



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 1A4O / pdb_00001a4o
Title : 14-3-3 PROTEIN ZETA ISOFORM
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Deposited on : 1998-02-01
Resolution : 2.80 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

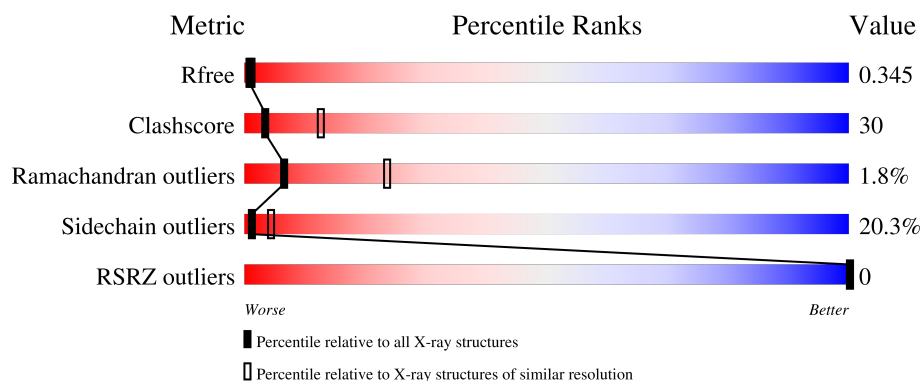
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	245	
1	B	245	
1	C	245	
1	D	245	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6360 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.

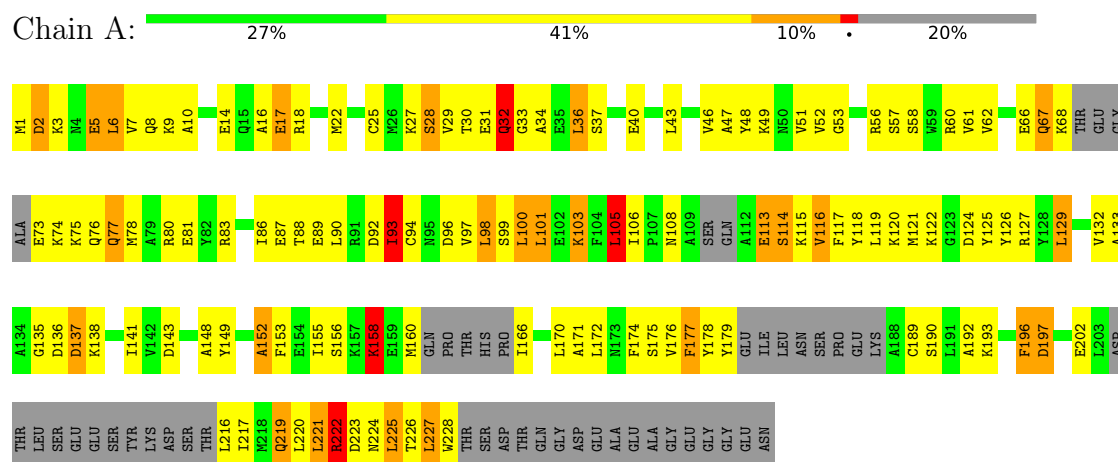
- Molecule 1 is a protein called 14-3-3 PROTEIN ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	B	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	C	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	D	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			

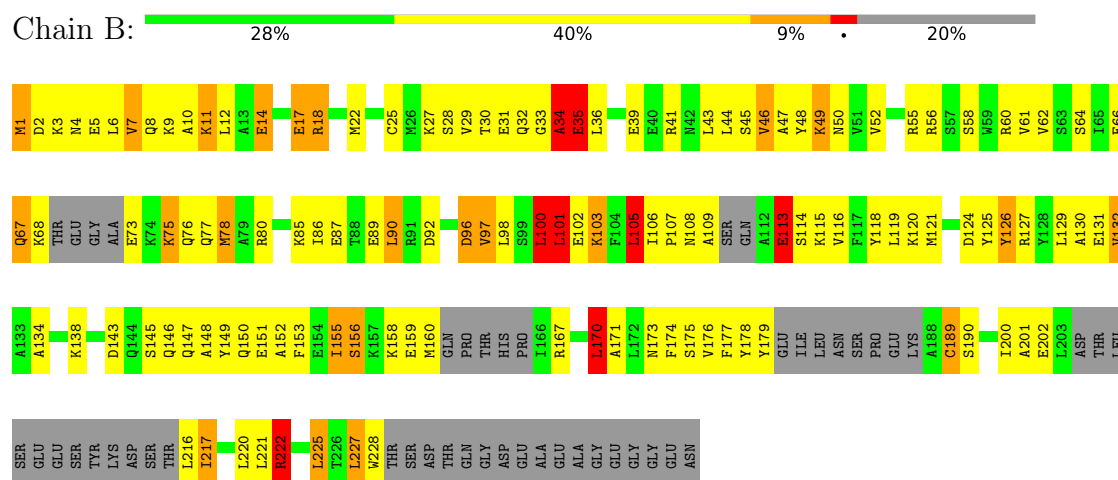
3 Residue-property plots

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.

