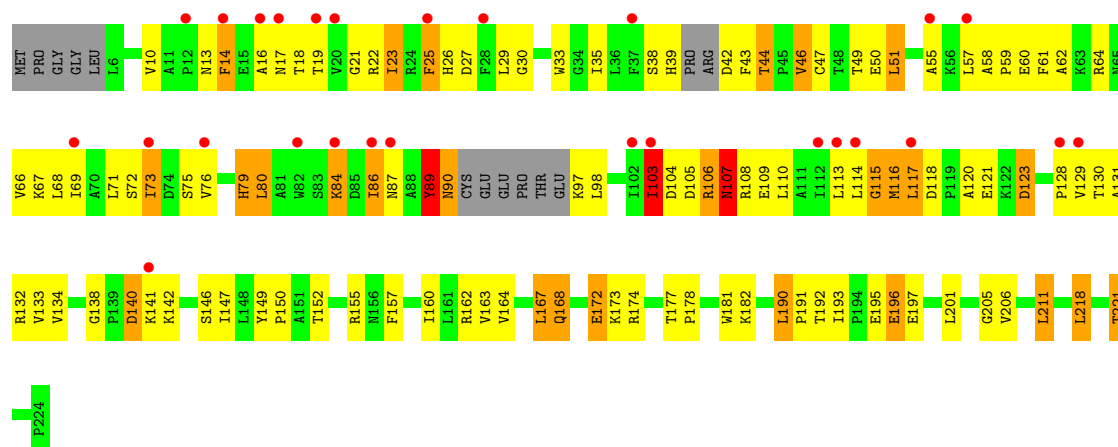
• Molecule 1: Peroxiredoxin-6

Chain C: 

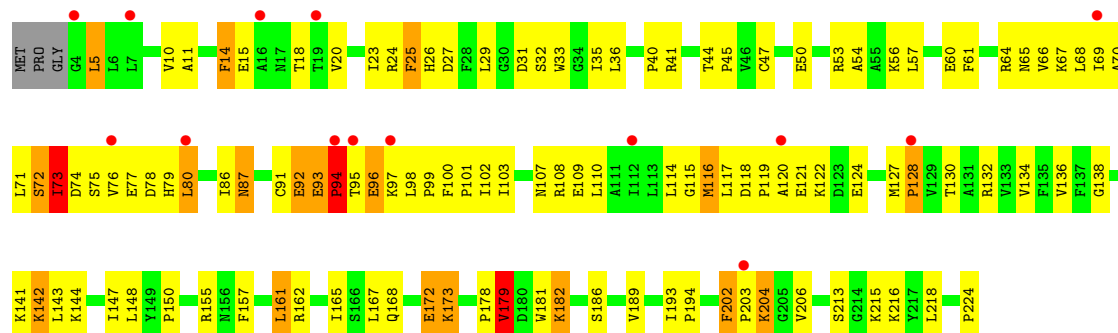


• Molecule 1: Peroxiredoxin-6

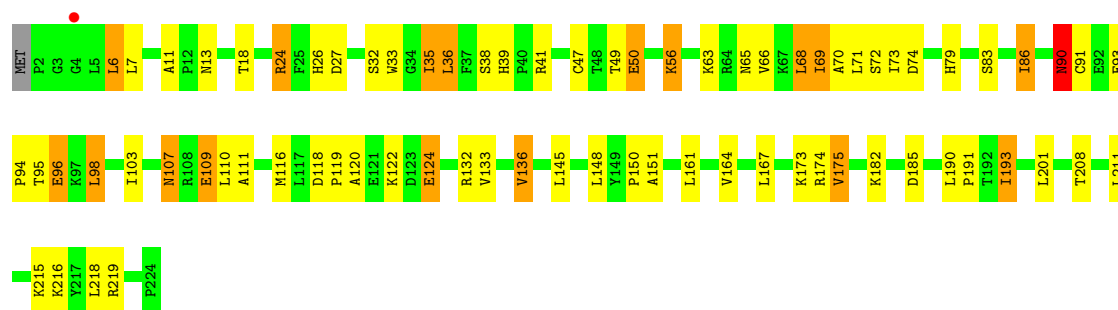
Chain D: 



• Molecule 1: Peroxiredoxin-6



• Molecule 1: Peroxiredoxin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.35Å 106.35Å 165.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.89 – 2.50 37.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (37.89-2.50) 98.7 (37.89-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.233 , 0.290 0.237 , 0.238	Depositor DCC
R_{free} test set	2926 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.3	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	0.94	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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	0.59	0/1789	0.98	4/2428 (0.2%)
1	B	0.64	0/1789	1.03	9/2428 (0.4%)
1	C	0.61	1/1731 (0.1%)	1.18	18/2349 (0.8%)
1	D	0.49	0/1708	1.43	29/2314 (1.3%)
1	E	0.64	1/1789 (0.1%)	1.35	23/2428 (0.9%)
1	F	0.56	0/1801	1.02	7/2444 (0.3%)
All	All	0.59	2/10607 (0.0%)	1.17	90/14391 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	94	PRO	N-CD	-14.68	1.27	1.47
1	C	224	PRO	N-CD	5.57	1.55	1.47

