Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:18 PM GMT

PDB ID	:	1A4O
Title	:	14-3-3 PROTEIN ZETA ISOFORM
Authors	:	Liu, D.; Bienkowska, J.; Petosa, C.; Collier, R.J.; Fu, H.; Liddington, R.C.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

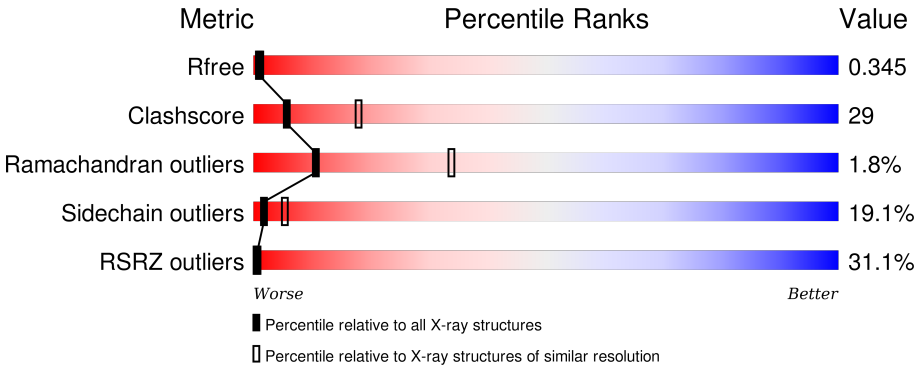
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	24% 33% 36% 11% • 20%
1	B	245	25% 31% 40% 8% • 20%
1	C	245	26% 32% 38% 9% • 20%
1	D	245	25% 25% 45% 10% 20%

2 Entry composition (i)

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.

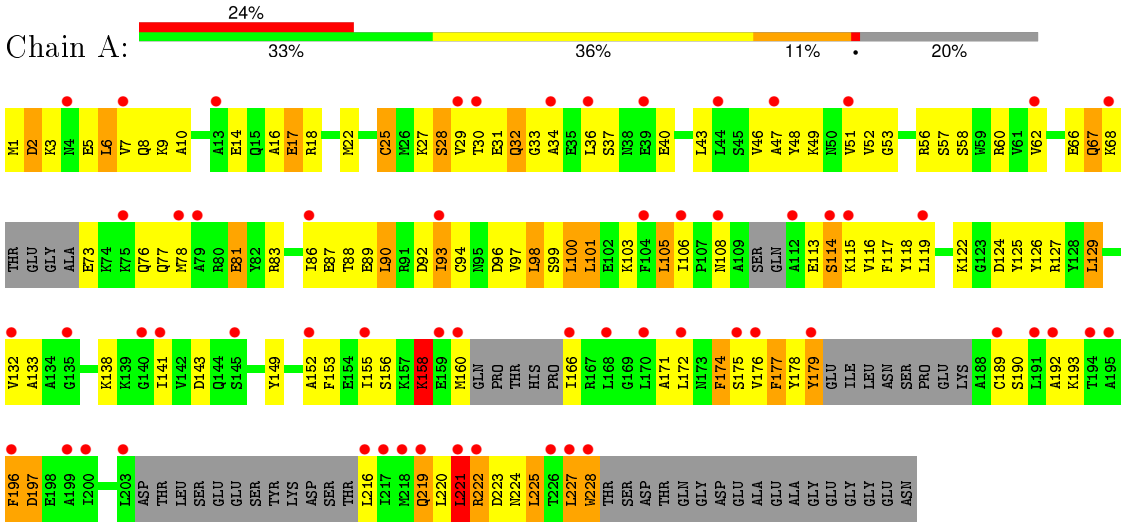
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	B	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	C	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			
1	D	197	Total	C	N	O	S	0	0	0
			1590	1004	269	307	10			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