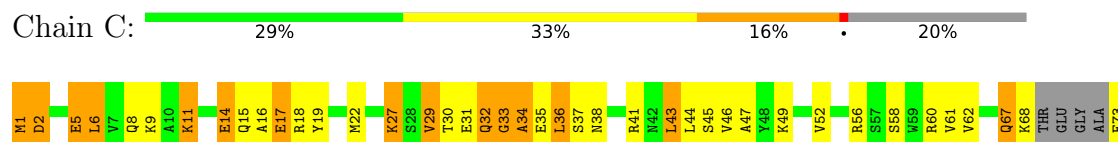
• Molecule 1: 14-3-3 PROTEIN ZETA



• Molecule 1: 14-3-3 PROTEIN ZETA



• Molecule 1: 14-3-3 PROTEIN ZETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	94.90Å 94.90Å 236.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-2.80) 97.0 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.310 , 0.345 0.317 , 0.345	Depositor DCC
R_{free} test set	2327 reflections (8.21%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.446 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.58	0/1605	1.30	21/2144 (1.0%)
1	B	0.61	0/1605	1.36	24/2144 (1.1%)
1	C	0.59	0/1605	1.32	19/2144 (0.9%)
1	D	0.60	0/1605	1.37	20/2144 (0.9%)
All	All	0.59	0/6420	1.34	84/8576 (1.0%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	GLU	N-CA-C	-10.38	99.38	113.18
1	C	5	GLU	N-CA-C	-9.56	102.12	113.88
1	A	222	ARG	N-CA-C	-9.01	101.42	111.14
1	D	64	SER	N-CA-C	-8.85	101.58	111.14
1	A	32	GLN	N-CA-C	-8.80	100.30	108.75
1	B	34	ALA	N-CA-C	8.43	128.76	110.80
1	D	177	PHE	N-CA-C	-8.24	102.30	111.28
1	C	177	PHE	N-CA-C	-8.18	102.33	111.82
1	C	137	ASP	N-CA-C	-7.96	102.55	111.07
1	B	77	GLN	N-CA-C	-7.89	102.68	111.28
1	C	152	ALA	N-CA-C	-7.86	102.79	111.36
1	A	177	PHE	N-CA-C	-7.31	103.02	112.23
1	B	201	ALA	N-CA-C	-7.29	101.54	112.54
1	A	77	GLN	N-CA-C	-7.27	103.44	111.36
1	A	226	THR	N-CA-C	-7.12	103.60	111.36
1	A	93	ILE	CB-CA-C	-7.11	102.73	112.04
1	A	5	GLU	N-CA-C	-7.07	104.79	113.41
1	D	27	LYS	N-CA-C	-7.06	103.66	111.36
1	B	202	GLU	N-CA-C	-6.93	104.49	114.12
1	B	80	ARG	N-CA-C	-6.85	103.87	111.82
1	A	75	LYS	N-CA-C	-6.74	104.78	112.87
1	D	33	GLY	N-CA-C	-6.72	100.43	110.71
1	D	77	GLN	N-CA-C	-6.63	104.13	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	GLY	N-CA-C	-6.58	97.59	113.18
1	C	27	LYS	N-CA-C	-6.58	103.38	111.40
1	D	9	LYS	N-CA-C	-6.44	103.49	112.45
1	B	103	LYS	N-CA-C	6.34	120.66	112.41
1	B	227	LEU	N-CA-C	-6.33	105.21	113.12
1	A	113	GLU	N-CA-C	-6.29	104.35	111.14
1	B	113	GLU	N-CA-C	-6.23	105.80	113.41
1	C	75	LYS	N-CA-C	-6.12	104.38	112.34
1	B	222	ARG	N-CA-C	-6.12	104.52	111.07
1	D	80	ARG	N-CA-C	-6.11	104.53	112.23
1	B	35	GLU	N-CA-C	-6.11	97.79	110.80
1	B	155	ILE	N-CA-C	-6.05	104.84	113.07
1	A	120	LYS	N-CA-C	-6.00	104.08	111.40
1	B	75	LYS	N-CA-C	-5.94	105.29	112.54
1	C	149	TYR	N-CA-C	-5.92	104.51	110.97
1	B	33	GLY	N-CA-C	-5.92	99.15	113.18
1	C	33	GLY	N-CA-C	-5.87	101.72	110.71
1	D	226	THR	N-CA-C	-5.86	105.02	111.82
1	C	34	ALA	N-CA-C	5.83	123.22	110.80
1	A	152	ALA	N-CA-C	-5.76	105.08	111.36
1	C	148	ALA	N-CA-C	-5.74	105.30	112.93
1	B	105	LEU	N-CA-C	5.66	119.81	111.04
1	D	222	ARG	N-CA-C	-5.65	105.03	111.14
1	A	137	ASP	N-CA-C	-5.61	104.38	111.11
1	B	134	ALA	N-CA-C	5.59	122.71	110.80
1	C	74	LYS	N-CA-C	-5.58	105.28	111.36
1	C	19	TYR	N-CA-C	5.57	117.43	111.36
1	D	75	LYS	N-CA-C	-5.53	105.63	112.38
1	C	103	LYS	N-CA-C	5.53	119.66	113.02
1	C	35	GLU	N-CA-C	-5.52	104.45	110.91
1	D	117	PHE	N-CA-C	-5.51	104.97	110.97
1	D	103	LYS	N-CA-C	5.49	119.97	113.28
1	B	6	LEU	N-CA-C	-5.43	105.52	111.82
1	D	120	LYS	N-CA-C	-5.43	104.77	111.40
1	A	217	ILE	N-CA-C	5.43	120.63	109.34
1	B	148	ALA	N-CA-C	-5.42	104.23	112.04
1	B	41	ARG	N-CA-C	5.40	117.92	111.71
1	A	105	LEU	N-CA-C	5.40	119.40	111.04
1	B	156	SER	N-CA-C	-5.37	104.66	111.11
1	B	159	GLU	N-CA-C	-5.37	106.50	112.57
1	A	61	VAL	N-CA-C	5.35	115.56	110.42
1	D	126	TYR	N-CA-C	-5.34	105.63	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	N-CA-C	-5.33	105.84	112.93
1	B	126	TYR	N-CA-C	-5.32	105.53	112.23
1	B	11	LYS	N-CA-C	-5.31	105.54	112.23
1	D	222	ARG	CA-C-N	5.26	127.33	120.28
1	D	222	ARG	C-N-CA	5.26	127.33	120.28
1	C	126	TYR	N-CA-C	-5.23	105.64	112.23
1	B	100	LEU	N-CA-C	-5.20	104.87	111.11
1	A	103	LYS	N-CA-C	5.18	119.31	112.89
1	A	136	ASP	N-CA-C	-5.17	106.08	112.38
1	C	105	LEU	N-CA-C	5.16	121.80	110.80
1	A	80	ARG	N-CA-C	-5.16	105.74	111.36
1	D	221	LEU	CA-CB-CG	5.14	134.28	116.30
1	B	170	LEU	N-CA-C	-5.08	105.65	111.14
1	C	77	GLN	N-CA-C	-5.08	105.93	111.82
1	D	41	ARG	N-CA-C	5.08	116.50	110.97
1	D	134	ALA	N-CA-C	5.06	121.57	110.80
1	C	151	GLU	N-CA-C	-5.05	107.18	113.55
1	C	122	LYS	N-CA-C	-5.05	106.22	112.38
1	A	202	GLU	N-CA-C	-5.04	107.17	113.72

There are no chirality outliers.

There are no planarity outliers.