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	LEU	CB-CA-C	-19.23	80.06	111.02
1	E	172	GLU	N-CA-C	17.02	131.56	111.82
1	E	120	ALA	N-CA-C	16.60	132.11	111.69
1	E	94	PRO	N-CA-CB	-15.91	85.09	102.60
1	D	195	GLU	N-CA-C	15.15	129.13	111.71
1	E	93	GLU	CB-CA-C	-12.66	90.35	109.97
1	C	120	ALA	N-CA-CB	-12.59	93.17	110.67
1	D	114	LEU	N-CA-C	12.41	127.73	112.59
1	D	115	GLY	N-CA-C	12.33	133.05	115.30
1	D	120	ALA	N-CA-C	12.05	125.57	111.11
1	E	93	GLU	N-CA-C	11.73	121.86	108.25
1	D	103	ILE	CB-CA-C	-11.58	95.51	111.49
1	C	119	PRO	N-CA-C	11.54	128.86	113.98
1	D	109	GLU	N-CA-C	11.03	125.26	111.69
1	E	172	GLU	CB-CA-C	-10.35	90.80	110.67
1	E	94	PRO	CA-N-CD	10.24	125.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	GLU	N-CA-C	10.07	124.91	112.23
1	C	109	GLU	N-CA-CB	9.91	127.23	110.49
1	E	72	SER	N-CA-C	9.70	125.77	113.55
1	D	117	LEU	CB-CA-C	9.53	121.52	109.80
1	B	109	GLU	N-CA-C	9.30	121.50	111.36
1	E	94	PRO	N-CD-CG	-9.18	92.79	103.80
1	D	196	GLU	N-CA-C	-8.96	101.92	113.12
1	C	206	VAL	N-CA-C	8.87	127.79	109.34
1	D	43	PHE	CB-CA-C	-8.74	99.04	111.80
1	C	205	GLY	N-CA-C	-8.62	99.41	112.60
1	D	109	GLU	N-CA-CB	-8.54	97.48	110.20
1	C	206	VAL	N-CA-CB	-8.42	97.34	111.23
1	D	107	ASN	N-CA-C	-8.41	97.56	110.10
1	C	223	GLN	N-CA-C	-8.35	99.04	109.64
1	F	109	GLU	N-CA-C	8.29	121.06	111.11
1	D	195	GLU	CB-CA-C	-8.10	95.65	110.63
1	E	120	ALA	CB-CA-C	-7.92	96.20	110.70
1	C	109	GLU	N-CA-C	-7.86	94.05	110.80
1	F	110	LEU	N-CA-C	-7.72	103.99	113.41
1	C	108	ARG	N-CA-C	-7.71	94.39	110.80
1	D	172	GLU	CB-CA-C	-7.66	94.75	110.38
1	D	104	ASP	N-CA-C	7.47	121.66	109.85
1	D	90	ASN	N-CA-CB	-7.43	97.86	110.50
1	B	110	LEU	N-CA-C	-7.35	103.27	112.90
1	E	97	LYS	CB-CA-C	-7.33	99.60	110.16
1	D	104	ASP	N-CA-CB	-7.21	99.53	111.20
1	D	55	ALA	N-CA-C	7.14	120.89	111.75
1	E	202	PHE	CA-C-N	7.12	126.64	119.24
1	E	202	PHE	C-N-CA	7.12	126.64	119.24
1	E	92	GLU	N-CA-C	-7.11	98.46	109.76
1	F	109	GLU	CB-CA-C	-7.08	99.48	110.81
1	E	173	LYS	N-CA-C	-7.06	98.43	109.72
1	F	90	ASN	N-CA-C	6.97	121.23	113.21
1	C	223	GLN	CB-CA-C	6.88	120.38	109.52
1	D	107	ASN	CB-CA-C	6.84	120.57	109.90
1	C	193	ILE	N-CA-C	6.82	115.63	108.95
1	E	127	MET	CA-C-N	6.57	128.05	119.84
1	E	127	MET	C-N-CA	6.57	128.05	119.84
1	D	25	PHE	CB-CA-C	-6.54	98.28	109.65
1	B	109	GLU	CB-CA-C	-6.52	99.76	110.85
1	D	44	THR	N-CA-C	-6.45	100.27	109.62
1	C	100	PHE	CA-C-N	-6.44	113.64	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	PHE	C-N-CA	-6.44	113.64	120.66
1	E	203	PRO	CB-CA-C	-6.35	102.46	113.20
1	C	93	GLU	CA-C-N	6.28	127.69	119.84
1	C	93	GLU	C-N-CA	6.28	127.69	119.84
1	A	193	ILE	CA-C-N	6.27	126.63	119.92
1	A	193	ILE	C-N-CA	6.27	126.63	119.92
1	E	124	GLU	N-CA-C	6.21	124.04	110.80
1	D	142	LYS	N-CA-CB	6.16	121.60	111.62
1	B	132	ARG	N-CA-C	5.89	118.77	108.52
1	D	173	LYS	N-CA-C	-5.85	100.36	109.72
1	E	94	PRO	N-CA-C	5.82	127.24	112.10
1	D	89	TYR	N-CA-C	-5.72	98.57	108.52
1	D	55	ALA	CB-CA-C	-5.68	99.45	110.46
1	B	131	ALA	CB-CA-C	-5.65	100.69	111.48
1	D	120	ALA	CB-CA-C	-5.64	101.78	110.81
1	C	222	PRO	CB-CA-C	5.63	120.08	111.40
1	B	179	VAL	CB-CA-C	-5.58	102.89	111.71
1	D	117	LEU	N-CA-C	-5.54	102.43	110.64
1	F	175	VAL	N-CA-CB	5.47	119.99	110.96
1	E	204	LYS	N-CA-CB	5.40	119.32	110.90
1	F	91	CYS	N-CA-C	5.39	118.87	111.54
1	D	79	HIS	N-CA-C	-5.38	105.33	111.14
1	C	120	ALA	CB-CA-C	-5.28	100.21	109.07
1	B	93	GLU	CA-C-N	5.25	126.40	119.84
1	B	93	GLU	C-N-CA	5.25	126.40	119.84
1	F	174	ARG	N-CA-C	-5.21	99.70	110.80
1	E	179	VAL	CB-CA-C	-5.20	102.93	111.51
1	E	96	GLU	CB-CA-C	-5.18	100.21	110.27
1	C	120	ALA	N-CA-C	5.16	120.58	113.97
1	A	177	THR	CA-C-N	5.09	125.10	120.21
1	A	177	THR	C-N-CA	5.09	125.10	120.21
1	B	41	ARG	N-CA-C	5.00	116.01	108.46

There are no chirality outliers.