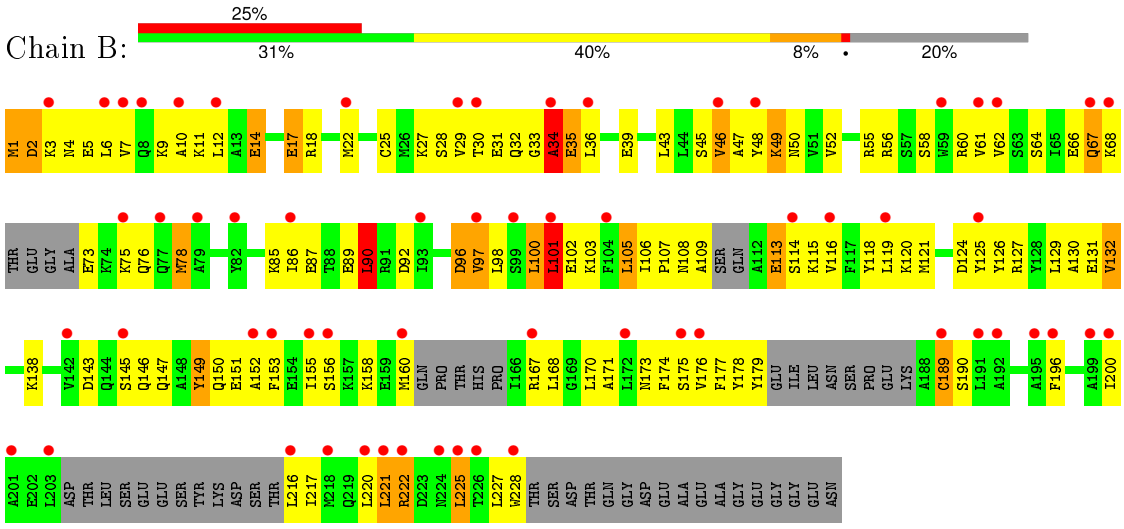
- Molecule 1: 14-3-3 PROTEIN ZETA

Chain A:



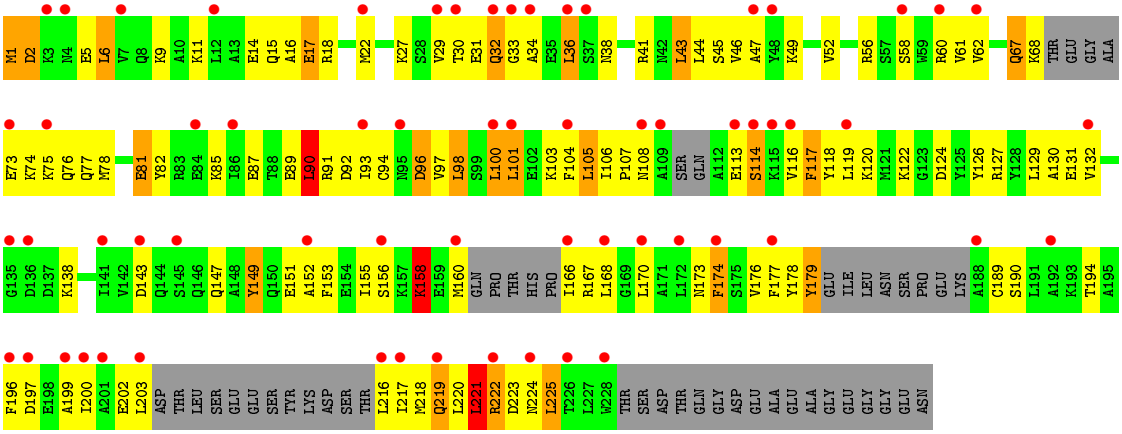
- Molecule 1: 14-3-3 PROTEIN ZETA

Chain B:

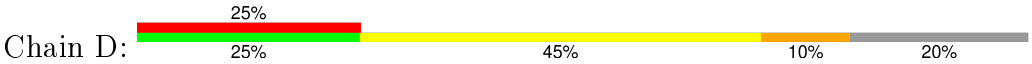


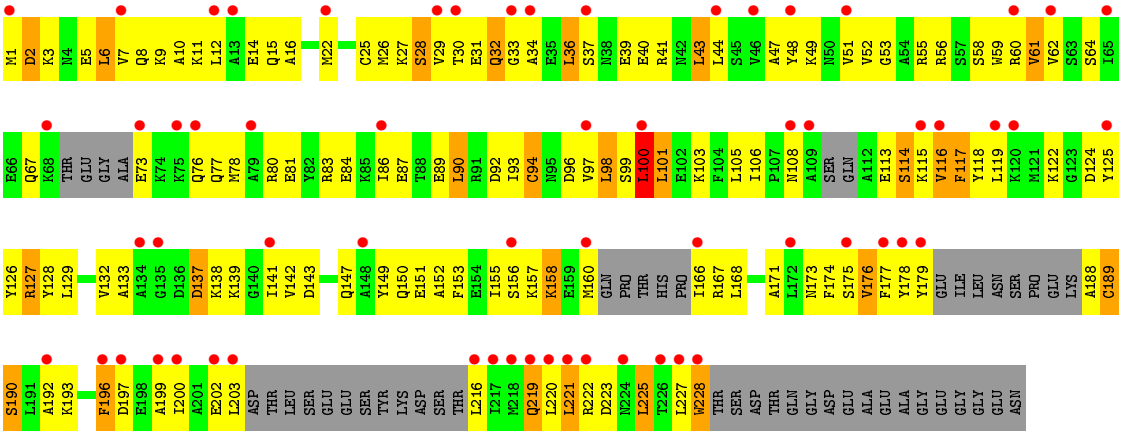
- Molecule 1: 14-3-3 PROTEIN ZETA

Chain C:



- Molecule 1: 14-3-3 PROTEIN ZETA





4 Data and refinement statistics (i)

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 8.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-2.80) 97.8 (8.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [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	No test flags present.	DCC
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 60.7	EDS
Estimated twinning fraction	0.446 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 28360 reflections	Xtriage
F_o,F_c correlation	0.83	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	1/1605 (0.1%)	0.85	3/2144 (0.1%)
1	B	0.51	0/1605	0.90	6/2144 (0.3%)
1	C	0.49	0/1605	0.85	2/2144 (0.1%)
1	D	0.52	1/1605 (0.1%)	0.89	4/2144 (0.2%)
All	All	0.50	2/6420 (0.0%)	0.87	15/8576 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	CYS	CB-SG	-5.73	1.72	1.81
1	D	94	CYS	CB-SG	-5.12	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	221	LEU	CA-CB-CG	8.25	134.28	115.30
1	C	221	LEU	CA-CB-CG	7.97	133.63	115.30
1	B	90	LEU	CA-CB-CG	7.16	131.76	115.30
1	B	34	ALA	N-CA-C	6.58	128.76	111.00
1	D	90	LEU	CA-CB-CG	6.37	129.94	115.30
1	A	33	GLY	N-CA-C	-6.20	97.59	113.10
1	B	221	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	90	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	221	LEU	CA-CB-CG	5.99	129.08	115.30
1	B	6	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	33	GLY	N-CA-C	-5.58	99.15	113.10
1	A	90	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	100	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	168	LEU	CA-CB-CG	5.11	127.04	115.30
1	D	33	GLY	N-CA-C	-5.07	100.43	113.10