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	1590	0	1599	92	0
1	B	1590	0	1599	82	0
1	C	1590	0	1599	112	0
1	D	1590	0	1599	111	0
All	All	6360	0	6396	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:HG11	1:B:160:MET:HE1	1.39	1.04
1:A:116:VAL:HG11	1:A:160:MET:HE1	1.47	0.93
1:B:30:THR:HG21	1:B:100:LEU:HG	1.56	0.85
1:C:196:PHE:CE1	1:C:200:ILE:HD11	2.13	0.83
1:C:116:VAL:HG11	1:C:160:MET:CE	2.10	0.82
1:B:14:GLU:HB2	1:B:22:MET:SD	2.19	0.81
1:A:216:LEU:HG	1:A:220:LEU:CD1	2.12	0.80
1:A:192:ALA:O	1:A:196:PHE:HB3	1.82	0.80
1:A:67:GLN:OE1	1:A:68:LYS:HG3	1.82	0.79
1:C:116:VAL:HG11	1:C:160:MET:HE1	1.67	0.77
1:D:156:SER:HA	1:D:160:MET:HE3	1.65	0.77
1:A:113:GLU:HG3	1:A:114:SER:N	1.99	0.77
1:A:216:LEU:HG	1:A:220:LEU:HD11	1.67	0.76
1:D:116:VAL:HG11	1:D:160:MET:SD	2.25	0.76
1:C:219:GLN:NE2	1:C:223:ASP:HB2	2.01	0.75
1:D:58:SER:HB3	1:D:86:ILE:HD13	1.67	0.75
1:D:89:GLU:O	1:D:93:ILE:HG12	1.85	0.75
1:A:27:LYS:HG3	1:A:100:LEU:HD21	1.70	0.73
1:C:153:PHE:HA	1:C:170:LEU:HD21	1.70	0.73
1:C:173:ASN:HA	1:C:176:VAL:HG12	1.71	0.72
1:D:174:PHE:O	1:D:177:PHE:HB3	1.88	0.72
1:C:166:ILE:HG23	1:C:167:ARG:H	1.54	0.72
1:C:178:TYR:O	1:C:179:TYR:HB2	1.90	0.72
1:A:94:CYS:O	1:A:98:LEU:HB2	1.90	0.72
1:D:7:VAL:HG23	1:D:29:VAL:HG21	1.71	0.72
1:B:113:GLU:O	1:B:116:VAL:HG12	1.91	0.71
1:D:119:LEU:HD23	1:D:151:GLU:HB3	1.71	0.71
1:B:56:ARG:O	1:B:60:ARG:HG3	1.92	0.69
1:A:10:ALA:HB2	1:A:25:CYS:HB2	1.74	0.69
1:A:174:PHE:O	1:A:177:PHE:HB3	1.93	0.68
1:C:200:ILE:HG23	1:C:203:LEU:CD1	2.23	0.68
1:D:156:SER:HA	1:D:160:MET:CE	2.23	0.68
1:B:120:LYS:HG3	1:B:170:LEU:HD12	1.74	0.68
1:D:30:THR:OG1	1:D:105:LEU:HD11	1.93	0.68
1:D:14:GLU:HB2	1:D:22:MET:SD	2.34	0.68
1:A:155:ILE:HG22	1:A:155:ILE:O	1.92	0.68
1:D:116:VAL:HG11	1:D:160:MET:HE1	1.75	0.67
1:B:109:ALA:CB	1:B:115:LYS:HG2	2.24	0.67
1:A:30:THR:HG21	1:A:100:LEU:HG	1.76	0.67
1:C:168:LEU:HD21	1:C:218:MET:HG2	1.77	0.67
1:C:87:GLU:HG2	1:C:132:VAL:HG13	1.78	0.66
1:D:196:PHE:O	1:D:200:ILE:HG13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:VAL:HA	1:D:100:LEU:HD22	1.77	0.66
1:B:30:THR:CG2	1:B:100:LEU:HG	2.26	0.65
1:D:116:VAL:HG11	1:D:160:MET:CE	2.27	0.65
1:A:101:LEU:HD12	1:A:105:LEU:HD23	1.78	0.65
1:C:85:LYS:O	1:C:89:GLU:HG3	1.96	0.65
1:B:119:LEU:HB3	1:B:152:ALA:HB2	1.78	0.65
1:C:73:GLU:HA	1:C:76:GLN:HB3	1.79	0.65
1:D:127:ARG:HD3	1:D:149:TYR:OH	1.98	0.64
1:B:200:ILE:HG22	1:B:200:ILE:O	1.98	0.64
1:B:216:LEU:O	1:B:220:LEU:HD13	1.98	0.64
1:D:101:LEU:HA	1:D:105:LEU:HB2	1.79	0.64
1:A:106:ILE:HG22	1:A:118:TYR:HB3	1.81	0.63
1:A:221:LEU:O	1:A:225:LEU:HD22	1.98	0.63
1:B:58:SER:O	1:B:62:VAL:HG12	1.99	0.63
1:A:101:LEU:HD11	1:A:121:MET:HE2	1.80	0.63
1:A:47:ALA:O	1:A:51:VAL:HG23	1.99	0.63
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.80	0.63
1:C:77:GLN:O	1:C:81:GLU:HB2	1.98	0.63
1:D:49:LYS:HA	1:D:52:VAL:HG12	1.79	0.63
1:D:94:CYS:O	1:D:98:LEU:HB2	1.99	0.62
1:B:3:LYS:HG3	1:B:29:VAL:HG13	1.82	0.62
1:C:101:LEU:HA	1:C:105:LEU:HB2	1.80	0.62
1:D:77:GLN:O	1:D:81:GLU:HB2	1.99	0.62
1:D:192:ALA:HB3	1:D:225:LEU:HD11	1.80	0.62
1:A:178:TYR:O	1:A:179:TYR:HB2	2.00	0.61
1:A:127:ARG:HD3	1:A:149:TYR:OH	2.00	0.61
1:A:14:GLU:HB2	1:A:22:MET:SD	2.41	0.61
1:A:92:ASP:O	1:A:96:ASP:HB2	2.01	0.61
1:D:92:ASP:O	1:D:96:ASP:HB2	2.00	0.61
1:D:3:LYS:HG3	1:D:29:VAL:HG22	1.82	0.61
1:C:122:LYS:HE2	1:C:126:TYR:HE2	1.66	0.60
1:C:153:PHE:O	1:C:156:SER:HB2	2.01	0.60
1:C:194:THR:O	1:C:197:ASP:HB3	2.01	0.60
1:A:193:LYS:HA	1:A:196:PHE:HD2	1.67	0.60
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.83	0.60
1:D:124:ASP:O	1:D:127:ARG:HB3	2.02	0.60
1:A:216:LEU:HG	1:A:220:LEU:HD13	1.83	0.59
1:C:92:ASP:O	1:C:96:ASP:HB2	2.02	0.59
1:D:101:LEU:HD12	1:D:105:LEU:HD22	1.85	0.59
1:C:90:LEU:HD21	1:C:132:VAL:HG21	1.83	0.59
1:A:219:GLN:HE21	1:A:223:ASP:HB2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASN:O	1:D:176:VAL:HG12	2.04	0.58
1:B:9:LYS:HD2	1:B:25:CYS:SG	2.44	0.58
1:B:48:TYR:O	1:B:52:VAL:HG12	2.03	0.58
1:C:56:ARG:O	1:C:60:ARG:HG3	2.04	0.58
1:A:27:LYS:O	1:A:30:THR:HG22	2.04	0.58
1:A:176:VAL:HG23	1:A:228:TRP:HZ2	1.68	0.57
1:D:133:ALA:HB2	1:D:141:ILE:HD12	1.86	0.57
1:A:115:LYS:HB3	1:A:115:LYS:HZ2	1.70	0.57
1:A:90:LEU:HD21	1:A:132:VAL:HG21	1.85	0.57
1:B:92:ASP:O	1:B:96:ASP:HB2	2.05	0.57