There are no planarity outliers.

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	1747	0	1778	35	0
1	B	1747	0	1778	36	0
1	C	1692	0	1716	44	0
1	D	1670	0	1705	83	0
1	E	1747	0	1778	79	0
1	F	1758	0	1789	48	0
2	A	23	0	0	0	0
2	B	31	0	0	0	0
2	C	18	0	0	1	0
2	D	10	0	0	0	0
2	E	20	0	0	1	0
2	F	22	0	0	1	0
All	All	10485	0	10544	303	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 14.

All (303) 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:D:89:TYR:O	1:D:89:TYR:CD2	1.90	1.25
1:E:80:LEU:HG	1:E:96:GLU:OE2	1.64	0.97
1:E:80:LEU:O	1:E:96:GLU:HG2	1.72	0.89
1:A:50:GLU:HG2	1:B:179:VAL:HG13	1.52	0.88
1:D:105:ASP:O	1:D:107:ASN:O	1.92	0.87
1:C:204:LYS:HG3	1:C:205:GLY:O	1.76	0.84
1:F:47:CYS:SG	1:F:132:ARG:NH2	2.53	0.82
1:A:7:LEU:HD13	1:B:148:LEU:HD13	1.63	0.80
1:B:69:ILE:HG13	1:B:101:PRO:HG2	1.63	0.79
1:D:89:TYR:O	1:D:89:TYR:HD2	1.61	0.75
1:D:18:THR:OG1	1:D:19:THR:N	2.13	0.75
1:E:87:ASN:O	1:E:92:GLU:O	2.05	0.75
1:E:80:LEU:HG	1:E:96:GLU:CD	2.13	0.73
1:A:7:LEU:HB3	1:B:119:PRO:HD3	1.70	0.72
1:C:207:PHE:HB2	1:C:220:TYR:HB2	1.71	0.72
1:D:89:TYR:O	1:D:89:TYR:CG	2.43	0.72
1:E:91:CYS:O	1:E:93:GLU:OE1	2.09	0.70
1:E:172:GLU:O	1:E:172:GLU:OE2	2.09	0.69
1:B:208:THR:HB	1:B:219:ARG:HG2	1.75	0.68
1:C:197:GLU:HG2	1:C:201:LEU:HB2	1.78	0.65
1:E:5:LEU:HD12	1:E:114:LEU:HD22	1.78	0.65
1:E:93:GLU:OE1	1:E:93:GLU:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:HIS:HB2	1:D:47:CYS:SG	2.37	0.64
1:E:93:GLU:HB2	1:E:94:PRO:HB3	1.78	0.64
1:F:36:LEU:HD23	1:F:69:ILE:HG23	1.80	0.64
1:B:73:ILE:HG21	1:B:108:ARG:CZ	2.27	0.63
1:E:80:LEU:CG	1:E:96:GLU:OE2	2.44	0.63
1:C:121:GLU:O	1:C:129:VAL:HG22	1.99	0.62
1:E:95:THR:OG1	1:E:96:GLU:N	2.30	0.62
1:C:219:ARG:N	2:C:301:HOH:O	2.33	0.61
1:D:16:ALA:H	1:D:23:ILE:HD11	1.65	0.61
1:E:115:GLY:HA3	1:F:6:LEU:HD11	1.82	0.61
1:C:179:VAL:HG13	1:D:50:GLU:HG2	1.82	0.61
1:D:163:VAL:O	1:D:167:LEU:HG	2.00	0.61
1:A:56:LYS:HE2	1:A:90:ASN:HB2	1.83	0.61
1:E:11:ALA:O	1:E:26:HIS:NE2	2.31	0.61
1:D:46:VAL:HB	1:D:132:ARG:HH22	1.65	0.61
1:D:89:TYR:O	1:D:90:ASN:O	2.19	0.61
1:E:150:PRO:HG3	1:F:167:LEU:HD21	1.83	0.61
1:D:13:ASN:HB2	1:D:26:HIS:CE1	2.36	0.60
1:E:167:LEU:HD21	1:F:150:PRO:HG3	1.83	0.60
1:A:148:LEU:HD22	1:B:7:LEU:HG	1.84	0.60
1:D:61:PHE:HB3	1:D:66:VAL:HB	1.84	0.60
1:C:173:LYS:HG3	1:C:224:PRO:HB2	1.83	0.60
1:A:32:SER:HB3	1:A:65:ASN:OD1	2.02	0.59
1:B:36:LEU:HD23	1:B:69:ILE:HG23	1.84	0.59
1:E:33:TRP:CZ3	1:E:144:LYS:HG3	2.37	0.59
1:E:33:TRP:HZ3	1:E:144:LYS:HG3	1.68	0.59
1:A:41:ARG:O	1:A:44:THR:OG1	2.19	0.58
1:E:5:LEU:HD22	1:E:143:LEU:HD22	1.85	0.58
1:D:130:THR:OG1	1:D:131:ALA:N	2.36	0.58
1:B:196:GLU:HA	1:B:199:LYS:HD2	1.86	0.58
1:B:63:LYS:HG3	1:B:64:ARG:HG3	1.85	0.58
1:D:58:ALA:N	1:D:59:PRO:HD2	2.18	0.58
1:E:79:HIS:HB3	1:E:102:ILE:HD12	1.85	0.58
1:E:69:ILE:HG13	1:E:101:PRO:HG2	1.85	0.57
1:D:57:LEU:HD22	1:D:60:GLU:HG3	1.86	0.57
1:E:41:ARG:NH2	1:E:74:ASP:OD1	2.30	0.57
1:E:71:LEU:HD22	1:E:116:MET:HE2	1.87	0.57
1:B:38:SER:OG	1:B:133:VAL:HG12	2.04	0.57
1:D:105:ASP:C	1:D:107:ASN:O	2.48	0.57
1:B:38:SER:OG	1:B:131:ALA:O	2.23	0.56
1:D:205:GLY:O	1:D:221:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ARG:HD2	1:D:181:TRP:O	2.05	0.56
1:F:182:LYS:NZ	1:F:185:ASP:OD2	2.27	0.56
1:C:179:VAL:O	1:C:180:ASP:C	2.48	0.56
1:D:118:ASP:HB2	1:D:131:ALA:HB2	1.87	0.56
1:D:132:ARG:C	1:D:155:ARG:HH12	2.13	0.56
1:E:24:ARG:HB2	1:E:27:ASP:HB2	1.87	0.56
1:D:72:SER:HB3	1:D:79:HIS:NE2	2.20	0.56
1:B:209:LYS:HB3	1:B:218:LEU:HD23	1.87	0.55