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	1590	0	1599	86	0
1	B	1590	0	1599	83	0
1	C	1590	0	1599	107	0
1	D	1590	0	1599	108	0
All	All	6360	0	6396	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (373) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG23	1:D:29:VAL:HG21	1.71	0.72
1:C:116:VAL:HG11	1:C:160:MET:HE1	1.73	0.71
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: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:A:174:PHE:O	1:A:177:PHE:HB3	1.93	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:O	1:A:155:ILE:HG22	1.92	0.68
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:116:VAL:HG11	1:D:160:MET:HE1	1.77	0.66
1:D:196:PHE:O	1:D:200:ILE:HG13	1.95	0.66
1:B:116:VAL:HG11	1:B:160:MET:CE	2.25	0.66
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:B:116:VAL:HG11	1:B:160:MET:HE1	1.79	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:B:58:SER:O	1:B:62:VAL:HG12	1.99	0.63
1:A:221:LEU:O	1:A:225:LEU:HD22	1.98	0.63
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.80	0.63
1:A:47:ALA:O	1:A:51:VAL:HG23	1.99	0.63
1:D:49:LYS:HA	1:D:52:VAL:HG12	1.79	0.63
1:C:77:GLN:O	1:C:81:GLU:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:116:VAL:HG11	1:A:160:MET:CE	2.30	0.60
1:C:122:LYS:HE2	1:C:126:TYR:HE2	1.66	0.60
1:D:156:SER:HA	1:D:160:MET:HE2	1.83	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
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:D:133:ALA:HB2	1:D:141:ILE:HD12	1.86	0.57
1:A:176:VAL:HG23	1:A:228:TRP:HZ2	1.68	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:B:7:VAL:HG23	1:B:29:VAL:HG21	1.86	0.57
1:A:122:LYS:O	1:A:126:TYR:HD2	1.87	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:99:SER:O	1:A:103:LYS:HB2	2.05	0.56
1:A:73:GLU:O	1:A:76:GLN:HB3	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:O	1:D:30:THR:HG22	2.06	0.56
1:B:174:PHE:O	1:B:177:PHE:HB3	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:116:VAL:HG13	1:A:166:ILE:HD11	1.87	0.55
1:A:56:ARG:O	1:A:60:ARG:HG3	2.06	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: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:D:166:ILE:HG23	1:D:167:ARG:H	1.72	0.55
1:B:143:ASP:O	1:B:147:GLN:HG2	2.06	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:D:139:LYS:O	1:D:142:VAL:HG12	2.07	0.54
1:C:46:VAL:HA	1:C:49:LYS:HG2	1.89	0.54
1:C:143:ASP:O	1:C:147:GLN:HG2	2.08	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:178:TYR:O	1:B:179:TYR:HB2	2.08	0.54
1:B:67:GLN:OE1	1:B:68:LYS:HG3	2.07	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:D:6:LEU:HG	1:D:28:SER:HB3	1.89	0.53
1:C:36:LEU:HD22	1:C:105:LEU:HD11	1.91	0.53
1:D:133:ALA:HB3	1:D:138:LYS:HA	1.91	0.53
1:B:35:GLU:OE1	1:B:35:GLU:HA	2.09	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:B:52:VAL:HG11	1:B:125:TYR:CE2	2.45	0.52
1:A:27:LYS:O	1:A:31:GLU:HG2	2.10	0.52
1:D:171:ALA:O	1:D:175:SER:HB2	2.10	0.52
1:B:97:VAL:HA	1:B:100:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:O	1:D:158:LYS:HB3	2.09	0.52
1:B:73:GLU:O	1:B:76:GLN:HB3	2.10	0.52
1:C:106:ILE:CG1	1:C:107:PRO:HD3	2.40	0.52
1:D:48:TYR:O	1:D:52:VAL:HG12	2.10	0.52
1:B:87:GLU:HG3	1:B:132:VAL:HG22	1.90	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: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:113:GLU:O	1:A:166:ILE:HD11	2.11	0.51
1:A:116:VAL:HG11	1:A:160:MET:HE1	1.91	0.51
1:A:37:SER:HB3	1:A:40:GLU:HG3	1.93	0.51
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:D:94:CYS:HB2	1:D:129:LEU:HD13	1.92	0.51
1:C:2:ASP:O	1:C:6:LEU:HD22	2.11	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: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:D:133:ALA:CB	1:D:138:LYS:HA	2.41	0.50