1:A:122:LYS:O	1:A:126:TYR:HD2	1.87	0.57
1:B:7:VAL:HG23	1:B:29:VAL:HG21	1.86	0.57
1:B:109:ALA:HB1	1:B:115:LYS:HG2	1.86	0.57
1:C:106:ILE:HG12	1:C:107:PRO:HD3	1.85	0.57
1:D:58:SER:O	1:D:62:VAL:HG12	2.05	0.56
1:A:73:GLU:O	1:A:76:GLN:HB3	2.05	0.56
1:A:99:SER:O	1:A:103:LYS:HB2	2.05	0.56
1:B:116:VAL:HG11	1:B:160:MET:CE	2.25	0.56
1:C:14:GLU:HB2	1:C:22:MET:SD	2.46	0.56
1:D:199:ALA:O	1:D:202:GLU:HB3	2.05	0.56
1:C:75:LYS:O	1:C:78:MET:HG3	2.05	0.56
1:B:174:PHE:O	1:B:177:PHE:HB3	2.06	0.56
1:D:27:LYS:O	1:D:30:THR:HG22	2.06	0.56
1:C:31:GLU:HA	1:C:104:PHE:CE2	2.41	0.56
1:B:45:SER:O	1:B:49:LYS:HB3	2.06	0.56
1:B:149:TYR:O	1:B:153:PHE:HB2	2.04	0.56
1:A:56:ARG:O	1:A:60:ARG:HG3	2.06	0.55
1:A:116:VAL:HG13	1:A:166:ILE:HD11	1.87	0.55
1:B:160:MET:HE3	1:B:167:ARG:HB2	1.87	0.55
1:D:178:TYR:O	1:D:179:TYR:HB2	2.05	0.55
1:B:155:ILE:HG22	1:B:155:ILE:O	2.05	0.55
1:C:160:MET:HE3	1:C:167:ARG:HB2	1.88	0.55
1:C:97:VAL:HA	1:C:100:LEU:HD22	1.88	0.55
1:D:73:GLU:O	1:D:76:GLN:HB3	2.06	0.55
1:B:39:GLU:O	1:B:43:LEU:HB2	2.07	0.55
1:B:143:ASP:O	1:B:147:GLN:HG2	2.06	0.55
1:D:166:ILE:HG23	1:D:167:ARG:H	1.72	0.55
1:B:75:LYS:O	1:B:78:MET:HG3	2.07	0.54
1:D:219:GLN:NE2	1:D:223:ASP:HB2	2.22	0.54
1:C:46:VAL:HA	1:C:49:LYS:HG2	1.89	0.54
1:D:139:LYS:O	1:D:142:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:O	1:C:147:GLN:HG2	2.08	0.54
1:D:200:ILE:C	1:D:202:GLU:H	2.16	0.54
1:A:30:THR:CG2	1:A:100:LEU:HG	2.38	0.54
1:C:87:GLU:CG	1:C:132:VAL:HG13	2.37	0.54
1:C:216:LEU:O	1:C:220:LEU:HD13	2.08	0.54
1:C:67:GLN:OE1	1:C:68:LYS:HG3	2.07	0.54
1:B:67:GLN:OE1	1:B:68:LYS:HG3	2.07	0.54
1:B:178:TYR:O	1:B:179:TYR:HB2	2.08	0.54
1:C:89:GLU:O	1:C:93:ILE:HG12	2.07	0.54
1:A:48:TYR:O	1:A:52:VAL:HG12	2.08	0.54
1:C:130:ALA:O	1:C:138:LYS:HE3	2.08	0.53
1:D:9:LYS:HD2	1:D:25:CYS:SG	2.47	0.53
1:D:150:GLN:HA	1:D:153:PHE:HB3	1.89	0.53
1:B:119:LEU:HD23	1:B:151:GLU:HB3	1.90	0.53
1:C:117:PHE:CD1	1:C:117:PHE:C	2.86	0.53
1:C:36:LEU:HD22	1:C:105:LEU:HD11	1.91	0.53
1:D:6:LEU:HG	1:D:28:SER:HB3	1.89	0.53
1:B:35:GLU:HA	1:B:35:GLU:OE1	2.09	0.53
1:D:133:ALA:HB3	1:D:138:LYS:HA	1.91	0.53
1:D:113:GLU:O	1:D:166:ILE:HD11	2.08	0.53
1:A:9:LYS:HD2	1:A:25:CYS:SG	2.49	0.52
1:C:78:MET:HE1	1:D:9:LYS:HA	1.90	0.52
1:A:27:LYS:O	1:A:31:GLU:HG2	2.10	0.52
1:B:52:VAL:HG11	1:B:125:TYR:CE2	2.45	0.52
1:D:171:ALA:O	1:D:175:SER:HB2	2.10	0.52
1:B:73:GLU:O	1:B:76:GLN:HB3	2.10	0.52
1:B:97:VAL:HA	1:B:100:LEU:HD22	1.92	0.52
1:D:155:ILE:O	1:D:158:LYS:HB3	2.09	0.52
1:C:106:ILE:CG1	1:C:107:PRO:HD3	2.40	0.52
1:B:87:GLU:HG3	1:B:132:VAL:HG22	1.90	0.52
1:D:48:TYR:O	1:D:52:VAL:HG12	2.10	0.52
1:A:93:ILE:O	1:A:97:VAL:HG12	2.09	0.52
1:B:173:ASN:O	1:B:176:VAL:HG12	2.09	0.52
1:A:116:VAL:HG11	1:A:160:MET:CE	2.30	0.52
1:C:219:GLN:HE22	1:C:223:ASP:HB2	1.75	0.52
1:D:216:LEU:O	1:D:220:LEU:HD13	2.10	0.52
1:C:200:ILE:HG23	1:C:203:LEU:HD12	1.91	0.51
1:B:189:CYS:HA	1:B:225:LEU:HD11	1.91	0.51
1:A:37:SER:HB3	1:A:40:GLU:HG3	1.93	0.51
1:A:113:GLU:O	1:A:166:ILE:HD11	2.11	0.51
1:D:101:LEU:HD11	1:D:121:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:LEU:HD12	1:D:105:LEU:CD2	2.40	0.51
1:C:113:GLU:HG3	1:C:114:SER:N	2.25	0.51
1:C:2:ASP:O	1:C:6:LEU:HD22	2.11	0.51
1:D:94:CYS:HB2	1:D:129:LEU:HD13	1.92	0.51
1:D:44:LEU:HD21	1:D:105:LEU:HD21	1.92	0.51
1:D:56:ARG:O	1:D:60:ARG:HG3	2.10	0.51
1:C:200:ILE:HG23	1:C:203:LEU:HD11	1.91	0.50
1:D:27:LYS:O	1:D:31:GLU:HG2	2.11	0.50
1:D:52:VAL:HG11	1:D:125:TYR:HE1	1.75	0.50
1:D:188:ALA:C	1:D:190:SER:H	2.19	0.50
1:A:193:LYS:O	1:A:197:ASP:N	2.45	0.50
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.93	0.50
1:A:129:LEU:HB3	1:A:141:ILE:HG21	1.94	0.50
1:A:156:SER:O	1:A:158:LYS:N	2.43	0.50
1:A:103:LYS:HE3	1:D:31:GLU:O	2.11	0.50
1:B:153:PHE:O	1:B:156:SER:HB2	2.11	0.50
1:D:133:ALA:CB	1:D:138:LYS:HA	2.41	0.50
1:A:16:ALA:HA	1:B:61:VAL:HG11	1.94	0.50
1:B:222:ARG:O	1:B:225:LEU:HB2	2.11	0.50
1:C:156:SER:O	1:C:158:LYS:N	2.44	0.50
1:B:17:GLU:O	1:B:17:GLU:HG2	2.11	0.49
1:C:17:GLU:O	1:C:17:GLU:HG2	2.12	0.49
1:C:222:ARG:HA	1:C:225:LEU:HD22	1.94	0.49
1:D:113:GLU:HG3	1:D:114:SER:N	2.27	0.49
1:A:5:GLU:O	1:A:9:LYS:HB2	2.12	0.49
1:B:22:MET:SD	1:B:47:ALA:HB2	2.53	0.49
1:B:121:MET:O	1:B:125:TYR:HD1	1.95	0.49
1:C:113:GLU:O	1:C:166:ILE:HD11	2.12	0.49