1:F:193:ILE:O	1:F:219:ARG:NH2	2.39	0.55
1:B:50:GLU:OE1	1:B:132:ARG:NH1	2.40	0.55
1:D:39:HIS:CD2	1:D:72:SER:HB2	2.42	0.55
1:B:32:SER:HB3	1:B:65:ASN:OD1	2.06	0.55
1:C:73:ILE:HG12	1:C:129:VAL:HG12	1.88	0.55
1:D:160:ILE:O	1:D:164:VAL:HG23	2.07	0.55
1:A:35:ILE:HB	1:A:68:LEU:HD12	1.89	0.55
1:A:193:ILE:HD11	1:A:198:ALA:HA	1.89	0.55
1:C:108:ARG:O	1:C:112:ILE:HD12	2.05	0.55
1:D:57:LEU:O	1:D:61:PHE:CD2	2.60	0.55
1:E:93:GLU:O	1:E:93:GLU:HG2	2.05	0.55
1:E:136:VAL:HG23	1:E:144:LYS:HB2	1.89	0.54
1:E:179:VAL:HG13	1:F:50:GLU:HG3	1.89	0.54
1:C:90:ASN:O	1:C:92:GLU:HG3	2.08	0.54
1:E:54:ALA:HB2	1:E:157:PHE:CE1	2.44	0.53
1:E:134:VAL:HB	1:E:147:ILE:HG12	1.90	0.53
1:F:41:ARG:NH2	1:F:124:GLU:OE1	2.39	0.53
1:D:25:PHE:CG	1:D:25:PHE:O	2.61	0.53
1:D:177:THR:HB	1:D:181:TRP:CG	2.43	0.53
1:D:164:VAL:HA	1:D:167:LEU:HD11	1.89	0.53
1:F:56:LYS:NZ	1:F:90:ASN:HB2	2.23	0.53
1:D:178:PRO:HD2	1:D:181:TRP:HB2	1.92	0.52
1:B:33:TRP:HB2	1:B:66:VAL:HG22	1.90	0.51
1:F:35:ILE:HB	1:F:68:LEU:HD12	1.92	0.51
1:C:175:VAL:HG11	1:C:224:PRO:HG2	1.92	0.51
1:C:179:VAL:HG11	1:D:50:GLU:HA	1.92	0.51
1:E:70:ALA:HB2	1:E:100:PHE:HE1	1.76	0.51
1:E:189:VAL:HG22	1:E:202:PHE:CE2	2.46	0.51
1:C:33:TRP:CD1	1:C:168:GLN:HE21	2.29	0.50
1:C:208:THR:HG22	1:C:209:LYS:H	1.75	0.50
1:A:46:VAL:HG13	1:B:178:PRO:HA	1.92	0.50
1:E:178:PRO:HD2	1:E:181:TRP:HB2	1.94	0.50
1:A:173:LYS:HD3	1:A:224:PRO:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LYS:HB2	1:E:142:LYS:NZ	2.26	0.50
1:F:38:SER:HB3	1:F:116:MET:HE2	1.93	0.50
1:A:204:LYS:H	1:A:204:LYS:HZ2	1.58	0.50
1:E:75:SER:O	1:E:78:ASP:HB2	2.12	0.50
1:E:40:PRO:HG2	1:E:47:CYS:SG	2.52	0.50
1:F:11:ALA:O	1:F:26:HIS:NE2	2.29	0.50
1:C:118:ASP:HB2	1:C:131:ALA:HB2	1.94	0.50
1:A:211:LEU:O	1:A:214:GLY:N	2.31	0.49
1:E:45:PRO:HD2	1:F:191:PRO:HG3	1.94	0.49
1:B:196:GLU:O	1:B:200:LYS:HG2	2.11	0.49
1:C:208:THR:HG23	1:C:219:ARG:HG3	1.94	0.49
1:D:39:HIS:NE2	1:D:72:SER:HB2	2.27	0.49
1:E:31:ASP:H	1:E:141:LYS:HZ1	1.60	0.49
1:F:41:ARG:HH22	1:F:124:GLU:CD	2.19	0.49
1:A:33:TRP:HB2	1:A:66:VAL:HG22	1.94	0.49
1:C:162:ARG:HD2	1:C:181:TRP:O	2.12	0.49
1:C:138:GLY:HA3	1:C:144:LYS:HE3	1.94	0.49
1:E:41:ARG:HB3	1:E:44:THR:OG1	2.13	0.49
1:F:27:ASP:HB3	2:F:308:HOH:O	2.13	0.49
1:F:132:ARG:NH1	1:F:151:ALA:O	2.41	0.49
1:B:32:SER:HB3	1:B:65:ASN:CG	2.38	0.49
1:E:32:SER:OG	1:E:65:ASN:OD1	2.21	0.49
1:E:161:LEU:O	1:E:165:ILE:HG12	2.13	0.49
1:D:123:ASP:OD2	1:D:123:ASP:N	2.46	0.49
1:F:107:ASN:OD1	1:F:107:ASN:N	2.46	0.49
1:A:50:GLU:OE1	1:A:132:ARG:NH1	2.42	0.48
1:B:45:PRO:O	1:B:49:THR:HG23	2.14	0.48
1:E:70:ALA:O	1:E:103:ILE:N	2.40	0.48
1:B:70:ALA:HB3	1:B:102:ILE:HG12	1.96	0.48
1:E:93:GLU:HB2	1:E:94:PRO:CB	2.42	0.48
1:F:83:SER:HB2	1:F:96:GLU:HA	1.95	0.48
1:C:45:PRO:HD2	1:D:191:PRO:HG3	1.95	0.48
1:D:14:PHE:CZ	1:D:25:PHE:HB2	2.49	0.48
1:F:56:LYS:HZ2	1:F:90:ASN:HB2	1.79	0.48
1:D:134:VAL:HB	1:D:147:ILE:HB	1.95	0.48
1:E:60:GLU:HB3	1:E:161:LEU:HD11	1.96	0.48
1:B:108:ARG:NH1	1:B:127:MET:HE2	2.29	0.48
1:D:141:LYS:O	1:D:141:LYS:HG2	2.13	0.47
1:F:72:SER:HB3	1:F:79:HIS:CE1	2.49	0.47
1:E:40:PRO:HA	1:E:130:THR:HG23	1.97	0.47
1:D:174:ARG:C	1:D:190:LEU:HD22	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:HA	1:A:23:ILE:O	2.14	0.47
1:A:119:PRO:HD3	1:B:7:LEU:HB3	1.97	0.47
1:C:179:VAL:HB	1:C:180:ASP:OD1	2.15	0.47
1:E:182:LYS:HB2	1:E:182:LYS:HE3	1.72	0.47
1:D:115:GLY:C	1:D:117:LEU:H	2.23	0.46
1:E:107:ASN:HB2	1:E:109:GLU:HG3	1.97	0.46
1:D:16:ALA:H	1:D:23:ILE:CD1	2.27	0.46