1:B:153:PHE:O	1:B:156:SER:HB2	2.11	0.50
1:C:17:GLU:HG2	1:C:17:GLU:O	2.12	0.50
1:C:156:SER:O	1:C:158:LYS:N	2.44	0.50
1:B:222:ARG:O	1:B:225:LEU:HB2	2.11	0.50
1:A:16:ALA:HA	1:B:61:VAL:HG11	1.94	0.50
1:B:17:GLU:HG2	1:B:17:GLU:O	2.11	0.49
1:D:113:GLU:HG3	1:D:114:SER:N	2.27	0.49
1:C:222:ARG:HA	1:C:225:LEU:HD22	1.94	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:B:22:MET:SD	1:B:47:ALA:HB2	2.53	0.49
1:A:5:GLU:O	1:A:9:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HG3	1:A:76:GLN:HG3	1.93	0.49
1:A:158:LYS:NZ	1:A:158:LYS:HB2	2.26	0.49
1:C:160:MET:HE3	1:C:167:ARG:HB2	1.94	0.49
1:A:115:LYS:HB3	1:A:115:LYS:NZ	2.28	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:117:PHE:CD1	1:C:117:PHE:C	2.86	0.49
1:C:27:LYS:HA	1:C:30:THR:HG22	1.94	0.49
1:D:200:ILE:C	1:D:202:GLU:H	2.16	0.48
1:A:28:SER:O	1:A:32:GLN:NE2	2.46	0.48
1:A:153:PHE:O	1:A:156:SER:HB2	2.13	0.48
1:C:73:GLU:CA	1:C:76:GLN:HB3	2.42	0.48
1:D:192:ALA:O	1:D:196:PHE:HB3	2.13	0.48
1:C:22:MET:SD	1:C:47:ALA:HB2	2.54	0.48
1:B:27:LYS:O	1:B:30:THR:HG22	2.13	0.48
1:D:158:LYS:HB2	1:D:158:LYS:NZ	2.28	0.48
1:D:39:GLU:O	1:D:43:LEU:HB2	2.13	0.48
1:A:117:PHE:HB2	1:A:166:ILE:HD12	1.95	0.48
1:C:219:GLN:HE21	1:C:223:ASP:HB2	1.77	0.48
1:C:155:ILE:HG22	1:C:155:ILE:O	2.14	0.48
1:A:106:ILE:HB	1:A:119:LEU:HD11	1.96	0.48
1:A:115:LYS:HB3	1:A:115:LYS:HZ2	1.79	0.48
1:B:1:MET:HB2	1:B:32:GLN:OE1	2.13	0.48
1:C:38:ASN:HA	1:C:41:ARG:HB3	1.95	0.48
1:D:6:LEU:HB3	1:D:29:VAL:HG23	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: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:D:156:SER:OG	1:D:167:ARG:HG3	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:C:116:VAL:HG11	1:C:160:MET:HE2	1.90	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:CG1	1:D:160:MET:HE1	2.42	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: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:HB3	1:D:115:LYS:NZ	2.29	0.47
1:D:7:VAL:CG2	1:D:29:VAL:HG21	2.41	0.47
1:D:1:MET:HB2	1:D:32:GLN:OE1	2.15	0.47
1:C:124:ASP:O	1:C:127:ARG:HB3	2.15	0.47
1:C:6:LEU:HB2	1:C:29:VAL:HG23	1.97	0.47
1:C:1:MET:HB2	1:C:32:GLN:OE1	2.15	0.47
1:A:97:VAL:HG11	1:A:125:TYR:CD2	2.50	0.47
1:B:127:ARG:O	1:B:131:GLU:HG3	2.15	0.47
1:A:17:GLU:O	1:A:17:GLU:HG2	2.13	0.47
1:B:55:ARG:HB3	1:B:90:LEU:HB2	1.95	0.47
1:C:73:GLU:O	1:C:76:GLN:HB3	2.15	0.46
1:D:129:LEU:HB3	1:D:141:ILE:HG21	1.96	0.46
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.97	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: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:D:156:SER:HA	1:D:160:MET:HE3	1.97	0.46
1:A:98:LEU:HA	1:A:98:LEU:HD12	1.82	0.46
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.46	0.46
1:A:90:LEU:CD2	1:A:132:VAL:HG21	2.46	0.46
1:A:66:GLU:CG	1:A:76:GLN:HG3	2.46	0.46
1:D:188:ALA:C	1:D:190:SER:H	2.19	0.46
1:C:166:ILE:HG23	1:C:167:ARG:N	2.26	0.45
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: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:D:30:THR:OG1	1:D:36:LEU:HD21	2.17	0.45
1:C:45:SER:O	1:C:49:LYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:O	1:C:131:GLU:HG3	2.16	0.45
1:C:32:GLN:HB3	1:C:33:GLY:H	1.50	0.45
1:C:202:GLU:HG2	1:C:202:GLU:O	2.17	0.45
1:D:6:LEU:CB	1:D:29:VAL:HG23	2.47	0.45
1:C:44:LEU:HD21	1:C:105:LEU:HD21	1.99	0.45
1:B:155:ILE:CG2	1:B:155:ILE:O	2.64	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:A:58:SER:O	1:A:62:VAL:HG12	2.17	0.45
1:C:61:VAL:HG11	1:D:16:ALA:HA	1.98	0.45
1:B:160:MET:HE3	1:B:160:MET:HB2	1.94	0.44
1:C:174:PHE:O	1:C:177:PHE:HB3	2.16	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
1:B:22:MET:HE2	1:B:43:LEU:O	2.17	0.44