1:A:66:GLU:HG3	1:A:76:GLN:HG3	1.93	0.49
1:A:158:LYS:HB2	1:A:158:LYS:NZ	2.26	0.49
1:B:10:ALA:HB2	1:B:25:CYS:HB2	1.94	0.49
1:D:106:ILE:HG22	1:D:118:TYR:HB3	1.94	0.49
1:B:97:VAL:HG11	1:B:125:TYR:CD2	2.48	0.49
1:B:103:LYS:HE3	1:C:31:GLU:O	2.12	0.49
1:B:221:LEU:O	1:B:225:LEU:HD22	2.13	0.49
1:D:122:LYS:O	1:D:126:TYR:HD2	1.95	0.49
1:C:27:LYS:HA	1:C:30:THR:HG22	1.94	0.49
1:A:28:SER:O	1:A:32:GLN:NE2	2.46	0.48
1:A:115:LYS:HB3	1:A:115:LYS:NZ	2.28	0.48
1:A:153:PHE:O	1:A:156:SER:HB2	2.13	0.48
1:D:188:ALA:C	1:D:190:SER:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:CA	1:C:76:GLN:HB3	2.42	0.48
1:C:22:MET:SD	1:C:47:ALA:HB2	2.54	0.48
1:D:192:ALA:O	1:D:196:PHE:HB3	2.13	0.48
1:B:27:LYS:O	1:B:30:THR:HG22	2.13	0.48
1:D:39:GLU:O	1:D:43:LEU:HB2	2.13	0.48
1:D:158:LYS:NZ	1:D:158:LYS:HB2	2.28	0.48
1:A:106:ILE:HB	1:A:119:LEU:HD11	1.96	0.48
1:A:117:PHE:HB2	1:A:166:ILE:HD12	1.95	0.48
1:B:1:MET:HB2	1:B:32:GLN:OE1	2.13	0.48
1:C:155:ILE:O	1:C:155:ILE:HG22	2.14	0.48
1:C:219:GLN:HE21	1:C:223:ASP:HB2	1.77	0.48
1:C:38:ASN:HA	1:C:41:ARG:HB3	1.95	0.48
1:B:5:GLU:O	1:B:9:LYS:HB2	2.13	0.48
1:C:119:LEU:HD22	1:C:151:GLU:HB3	1.94	0.48
1:D:6:LEU:HB3	1:D:29:VAL:HG23	1.95	0.48
1:C:196:PHE:HA	1:C:199:ALA:HB3	1.95	0.48
1:D:10:ALA:CB	1:D:26:MET:SD	3.01	0.48
1:D:41:ARG:O	1:D:44:LEU:HB3	2.14	0.47
1:D:87:GLU:HA	1:D:90:LEU:HD23	1.96	0.47
1:B:124:ASP:O	1:B:127:ARG:HB3	2.14	0.47
1:A:124:ASP:O	1:A:127:ARG:HB3	2.15	0.47
1:A:176:VAL:HG23	1:A:228:TRP:CZ2	2.48	0.47
1:C:119:LEU:HB2	1:C:152:ALA:HB2	1.96	0.47
1:D:156:SER:OG	1:D:167:ARG:HG3	2.14	0.47
1:B:85:LYS:O	1:B:89:GLU:HG3	2.13	0.47
1:D:51:VAL:HG13	1:D:55:ARG:NH1	2.29	0.47
1:C:9:LYS:HB2	1:D:78:MET:HE1	1.96	0.47
1:D:5:GLU:O	1:D:9:LYS:HB2	2.15	0.47
1:D:2:ASP:O	1:D:6:LEU:HD22	2.15	0.47
1:D:115:LYS:NZ	1:D:115:LYS:HB3	2.29	0.47
1:C:124:ASP:O	1:C:127:ARG:HB3	2.15	0.47
1:D:1:MET:HB2	1:D:32:GLN:OE1	2.15	0.47
1:D:7:VAL:CG2	1:D:29:VAL:HG21	2.41	0.47
1:C:1:MET:HB2	1:C:32:GLN:OE1	2.15	0.47
1:C:6:LEU:HB2	1:C:29:VAL:HG23	1.97	0.47
1:C:117:PHE:C	1:C:117:PHE:HD1	2.22	0.47
1:A:17:GLU:O	1:A:17:GLU:HG2	2.13	0.47
1:A:97:VAL:HG11	1:A:125:TYR:CD2	2.50	0.47
1:B:55:ARG:HB3	1:B:90:LEU:HB2	1.95	0.47
1:B:127:ARG:O	1:B:131:GLU:HG3	2.15	0.47
1:B:22:MET:HE1	1:B:46:VAL:CG1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:O	1:C:76:GLN:HB3	2.15	0.46
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.97	0.46
1:D:117:PHE:CD1	1:D:117:PHE:C	2.92	0.46
1:D:129:LEU:HB3	1:D:141:ILE:HG21	1.96	0.46
1:C:15:GLN:O	1:D:61:VAL:HG21	2.15	0.46
1:D:193:LYS:O	1:D:197:ASP:N	2.48	0.46
1:C:173:ASN:O	1:C:176:VAL:HG12	2.16	0.46
1:C:119:LEU:CD2	1:C:151:GLU:HB3	2.46	0.46
1:C:106:ILE:HG22	1:C:118:TYR:HB3	1.97	0.46
1:C:218:MET:HE2	1:C:218:MET:HB3	1.87	0.46
1:A:115:LYS:O	1:A:119:LEU:HD13	2.15	0.46
1:D:59:TRP:CE2	1:D:83:ARG:HD3	2.50	0.46
1:A:66:GLU:CG	1:A:76:GLN:HG3	2.46	0.46
1:A:90:LEU:CD2	1:A:132:VAL:HG21	2.46	0.46
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.82	0.46
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.46	0.46
1:A:52:VAL:HG13	1:A:53:GLY:N	2.31	0.45
1:B:86:ILE:O	1:B:90:LEU:HB3	2.16	0.45
1:B:171:ALA:O	1:B:175:SER:HB2	2.16	0.45
1:C:166:ILE:HG23	1:C:167:ARG:N	2.26	0.45
1:D:99:SER:O	1:D:103:LYS:HB2	2.16	0.45
1:B:31:GLU:O	1:C:103:LYS:HE3	2.16	0.45
1:B:34:ALA:HB1	1:B:35:GLU:H	1.44	0.45
1:B:66:GLU:O	1:B:66:GLU:HG2	2.16	0.45
1:C:45:SER:O	1:C:49:LYS:HB3	2.16	0.45
1:D:30:THR:OG1	1:D:36:LEU:HD21	2.17	0.45
1:C:32:GLN:HB3	1:C:33:GLY:H	1.50	0.45
1:C:127:ARG:O	1:C:131:GLU:HG3	2.16	0.45
1:C:202:GLU:O	1:C:202:GLU:HG2	2.17	0.45
1:A:135:GLY:C	1:A:137:ASP:N	2.74	0.45
1:B:155:ILE:O	1:B:155:ILE:CG2	2.64	0.45
1:C:44:LEU:HD21	1:C:105:LEU:HD21	1.99	0.45
1:D:6:LEU:CB	1:D:29:VAL:HG23	2.47	0.45
1:A:58:SER:O	1:A:62:VAL:HG12	2.17	0.45
1:A:216:LEU:O	1:A:220:LEU:HD13	2.17	0.45
1:B:113:GLU:HG3	1:B:114:SER:N	2.32	0.45
1:C:61:VAL:HG11	1:D:16:ALA:HA	1.98	0.45
1:C:174:PHE:O	1:C:177:PHE:HB3	2.16	0.44
1:A:36:LEU:O	1:A:37:SER:C	2.60	0.44
1:B:11:LYS:HG3	1:B:43:LEU:HD21	1.99	0.44
1:D:178:TYR:O	1:D:179:TYR:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:CG	1:A:132:VAL:HG13	2.47	0.44
1:B:101:LEU:HD12	1:B:105:LEU:HD23	1.98	0.44
1:A:3:LYS:O	1:A:7:VAL:HG23	2.17	0.44
1:C:196:PHE:HE1	1:C:200:ILE:HD11	1.79	0.44