1:E:122:LYS:HA	1:E:128:PRO:HA	1.97	0.46
1:B:83:SER:HB3	1:B:98:LEU:HD13	1.97	0.46
1:D:84:LYS:HZ1	1:D:97:LYS:N	2.13	0.46
1:C:43:PHE:H	1:C:82:TRP:CD1	2.34	0.46
1:E:179:VAL:CG1	1:F:50:GLU:HA	2.45	0.46
1:D:44:THR:OG1	1:D:47:CYS:SG	2.72	0.46
1:D:138:GLY:C	1:D:140:ASP:H	2.23	0.46
1:D:33:TRP:HB2	1:D:66:VAL:HG22	1.98	0.46
1:E:41:ARG:HE	1:E:74:ASP:CG	2.24	0.46
1:F:13:ASN:OD1	1:F:24:ARG:HG2	2.16	0.46
1:C:93:GLU:HA	1:C:94:PRO:HD3	1.74	0.45
1:E:179:VAL:CG1	1:F:50:GLU:HG3	2.46	0.45
1:C:93:GLU:O	1:C:95:THR:HG23	2.16	0.45
1:F:18:THR:HG22	1:F:103:ILE:HA	1.99	0.45
1:F:41:ARG:HD2	1:F:74:ASP:OD2	2.16	0.45
1:F:182:LYS:HB2	1:F:182:LYS:HE2	1.61	0.45
1:D:121:GLU:O	1:D:129:VAL:HG11	2.16	0.45
1:E:56:LYS:NZ	2:E:301:HOH:O	2.40	0.45
1:B:25:PHE:CZ	1:B:29:LEU:HD21	2.52	0.45
1:D:38:SER:OG	1:D:39:HIS:N	2.49	0.45
1:F:72:SER:HB3	1:F:79:HIS:HE1	1.81	0.45
1:A:43:PHE:H	1:A:82:TRP:CD1	2.34	0.45
1:C:45:PRO:CD	1:D:191:PRO:HG3	2.46	0.45
1:D:76:VAL:HA	1:D:79:HIS:HB2	1.99	0.45
1:D:50:GLU:OE2	1:D:132:ARG:NE	2.47	0.45
1:B:82:TRP:O	1:B:86:ILE:HG12	2.16	0.45
1:D:17:ASN:HB2	1:D:106:ARG:NH2	2.32	0.45
1:D:27:ASP:HA	1:D:30:GLY:HA2	1.99	0.45
1:D:108:ARG:HG2	1:D:128:PRO:HG2	1.98	0.45
1:E:68:LEU:O	1:E:100:PHE:HB2	2.16	0.45
1:E:98:LEU:HA	1:E:99:PRO:HD3	1.78	0.44
1:E:73:ILE:HD13	1:E:73:ILE:O	2.17	0.44
1:F:35:ILE:HD13	1:F:136:VAL:HG12	1.98	0.44
1:C:15:GLU:HB3	1:C:22:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD12	1:C:80:LEU:HA	1.83	0.44
1:E:71:LEU:HA	1:E:103:ILE:HB	1.99	0.44
1:E:119:PRO:HD3	1:F:7:LEU:HB3	1.99	0.44
1:E:162:ARG:HD2	1:E:181:TRP:O	2.17	0.44
1:C:69:ILE:HD12	1:C:101:PRO:HG2	1.99	0.44
1:C:200:LYS:HZ3	1:C:201:LEU:N	2.16	0.44
1:E:61:PHE:HB3	1:E:66:VAL:HB	1.99	0.44
1:D:211:LEU:HD21	1:D:218:LEU:HB2	1.99	0.44
1:E:108:ARG:NH1	1:E:128:PRO:O	2.50	0.44
1:F:39:HIS:HB2	1:F:47:CYS:SG	2.58	0.44
1:F:32:SER:HB3	1:F:65:ASN:OD1	2.17	0.44
1:F:111:ALA:HA	1:F:116:MET:HG2	1.99	0.44
1:D:22:ARG:HB2	1:D:22:ARG:CZ	2.47	0.44
1:E:213:SER:C	1:E:215:LYS:H	2.25	0.44
1:B:147:ILE:HD12	1:B:149:TYR:CE1	2.53	0.44
1:D:110:LEU:HD12	1:D:110:LEU:HA	1.86	0.44
1:D:116:MET:O	1:D:117:LEU:C	2.61	0.44
1:F:32:SER:HA	1:F:65:ASN:HD21	1.82	0.44
1:F:136:VAL:HG22	1:F:145:LEU:HB3	1.99	0.43
1:B:138:GLY:HA3	1:B:144:LYS:HE2	2.00	0.43
1:D:71:LEU:HD23	1:D:103:ILE:O	2.18	0.43
1:A:173:LYS:HD3	1:A:224:PRO:CB	2.48	0.43
1:B:98:LEU:C	1:B:100:PHE:H	2.27	0.43
1:C:75:SER:HA	1:C:106:ARG:HD2	2.01	0.43
1:E:93:GLU:HB2	1:E:94:PRO:CA	2.48	0.43
1:E:122:LYS:HE2	1:E:128:PRO:HG3	1.99	0.43
1:C:124:GLU:OE2	1:C:125:LYS:HE3	2.18	0.43
1:E:72:SER:O	1:E:73:ILE:HG22	2.18	0.43
1:A:104:ASP:OD1	1:A:106:ARG:HD3	2.18	0.43
1:D:51:LEU:HB2	1:D:86:ILE:HG21	2.00	0.43
1:D:132:ARG:HB2	1:D:149:TYR:O	2.18	0.43
1:D:33:TRP:O	1:D:66:VAL:HA	2.18	0.43
1:E:173:LYS:HG2	1:E:224:PRO:HG2	2.00	0.43
1:F:70:ALA:O	1:F:103:ILE:N	2.51	0.43
1:B:33:TRP:CD1	1:B:168:GLN:HE21	2.36	0.43
1:B:147:ILE:HD11	1:B:155:ARG:HG2	2.01	0.43
1:C:104:ASP:OD1	1:C:106:ARG:HD3	2.19	0.43
1:E:33:TRP:CE3	1:E:138:GLY:HA2	2.54	0.43
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.79	0.43
1:A:121:GLU:HG3	1:A:151:ALA:HB3	2.00	0.42
1:C:195:GLU:HA	1:C:198:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:TRP:CE3	1:D:138:GLY:HA2	2.53	0.42
1:F:33:TRP:HB2	1:F:66:VAL:HG22	2.00	0.42
1:A:93:GLU:HA	1:A:94:PRO:HD3	1.83	0.42
1:A:199:LYS:H	1:A:199:LYS:HG3	1.63	0.42
1:C:6:LEU:HD23	1:D:117:LEU:HB3	2.00	0.42
1:F:118:ASP:OD2	1:F:119:PRO:HD2	2.19	0.42