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: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:A:3:LYS:O	1:A:7:VAL:HG23	2.17	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:C:106:ILE:N	1:C:107:PRO:HD2	2.32	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:74:LYS:C	1:C:76:GLN:N	2.71	0.44
1:C:147:GLN:O	1:C:151:GLU:HB2	2.18	0.44
1:D:188:ALA:C	1:D:190:SER:N	2.70	0.44
1:D:166:ILE:HG23	1:D:167:ARG:N	2.32	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:D:11:LYS:HG3	1:D:43:LEU:HD21	2.00	0.44
1:B:109:ALA:HB3	1:B:115:LYS:HG2	2.00	0.43
1:A:2:ASP:O	1:A:6:LEU:HD22	2.18	0.43
1:C:149:TYR:CE2	1:C:177:PHE:HB2	2.53	0.43
1:B:46:VAL:O	1:B:50:ASN:ND2	2.50	0.43
1:C:116:VAL:HG21	1:C:160:MET:HE1	1.99	0.43
1:D:137:ASP:O	1:D:141:ILE:HG13	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:86:ILE:O	1:A:86:ILE:HG22	2.19	0.43
1:A:77:GLN:O	1:A:81:GLU:HB2	2.18	0.43
1:A:113:GLU:CG	1:A:114:SER:N	2.77	0.43
1:C:155:ILE:HG23	1:C:158:LYS:HD2	2.01	0.43
1:C:62:VAL:HG23	1:D:12:LEU:HD11	2.00	0.43
1:A:222:ARG:O	1:A:225:LEU:HB2	2.19	0.43
1:A:83:ARG:O	1:A:87:GLU:HB2	2.18	0.43
1:C:18:ARG:CZ	1:D:86:ILE:HG12	2.48	0.43
1:D:119:LEU:CB	1:D:152:ALA:HB2	2.48	0.43
1:C:100:LEU:O	1:C:104:PHE:HB2	2.18	0.43
1:B:18:ARG:H	1:B:18:ARG:HG2	1.63	0.43
1:C:87:GLU:HG2	1:C:132:VAL:CG1	2.47	0.43
1:A:172:LEU:HD13	1:A:221:LEU:HB3	2.01	0.43
1:C:100:LEU:HD13	1:C:100:LEU:N	2.33	0.43
1:C:129:LEU:HA	1:C:129:LEU:HD12	1.84	0.43
1:A:6:LEU:HB3	1:A:29:VAL:HG23	2.01	0.43
1:D:52:VAL:HG11	1:D:125:TYR:CE1	2.54	0.42
1:A:49:LYS:HA	1:A:52:VAL:HG12	2.01	0.42
1:D:56:ARG:HD2	1:D:128:TYR:CD2	2.54	0.42
1:D:37:SER:HB3	1:D:40:GLU:HG3	2.01	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:D:76:GLN:O	1:D:80:ARG:N	2.50	0.42
1:C:217:ILE:HG13	1:C:217:ILE:H	1.51	0.42
1:A:62:VAL:HG23	1:B:12:LEU:HD11	2.00	0.42
1:C:117:PHE:C	1:C:117:PHE:HD1	2.22	0.42
1:D:37:SER:O	1:D:40:GLU:N	2.53	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:C:91:ARG:NH1	1:C:132:VAL:HG12	2.35	0.42
1:C:16:ALA:O	1:C:17:GLU:HB3	2.19	0.42
1:D:117:PHE:C	1:D:117:PHE:CD1	2.92	0.42
1:C:202:GLU:CG	1:C:202:GLU:O	2.68	0.41
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:D:143:ASP:O	1:D:147:GLN:HG2	2.20	0.41
1:B:103:LYS:HE2	1:B:103:LYS:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:HG3	1:B:132:VAL:CG2	2.49	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:B:200:ILE:CG2	1:B:200:ILE:O	2.68	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:HA	1:D:98:LEU:HD12	1.90	0.41
1:C:120:LYS:HE2	1:C:120:LYS:HB3	1.79	0.41
1:A:29:VAL:O	1:A:32:GLN:HB2	2.20	0.41
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:D:200:ILE:HG23	1:D:203:LEU:CD1	2.51	0.41
1:D:10:ALA:HB2	1:D:26:MET:SD	2.61	0.41
1:C:153:PHE:CA	1:C:170:LEU:HD21	2.45	0.40
1:A:97:VAL:HA	1:A:100:LEU:HD22	2.03	0.40
1:B:155:ILE:HG12	1:B:158:LYS:HE2	2.02	0.40
1:A:171:ALA:O	1:A:175:SER:HB2	2.21	0.40
1:D:155:ILE:O	1:D:158:LYS:CB	2.69	0.40
1:C:173:ASN:CA	1:C:176:VAL:HG12	2.46	0.40
1:B:160:MET:CE	1:B:167:ARG:HB2	2.51	0.40
1:B:4:ASN:HA	1:B:7:VAL:HB	2.04	0.40
1:C:173:ASN:HA	1:C:176:VAL:CG1	2.47	0.40
1:C:78:MET:HE1	1:D:9:LYS:HG2	2.04	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%)	12 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	185/245 (76%)	161 (87%)	20 (11%)	4 (2%)	8 28
1	C	185/245 (76%)	165 (89%)	17 (9%)	3 (2%)	12 38
1	D	185/245 (76%)	158 (85%)	24 (13%)	3 (2%)	12 38
All	All	740/980 (76%)	639 (86%)	88 (12%)	13 (2%)	11 34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ALA
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/209 (81%)	132 (78%)	37 (22%)	1 3
1	B	169/209 (81%)	138 (82%)	31 (18%)	2 6
1	C	169/209 (81%)	140 (83%)	29 (17%)	2 7
1	D	169/209 (81%)	137 (81%)	32 (19%)	2 5
All	All	676/836 (81%)	547 (81%)	129 (19%)	2 5