1:D:116:VAL:HG13	1:D:166:ILE:HD11	1.98	0.44
1:C:106:ILE:N	1:C:107:PRO:HD2	2.32	0.44
1:C:196:PHE:CE1	1:C:200:ILE:CD1	2.93	0.44
1:D:133:ALA:CB	1:D:141:ILE:HD12	2.47	0.44
1:B:119:LEU:CB	1:B:152:ALA:HB2	2.45	0.44
1:C:49:LYS:HA	1:C:52:VAL:HG12	1.99	0.44
1:C:94:CYS:O	1:C:98:LEU:HB2	2.17	0.44
1:C:116:VAL:HG21	1:C:160:MET:HE1	1.99	0.44
1:D:127:ARG:HD3	1:D:149:TYR:HH	1.82	0.44
1:C:147:GLN:O	1:C:151:GLU:HB2	2.18	0.44
1:A:89:GLU:O	1:A:93:ILE:HG12	2.18	0.44
1:A:106:ILE:HB	1:A:119:LEU:CD1	2.48	0.44
1:C:74:LYS:C	1:C:76:GLN:N	2.71	0.44
1:D:11:LYS:HG3	1:D:43:LEU:HD21	2.00	0.44
1:D:166:ILE:HG23	1:D:167:ARG:N	2.32	0.44
1:A:2:ASP:O	1:A:6:LEU:HD22	2.18	0.43
1:B:46:VAL:O	1:B:50:ASN:ND2	2.50	0.43
1:B:109:ALA:HB3	1:B:115:LYS:HG2	2.00	0.43
1:C:149:TYR:CE2	1:C:177:PHE:HB2	2.53	0.43
1:A:74:LYS:C	1:A:76:GLN:N	2.74	0.43
1:B:106:ILE:HG22	1:B:118:TYR:HB3	1.99	0.43
1:C:5:GLU:O	1:C:9:LYS:HB2	2.18	0.43
1:D:137:ASP:O	1:D:141:ILE:HG13	2.18	0.43
1:A:224:ASN:HA	1:A:227:LEU:HG	2.00	0.43
1:B:130:ALA:O	1:B:138:LYS:HE3	2.17	0.43
1:C:221:LEU:O	1:C:225:LEU:HD22	2.19	0.43
1:D:189:CYS:HB3	1:D:228:TRP:HE3	1.82	0.43
1:A:77:GLN:O	1:A:81:GLU:HB2	2.18	0.43
1:A:86:ILE:O	1:A:86:ILE:HG22	2.19	0.43
1:A:113:GLU:CG	1:A:114:SER:N	2.77	0.43
1:A:116:VAL:CG1	1:A:160:MET:HE1	2.35	0.43
1:C:62:VAL:HG23	1:D:12:LEU:HD11	2.00	0.43
1:C:155:ILE:HG23	1:C:158:LYS:HD2	2.01	0.43
1:A:83:ARG:O	1:A:87:GLU:HB2	2.18	0.43
1:A:222:ARG:O	1:A:225:LEU:HB2	2.19	0.43
1:B:18:ARG:H	1:B:18:ARG:HG2	1.63	0.43
1:C:18:ARG:CZ	1:D:86:ILE:HG12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:O	1:C:104:PHE:HB2	2.18	0.43
1:D:119:LEU:CB	1:D:152:ALA:HB2	2.48	0.43
1:A:172:LEU:HD13	1:A:221:LEU:HB3	2.01	0.43
1:C:87:GLU:HG2	1:C:132:VAL:CG1	2.47	0.43
1:C:100:LEU:N	1:C:100:LEU:HD13	2.33	0.43
1:C:129:LEU:HD12	1:C:129:LEU:HA	1.84	0.43
1:A:6:LEU:HB3	1:A:29:VAL:HG23	2.01	0.43
1:A:49:LYS:HA	1:A:52:VAL:HG12	2.01	0.42
1:D:37:SER:HB3	1:D:40:GLU:HG3	2.01	0.42
1:D:52:VAL:HG11	1:D:125:TYR:CE1	2.54	0.42
1:D:56:ARG:HD2	1:D:128:TYR:CD2	2.54	0.42
1:B:102:GLU:HA	1:B:106:ILE:HG12	2.00	0.42
1:C:94:CYS:CB	1:C:129:LEU:HD13	2.49	0.42
1:C:217:ILE:H	1:C:217:ILE:HG13	1.51	0.42
1:D:76:GLN:O	1:D:80:ARG:N	2.50	0.42
1:A:62:VAL:HG23	1:B:12:LEU:HD11	2.00	0.42
1:A:133:ALA:CB	1:A:138:LYS:HA	2.50	0.42
1:B:126:TYR:HB3	1:B:145:SER:HB2	2.00	0.42
1:D:37:SER:O	1:D:40:GLU:N	2.53	0.42
1:C:36:LEU:O	1:C:37:SER:C	2.63	0.42
1:C:91:ARG:NH1	1:C:132:VAL:HG12	2.35	0.42
1:C:9:LYS:CB	1:D:78:MET:HE1	2.49	0.42
1:C:16:ALA:O	1:C:17:GLU:HB3	2.19	0.42
1:B:106:ILE:N	1:B:107:PRO:HD2	2.34	0.41
1:C:58:SER:O	1:C:62:VAL:HG12	2.20	0.41
1:C:202:GLU:O	1:C:202:GLU:CG	2.68	0.41
1:D:143:ASP:O	1:D:147:GLN:HG2	2.20	0.41
1:B:87:GLU:HG3	1:B:132:VAL:CG2	2.49	0.41
1:B:103:LYS:HE2	1:B:103:LYS:HB2	1.96	0.41
1:A:57:SER:O	1:A:60:ARG:HB2	2.19	0.41
1:D:81:GLU:HA	1:D:84:GLU:OE1	2.20	0.41
1:B:146:GLN:HB2	1:B:177:PHE:CZ	2.56	0.41
1:C:61:VAL:HG21	1:D:15:GLN:O	2.21	0.41
1:C:219:GLN:HE21	1:C:219:GLN:C	2.29	0.41
1:C:116:VAL:HG11	1:C:160:MET:HE2	1.96	0.41
1:B:200:ILE:O	1:B:200:ILE:CG2	2.68	0.41
1:C:120:LYS:HE2	1:C:120:LYS:HB3	1.79	0.41
1:D:22:MET:HG2	1:D:47:ALA:HB2	2.01	0.41
1:D:52:VAL:HG13	1:D:53:GLY:N	2.36	0.41
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.90	0.41
1:A:29:VAL:O	1:A:32:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:H	1:B:217:ILE:HG13	1.60	0.41
1:C:11:LYS:HG3	1:C:43:LEU:HD21	2.03	0.41
1:A:74:LYS:C	1:A:76:GLN:H	2.29	0.41
1:D:10:ALA:HB2	1:D:26:MET:SD	2.61	0.41
1:D:200:ILE:HG23	1:D:203:LEU:CD1	2.51	0.41
1:C:153:PHE:CA	1:C:170:LEU:HD21	2.45	0.40
1:D:116:VAL:CG1	1:D:160:MET:HE1	2.49	0.40
1:A:97:VAL:HA	1:A:100:LEU:HD22	2.03	0.40
1:A:171:ALA:O	1:A:175:SER:HB2	2.21	0.40
1:B:155:ILE:HG12	1:B:158:LYS:HE2	2.02	0.40
1:D:155:ILE:O	1:D:158:LYS:CB	2.69	0.40
1:B:4:ASN:HA	1:B:7:VAL:HB	2.04	0.40
1:C:173:ASN:CA	1:C:176:VAL:HG12	2.46	0.40
1:C:173:ASN:HA	1:C:176:VAL:CG1	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/245 (76%)	155 (84%)	27 (15%)	3 (2%)	7	27
1	B	185/245 (76%)	161 (87%)	20 (11%)	4 (2%)	5	19
1	C	185/245 (76%)	165 (89%)	17 (9%)	3 (2%)	7	27
1	D	185/245 (76%)	158 (85%)	24 (13%)	3 (2%)	7	27
All	All	740/980 (76%)	639 (86%)	88 (12%)	13 (2%)	6	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA

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Mol	Chain	Res	Type
1	B	34	ALA
1	B	35	GLU
1	B	101	LEU
1	C	34	ALA
1	C	2	ASP
1	D	34	ALA
1	C	158	LYS
1	A	2	ASP
1	D	158	LYS
1	A	158	LYS
1	B	2	ASP
1	D	2	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/209 (81%)	135 (80%)	34 (20%)	1	4
1	B	169/209 (81%)	135 (80%)	34 (20%)	1	4
1	C	169/209 (81%)	133 (79%)	36 (21%)	1	4
1	D	169/209 (81%)	136 (80%)	33 (20%)	1	5
All	All	676/836 (81%)	539 (80%)	137 (20%)	1	4

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LEU
1	A	8	GLN
1	A	17	GLU
1	A	18	ARG
1	A	28	SER
1	A	32	GLN
1	A	36	LEU
1	A	43	LEU

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Mol	Chain	Res	Type
1	A	46	VAL
1	A	67	GLN
1	A	78	MET
1	A	88	THR
1	A	93	ILE
1	A	98	LEU
1	A	100	LEU
1	A	101	LEU
1	A	105	LEU
1	A	108	ASN
1	A	114	SER
1	A	116	VAL
1	A	129	LEU
1	A	143	ASP
1	A	158	LYS
1	A	170	LEU
1	A	189	CYS
1	A	190	SER
1	A	196	PHE
1	A	197	ASP
1	A	219	GLN
1	A	221	LEU
1	A	222	ARG
1	A	225	LEU
1	A	227	LEU
1	B	1	MET
1	B	7	VAL
1	B	8	GLN
1	B	14	GLU
1	B	17	GLU
1	B	18	ARG
1	B	28	SER
1	B	36	LEU
1	B	44	LEU
1	B	46	VAL
1	B	49	LYS
1	B	64	SER
1	B	67	GLN
1	B	78	MET
1	B	90	LEU
1	B	96	ASP
1	B	97	VAL

