Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:09 AM GMT

PDB ID	:	2FVZ
Title	:	Human Inositol Monophosphophosphatase 2
Authors	:	Ogg, D.; Hallberg, B.M.; Arrowsmith, C.; Berglund, H.; Collins, R.; Edwards, A.; Ehn, M.; Flodin, S.; Graslund, S.; Hammarstrom, M.; Hogbom, M.; Holmberg-Schiavone, L.; Kotenyova, T.; Kursula, P.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Van Den Berg, S.; Weigelt, J.; Thorsell, A.G.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-01-31
Resolution	:	2.40 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:

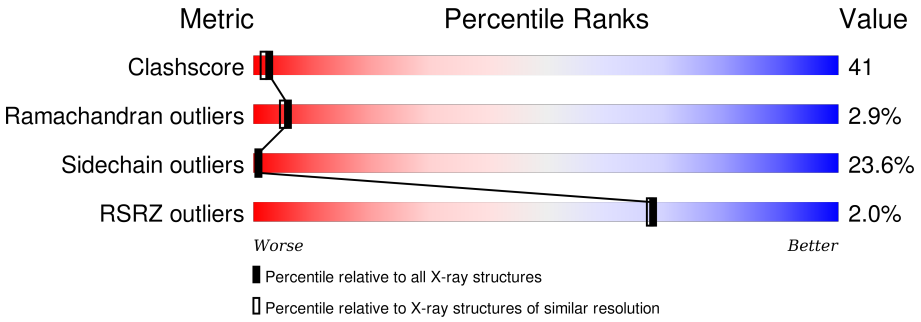
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	273	35% 44% 10% 11%
1	B	273	35% 42% 12% 11%
1	C	273	30% 44% 15% 11%
1	D	273	33% 38% 15% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7516 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 Inositol monophosphatase 2.

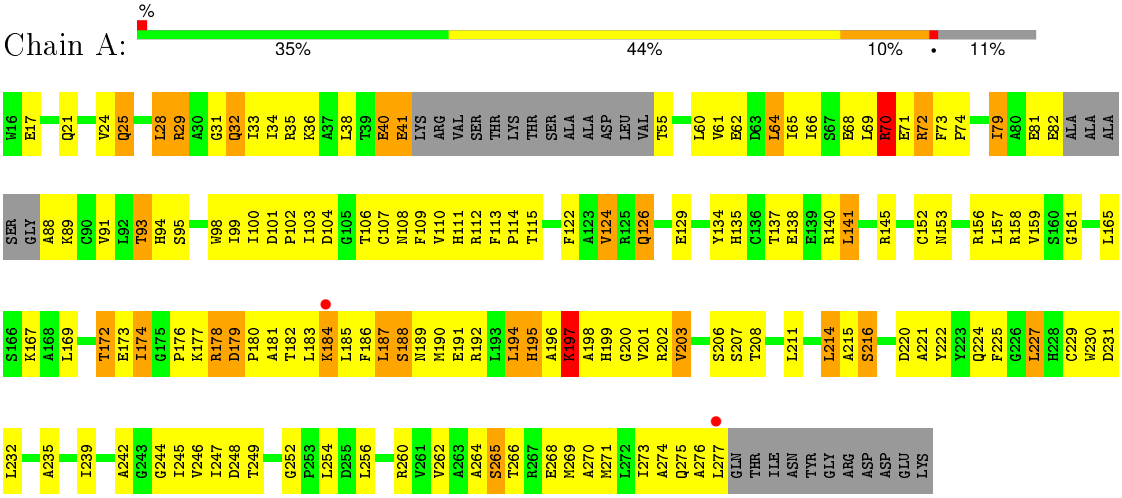
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1878	1185	337	344	12			
1	B	244	Total	C	N	O	S	0	0	0
			1878	1185	337	344	12			
1	C	244	Total	C	N	O	S	0	0	0
			1882	1188	338	344	12			
1	D	244	Total	C	N	O	S	0	0	0
			1878	1185	337	344	12			

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.