1:B:15:GLU:HG3	1:B:24:ARG:HD2	2.01	0.42
1:B:194:PRO:HD2	1:B:197:GLU:HB3	2.00	0.42
1:D:87:ASN:HD22	1:D:98:LEU:HD13	1.83	0.42
1:A:15:GLU:HB2	1:A:24:ARG:HD3	2.01	0.42
1:C:38:SER:OG	1:C:131:ALA:O	2.32	0.42
1:E:50:GLU:OE1	1:E:132:ARG:NH1	2.53	0.42
1:C:93:GLU:H	1:C:93:GLU:HG3	1.53	0.42
1:E:25:PHE:CE2	1:E:29:LEU:HD11	2.54	0.42
1:A:127:MET:HA	1:A:128:PRO:HD3	1.89	0.42
1:C:167:LEU:HD21	1:D:150:PRO:HG3	2.02	0.42
1:E:61:PHE:CD2	1:E:68:LEU:HD21	2.55	0.42
1:E:71:LEU:HD12	1:E:103:ILE:HG21	1.99	0.42
1:D:14:PHE:CE1	1:D:25:PHE:HB2	2.54	0.42
1:D:18:THR:HB	1:D:103:ILE:HG23	2.02	0.42
1:F:93:GLU:HA	1:F:94:PRO:HD3	1.81	0.42
1:D:35:ILE:HD11	1:D:164:VAL:HG21	2.00	0.42
1:D:58:ALA:N	1:D:59:PRO:CD	2.83	0.42
1:E:118:ASP:OD1	1:E:119:PRO:HD2	2.20	0.42
1:A:121:GLU:HG3	1:A:151:ALA:CB	2.50	0.42
1:C:209:LYS:HD2	1:C:209:LYS:HA	1.89	0.42
1:E:132:ARG:O	1:E:155:ARG:HD3	2.19	0.42
1:F:173:LYS:O	1:F:175:VAL:N	2.53	0.42
1:C:19:THR:HG22	1:C:80:LEU:HD13	2.02	0.41
1:C:59:PRO:O	1:C:63:LYS:HB3	2.19	0.41
1:D:18:THR:HG22	1:D:21:GLY:O	2.19	0.41
1:A:68:LEU:O	1:A:100:PHE:HB2	2.20	0.41
1:A:193:ILE:HA	1:A:194:PRO:HD3	1.72	0.41
1:B:73:ILE:O	1:B:73:ILE:HG22	2.20	0.41
1:D:164:VAL:O	1:D:168:GLN:HB2	2.20	0.41
1:A:195:GLU:O	1:A:199:LYS:HG3	2.20	0.41
1:F:6:LEU:HD12	1:F:6:LEU:HA	1.83	0.41
1:A:121:GLU:HB3	1:A:129:VAL:HG22	2.03	0.41
1:C:156:ASN:O	1:C:159:GLU:HB3	2.20	0.41
1:E:57:LEU:O	1:E:60:GLU:N	2.38	0.41
1:E:193:ILE:HA	1:E:194:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB3	1:A:222:PRO:HG2	2.02	0.41
1:B:174:ARG:HB3	1:B:190:LEU:HD12	2.02	0.41
1:E:64:ARG:HB3	1:E:168:GLN:HE22	1.84	0.41
1:F:120:ALA:O	1:F:122:LYS:HG3	2.20	0.41
1:C:179:VAL:CG1	1:D:50:GLU:HA	2.51	0.41
1:E:14:PHE:CD2	1:E:110:LEU:HD21	2.56	0.41
1:D:62:ALA:C	1:D:64:ARG:H	2.29	0.41
1:D:89:TYR:O	1:D:90:ASN:C	2.64	0.41
1:D:190:LEU:HD12	1:D:190:LEU:HA	1.95	0.41
1:E:24:ARG:NE	1:E:24:ARG:H	2.19	0.41
1:E:53:ARG:HD2	1:E:53:ARG:HA	1.82	0.41
1:F:215:LYS:HG2	1:F:216:LYS:H	1.85	0.41
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.60	0.41
1:D:73:ILE:HD11	1:D:130:THR:HG22	2.02	0.41
1:D:73:ILE:O	1:D:106:ARG:HA	2.21	0.41
1:A:124:GLU:CD	1:A:124:GLU:H	2.28	0.41
1:E:60:GLU:O	1:E:64:ARG:HD3	2.21	0.41
1:A:39:HIS:CE1	1:A:72:SER:HB2	2.56	0.40
1:D:76:VAL:HG22	1:D:80:LEU:HD13	2.02	0.40
1:D:193:ILE:H	1:D:193:ILE:HG13	1.69	0.40
1:E:15:GLU:HA	1:E:23:ILE:O	2.22	0.40
1:A:15:GLU:HB2	1:A:24:ARG:NH1	2.36	0.40
1:D:61:PHE:CG	1:D:68:LEU:HD11	2.56	0.40
1:F:56:LYS:HD2	1:F:56:LYS:HA	1.91	0.40
1:A:162:ARG:HD2	1:A:181:TRP:O	2.21	0.40
1:C:63:LYS:HG2	1:C:64:ARG:HG3	2.03	0.40
1:D:190:LEU:HA	1:D:191:PRO:HD3	1.96	0.40
1:E:179:VAL:HG22	1:F:49:THR:OG1	2.22	0.40
1:C:6:LEU:O	1:C:9:ASP:HB2	2.22	0.40
1:D:13:ASN:ND2	1:D:26:HIS:H	2.20	0.40
1:D:157:PHE:HA	1:D:160:ILE:HG12	2.03	0.40
1:F:39:HIS:CE1	1:F:72:SER:HB2	2.57	0.40
1:F:71:LEU:HA	1:F:103:ILE:HB	2.02	0.40
1:F:86:ILE:HD11	1:F:98:LEU:CD1	2.51	0.40
1:D:75:SER:HA	1:D:106:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/224 (98%)	201 (92%)	17 (8%)	1 (0%)	24	43
1	B	219/224 (98%)	201 (92%)	18 (8%)	0	100	100
1	C	210/224 (94%)	186 (89%)	23 (11%)	1 (0%)	24	43
1	D	205/224 (92%)	181 (88%)	24 (12%)	0	100	100
1	E	219/224 (98%)	185 (84%)	30 (14%)	4 (2%)	6	12
1	F	221/224 (99%)	200 (90%)	20 (9%)	1 (0%)	24	43
All	All	1293/1344 (96%)	1154 (89%)	132 (10%)	7 (0%)	24	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	73	ILE
1	A	19	THR
1	E	25	PHE
1	E	128	PRO
1	C	94	PRO
1	F	73	ILE
1	E	94	PRO