All (129) 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
1	A	46	VAL
1	A	67	GLN
1	A	78	MET
1	A	81	GLU
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	129	LEU
1	A	143	ASP
1	A	158	LYS
1	A	174	PHE
1	A	177	PHE
1	A	179	TYR
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	A	228	TRP
1	B	1	MET
1	B	2	ASP
1	B	14	GLU
1	B	17	GLU
1	B	28	SER
1	B	36	LEU

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Mol	Chain	Res	Type
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
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	149	TYR
1	B	150	GLN
1	B	189	CYS
1	B	190	SER
1	B	196	PHE
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	17	GLU
1	C	32	GLN
1	C	36	LEU
1	C	43	LEU
1	C	67	GLN
1	C	81	GLU
1	C	82	TYR
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

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Mol	Chain	Res	Type
1	C	117	PHE
1	C	149	TYR
1	C	158	LYS
1	C	174	PHE
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	28	SER
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	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	117	PHE
1	D	127	ARG
1	D	132	VAL
1	D	137	ASP
1	D	157	LYS
1	D	168	LEU
1	D	176	VAL
1	D	189	CYS
1	D	190	SER
1	D	196	PHE
1	D	219	GLN
1	D	221	LEU
1	D	222	ARG
1	D	225	LEU

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Mol	Chain	Res	Type
1	D	227	LEU
1	D	228	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	95	ASN
1	A	146	GLN
1	A	219	GLN
1	B	50	ASN
1	B	95	ASN
1	C	146	GLN
1	C	147	GLN
1	C	150	GLN
1	C	219	GLN
1	D	146	GLN
1	D	219	GLN