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Mol	Chain	Res	Type
1	B	98	LEU
1	B	100	LEU
1	B	101	LEU
1	B	105	LEU
1	B	108	ASN
1	B	113	GLU
1	B	129	LEU
1	B	132	VAL
1	B	150	GLN
1	B	170	LEU
1	B	189	CYS
1	B	190	SER
1	B	217	ILE
1	B	222	ARG
1	B	225	LEU
1	B	227	LEU
1	B	228	TRP
1	C	1	MET
1	C	6	LEU
1	C	8	GLN
1	C	11	LYS
1	C	14	GLU
1	C	17	GLU
1	C	29	VAL
1	C	32	GLN
1	C	36	LEU
1	C	43	LEU
1	C	67	GLN
1	C	81	GLU
1	C	83	ARG
1	C	90	LEU
1	C	96	ASP
1	C	98	LEU
1	C	100	LEU
1	C	101	LEU
1	C	105	LEU
1	C	108	ASN
1	C	114	SER
1	C	116	VAL
1	C	117	PHE
1	C	129	LEU
1	C	139	LYS

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Mol	Chain	Res	Type
1	C	149	TYR
1	C	158	LYS
1	C	170	LEU
1	C	179	TYR
1	C	189	CYS
1	C	190	SER
1	C	219	GLN
1	C	221	LEU
1	C	222	ARG
1	C	224	ASN
1	C	225	LEU
1	D	6	LEU
1	D	8	GLN
1	D	11	LYS
1	D	28	SER
1	D	30	THR
1	D	32	GLN
1	D	36	LEU
1	D	43	LEU
1	D	61	VAL
1	D	64	SER
1	D	67	GLN
1	D	74	LYS
1	D	78	MET
1	D	98	LEU
1	D	100	LEU
1	D	101	LEU
1	D	108	ASN
1	D	114	SER
1	D	116	VAL
1	D	132	VAL
1	D	142	VAL
1	D	157	LYS
1	D	158	LYS
1	D	168	LEU
1	D	176	VAL
1	D	190	SER
1	D	191	LEU
1	D	217	ILE
1	D	219	GLN
1	D	221	LEU
1	D	222	ARG

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Mol	Chain	Res	Type
1	D	225	LEU
1	D	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	108	ASN
1	A	146	GLN
1	A	219	GLN
1	A	224	ASN
1	B	4	ASN
1	B	15	GLN
1	B	95	ASN
1	B	173	ASN
1	C	146	GLN
1	C	147	GLN
1	C	150	GLN
1	C	219	GLN
1	D	146	GLN
1	D	173	ASN
1	D	219	GLN
1	D	224	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	197/245 (80%)	-1.64	0 100 100	12, 34, 57, 66	0
1	B	197/245 (80%)	-1.65	0 100 100	13, 34, 57, 67	0
1	C	197/245 (80%)	-1.68	0 100 100	13, 34, 57, 66	0
1	D	197/245 (80%)	-1.62	0 100 100	12, 33, 57, 67	0
All	All	788/980 (80%)	-1.65	0 100 100	12, 34, 57, 67	0

There are no RSRZ outliers to report.

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.