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	192/194 (99%)	174 (91%)	18 (9%)	8	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	192/194 (99%)	173 (90%)	19 (10%)	7	16
1	C	186/194 (96%)	169 (91%)	17 (9%)	9	19
1	D	183/194 (94%)	146 (80%)	37 (20%)	1	2
1	E	192/194 (99%)	165 (86%)	27 (14%)	3	7
1	F	193/194 (100%)	165 (86%)	28 (14%)	3	6
All	All	1138/1164 (98%)	992 (87%)	146 (13%)	4	9

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	15	GLU
1	A	17	ASN
1	A	18	THR
1	A	32	SER
1	A	36	LEU
1	A	53	ARG
1	A	68	LEU
1	A	76	VAL
1	A	86	ILE
1	A	144	LYS
1	A	161	LEU
1	A	173	LYS
1	A	193	ILE
1	A	200	LYS
1	A	204	LYS
1	A	209	LYS
1	A	210	GLU
1	B	23	ILE
1	B	24	ARG
1	B	29	LEU
1	B	36	LEU
1	B	76	VAL
1	B	97	LYS
1	B	98	LEU
1	B	106	ARG
1	B	113	LEU
1	B	117	LEU
1	B	125	LYS
1	B	127	MET

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	148	LEU
1	B	179	VAL
1	B	199	LYS
1	B	201	LEU
1	B	204	LYS
1	B	208	THR
1	C	9	ASP
1	C	10	VAL
1	C	29	LEU
1	C	36	LEU
1	C	63	LYS
1	C	67	LYS
1	C	76	VAL
1	C	80	LEU
1	C	95	THR
1	C	124	GLU
1	C	148	LEU
1	C	161	LEU
1	C	179	VAL
1	C	188	MET
1	C	200	LYS
1	C	210	GLU
1	C	211	LEU
1	D	10	VAL
1	D	14	PHE
1	D	23	ILE
1	D	42	ASP
1	D	46	VAL
1	D	49	THR
1	D	51	LEU
1	D	67	LYS
1	D	69	ILE
1	D	73	ILE
1	D	80	LEU
1	D	84	LYS
1	D	86	ILE
1	D	89	TYR
1	D	103	ILE
1	D	106	ARG
1	D	107	ASN
1	D	113	LEU