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 carbohydrates 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, 95^{th} 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%)	1.67	59 (29%)	1	0	12, 34, 57, 66	0
1	B	197/245 (80%)	1.60	61 (30%)	1	0	13, 34, 57, 67	0
1	C	197/245 (80%)	1.61	63 (31%)	1	0	13, 34, 57, 66	0
1	D	197/245 (80%)	1.66	62 (31%)	1	0	12, 33, 57, 67	0
All	All	788/980 (80%)	1.64	245 (31%)	1	0	12, 34, 57, 67	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	7.9
1	A	200	ILE	7.1
1	D	156	SER	6.3
1	D	224	ASN	6.2
1	D	68	LYS	6.2
1	B	224	ASN	5.7
1	B	228	TRP	5.4
1	D	197	ASP	5.2
1	D	216	LEU	5.1
1	D	192	ALA	5.1
1	B	200	ILE	5.0
1	D	196	PHE	5.0
1	B	196	PHE	4.8
1	A	226	THR	4.7
1	C	219	GLN	4.6
1	C	86	ILE	4.6
1	B	218	MET	4.6
1	A	228	TRP	4.6
1	B	192	ALA	4.5
1	B	34	ALA	4.5
1	B	199	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	196	PHE	4.5
1	C	216	LEU	4.4
1	C	228	TRP	4.4
1	D	62	VAL	4.3
1	D	33	GLY	4.3
1	A	166	ILE	4.3
1	A	47	ALA	4.3
1	A	189	CYS	4.3
1	B	155	ILE	4.2
1	D	178	TYR	4.2
1	D	86	ILE	4.2
1	B	68	LYS	4.2
1	B	75	LYS	4.1
1	A	196	PHE	4.1
1	D	200	ILE	4.1
1	C	33	GLY	4.1
1	B	216	LEU	4.1
1	A	155	ILE	4.0
1	C	166	ILE	4.0
1	C	132	VAL	4.0
1	A	217	ILE	4.0
1	A	219	GLN	3.9
1	B	36	LEU	3.9
1	A	199	ALA	3.9
1	D	108	ASN	3.9
1	A	216	LEU	3.9
1	D	30	THR	3.9
1	D	134	ALA	3.8
1	A	30	THR	3.7
1	A	192	ALA	3.7
1	C	34	ALA	3.7
1	A	62	VAL	3.7
1	A	175	SER	3.7
1	D	228	TRP	3.6
1	C	73	GLU	3.6
1	D	116	VAL	3.6
1	A	222	ARG	3.5
1	A	68	LYS	3.4
1	B	30	THR	3.4
1	B	116	VAL	3.4
1	B	222	ARG	3.4
1	C	145	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	203	LEU	3.3
1	A	227	LEU	3.3
1	A	78	MET	3.3
1	C	224	ASN	3.3
1	D	175	SER	3.3
1	C	3	LYS	3.3
1	D	115	LYS	3.3
1	D	141	ILE	3.2
1	D	217	ILE	3.2
1	C	200	ILE	3.2
1	C	116	VAL	3.2
1	B	172	LEU	3.1
1	D	120	LYS	3.1
1	A	218	MET	3.1
1	D	199	ALA	3.1
1	B	203	LEU	3.1
1	D	177	PHE	3.0
1	C	199	ALA	3.0
1	C	4	ASN	3.0
1	C	100	LEU	3.0
1	D	222	ARG	3.0
1	D	76	GLN	3.0
1	B	29	VAL	2.9
1	B	145	SER	2.9
1	C	156	SER	2.9
1	A	108	ASN	2.9
1	B	191	LEU	2.9
1	A	179	TYR	2.9
1	D	218	MET	2.9
1	B	175	SER	2.9
1	A	195	ALA	2.9
1	A	172	LEU	2.9
1	C	217	ILE	2.9
1	C	135	GLY	2.9
1	D	7	VAL	2.8
1	C	30	THR	2.8
1	A	168	LEU	2.8
1	B	86	ILE	2.8
1	D	100	LEU	2.8
1	B	67	GLN	2.8
1	D	44	LEU	2.8
1	A	36	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	221	LEU	2.8
1	B	189	CYS	2.8
1	D	48	TYR	2.8
1	C	222	ARG	2.8
1	B	82	TYR	2.7
1	A	203	LEU	2.7
1	D	202	GLU	2.6
1	B	221	LEU	2.6
1	C	160	MET	2.6
1	D	12	LEU	2.6
1	B	226	THR	2.6
1	A	145	SER	2.6
1	B	119	LEU	2.6
1	B	201	ALA	2.6
1	D	135	GLY	2.6
1	B	93	ILE	2.6
1	D	34	ALA	2.6
1	A	104	PHE	2.6
1	C	170	LEU	2.5
1	D	160	MET	2.5
1	B	101	LEU	2.5
1	C	172	LEU	2.5
1	A	119	LEU	2.5
1	C	168	LEU	2.5
1	B	114	SER	2.5
1	C	58	SER	2.5
1	C	143	ASP	2.5
1	C	197	ASP	2.5
1	B	10	ALA	2.5
1	B	195	ALA	2.5
1	D	75	LYS	2.5
1	D	29	VAL	2.5
1	A	141	ILE	2.5
1	B	104	PHE	2.5
1	C	114	SER	2.5
1	B	152	ALA	2.5
1	C	93	ILE	2.5
1	B	167	ARG	2.5
1	A	7	VAL	2.5
1	D	227	LEU	2.4
1	C	48	TYR	2.4
1	C	47	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	7	VAL	2.4
1	C	36	LEU	2.4
1	D	226	THR	2.4
1	A	13	ALA	2.4
1	B	125	TYR	2.4
1	B	61	VAL	2.4
1	D	1	MET	2.4
1	A	159	GLU	2.4
1	D	119	LEU	2.4
1	D	148	ALA	2.4
1	A	140	GLY	2.4
1	C	192	ALA	2.4
1	C	37	SER	2.4
1	D	51	VAL	2.4
1	A	160	MET	2.4
1	B	22	MET	2.4
1	C	177	PHE	2.4
1	C	201	ALA	2.4
1	A	93	ILE	2.4
1	A	106	ILE	2.4
1	B	142	VAL	2.4
1	D	221	LEU	2.4
1	C	109	ALA	2.4
1	A	114	SER	2.4
1	C	108	ASN	2.4
1	B	62	VAL	2.4
1	D	172	LEU	2.3
1	D	109	ALA	2.3
1	D	65	ILE	2.3
1	B	160	MET	2.3
1	C	188	ALA	2.3
1	D	166	ILE	2.3
1	D	125	TYR	2.3
1	B	77	GLN	2.3
1	D	179	TYR	2.3
1	C	104	PHE	2.3
1	D	97	VAL	2.3
1	C	75	LYS	2.3
1	A	132	VAL	2.3
1	B	97	VAL	2.3
1	D	220	LEU	2.3
1	B	48	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	75	LYS	2.3
1	A	115	LYS	2.3
1	B	3	LYS	2.3
1	D	22	MET	2.3
1	C	226	THR	2.3
1	C	62	VAL	2.3
1	B	6	LEU	2.3
1	B	8	GLN	2.3
1	B	156	SER	2.2
1	A	170	LEU	2.2
1	C	95	ASN	2.2
1	A	29	VAL	2.2
1	A	39	GLU	2.2
1	B	176	VAL	2.2
1	D	46	VAL	2.2
1	D	73	GLU	2.2
1	C	152	ALA	2.2
1	B	153	PHE	2.2
1	C	12	LEU	2.2
1	C	119	LEU	2.2
1	C	141	ILE	2.1
1	A	34	ALA	2.1
1	C	136	ASP	2.1
1	D	60	ARG	2.1
1	D	219	GLN	2.1
1	A	44	LEU	2.1
1	A	112	ALA	2.1
1	A	152	ALA	2.1
1	A	176	VAL	2.1
1	B	225	LEU	2.1
1	B	99	SER	2.1
1	C	115	LYS	2.1
1	A	194	THR	2.1
1	A	4	ASN	2.1
1	B	59	TRP	2.1
1	C	101	LEU	2.1
1	C	113	GLU	2.1
1	C	22	MET	2.1
1	C	32	GLN	2.1
1	C	29	VAL	2.1
1	C	60	ARG	2.1
1	C	84	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	79	ALA	2.0
1	A	51	VAL	2.0
1	A	191	LEU	2.0
1	B	12	LEU	2.0
1	B	46	VAL	2.0
1	B	220	LEU	2.0
1	D	37	SER	2.0
1	C	174	PHE	2.0
1	A	86	ILE	2.0
1	A	79	ALA	2.0
1	A	135	GLY	2.0
1	D	13	ALA	2.0
1	B	7	VAL	2.0
1	D	79	ALA	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 carbohydrates 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.