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Mol	Chain	Res	Type
1	D	116	MET
1	D	123	ASP
1	D	133	VAL
1	D	140	ASP
1	D	146	SER
1	D	152	THR
1	D	167	LEU
1	D	168	GLN
1	D	172	GLU
1	D	182	LYS
1	D	190	LEU
1	D	192	THR
1	D	196	GLU
1	D	197	GLU
1	D	201	LEU
1	D	206	VAL
1	D	211	LEU
1	D	218	LEU
1	D	221	THR
1	E	5	LEU
1	E	10	VAL
1	E	14	PHE
1	E	18	THR
1	E	20	VAL
1	E	35	ILE
1	E	36	LEU
1	E	67	LYS
1	E	73	ILE
1	E	76	VAL
1	E	77	GLU
1	E	80	LEU
1	E	86	ILE
1	E	87	ASN
1	E	116	MET
1	E	117	LEU
1	E	121	GLU
1	E	142	LYS
1	E	148	LEU
1	E	161	LEU
1	E	179	VAL
1	E	182	LYS
1	E	186	SER

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Mol	Chain	Res	Type
1	E	204	LYS
1	E	206	VAL
1	E	216	LYS
1	E	218	LEU
1	F	6	LEU
1	F	24	ARG
1	F	35	ILE
1	F	36	LEU
1	F	50	GLU
1	F	56	LYS
1	F	63	LYS
1	F	68	LEU
1	F	69	ILE
1	F	86	ILE
1	F	90	ASN
1	F	95	THR
1	F	96	GLU
1	F	98	LEU
1	F	107	ASN
1	F	109	GLU
1	F	124	GLU
1	F	133	VAL
1	F	136	VAL
1	F	148	LEU
1	F	161	LEU
1	F	164	VAL
1	F	190	LEU
1	F	193	ILE
1	F	201	LEU
1	F	208	THR
1	F	211	LEU
1	F	218	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	D	65	ASN
1	D	87	ASN
1	D	168	GLN
1	E	87	ASN
1	E	107	ASN

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Mol	Chain	Res	Type
1	E	168	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	221/224 (98%)	-0.44	1 (0%) 87 85	18, 34, 52, 65	0
1	B	221/224 (98%)	-0.42	0 100 100	18, 32, 60, 84	0
1	C	214/224 (95%)	-0.12	10 (4%) 36 32	17, 36, 114, 126	0
1	D	211/224 (94%)	0.72	27 (12%) 7 6	26, 81, 127, 142	0
1	E	221/224 (98%)	0.44	14 (6%) 26 23	25, 59, 98, 122	0
1	F	223/224 (99%)	-0.14	1 (0%) 88 86	20, 42, 66, 96	0
All	All	1311/1344 (97%)	-0.00	53 (4%) 42 38	17, 42, 105, 142	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	ILE	4.2
1	D	117	LEU	4.1
1	D	86	ILE	3.9
1	D	16	ALA	3.7
1	D	76	VAL	3.2
1	E	95	THR	3.2
1	D	84	LYS	3.1
1	D	25	PHE	3.1
1	E	120	ALA	3.1
1	C	208	THR	3.0
1	E	16	ALA	3.0
1	E	97	LYS	3.0
1	C	194	PRO	2.9
1	D	73	ILE	2.9
1	E	76	VAL	2.9
1	D	14	PHE	2.9
1	D	112	ILE	2.8
1	D	103	ILE	2.8
1	E	69	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	87	ASN	2.8
1	D	114	LEU	2.8
1	D	113	LEU	2.7
1	D	37	PHE	2.6
1	C	191	PRO	2.6
1	D	20	VAL	2.6
1	A	23	ILE	2.6
1	D	69	ILE	2.5
1	C	205	GLY	2.5
1	E	4	GLY	2.5
1	C	192	THR	2.5
1	D	28	PHE	2.4
1	E	19	THR	2.4
1	D	12	PRO	2.4
1	D	141	LYS	2.4
1	C	207	PHE	2.3
1	D	128	PRO	2.3
1	D	57	LEU	2.3
1	D	129	VAL	2.3
1	F	4	GLY	2.3
1	C	209	LYS	2.3
1	D	19	THR	2.2
1	C	190	LEU	2.2
1	D	82	TRP	2.2
1	D	17	ASN	2.1
1	E	128	PRO	2.1
1	E	203	PRO	2.1
1	D	55	ALA	2.1
1	E	94	PRO	2.1
1	C	211	LEU	2.0
1	C	220	TYR	2.0
1	E	7	LEU	2.0
1	E	80	LEU	2.0
1	E	112	ILE	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 [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.