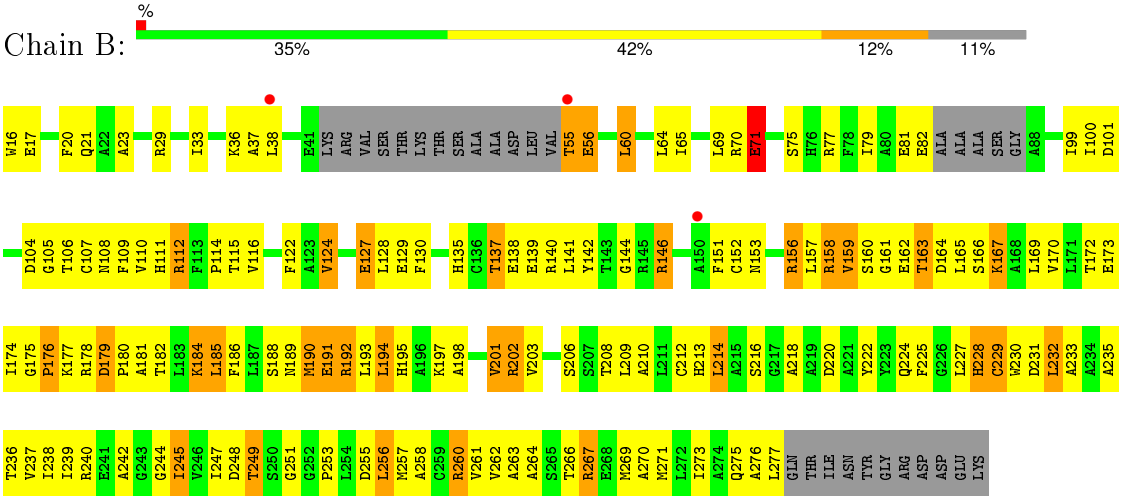
- Molecule 1: Inositol monophosphatase 2

Chain A:



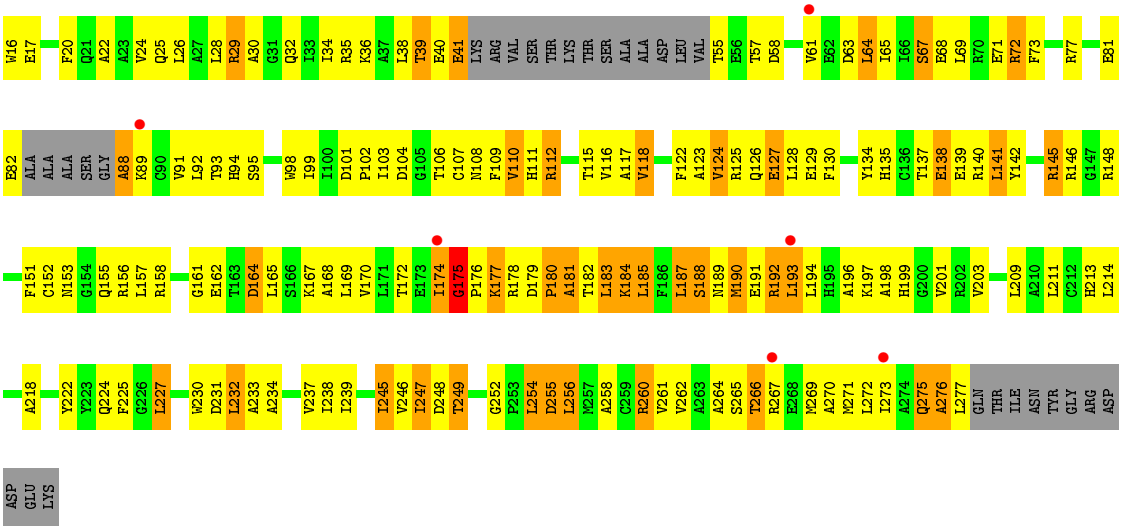
- Molecule 1: Inositol monophosphatase 2

Chain B:



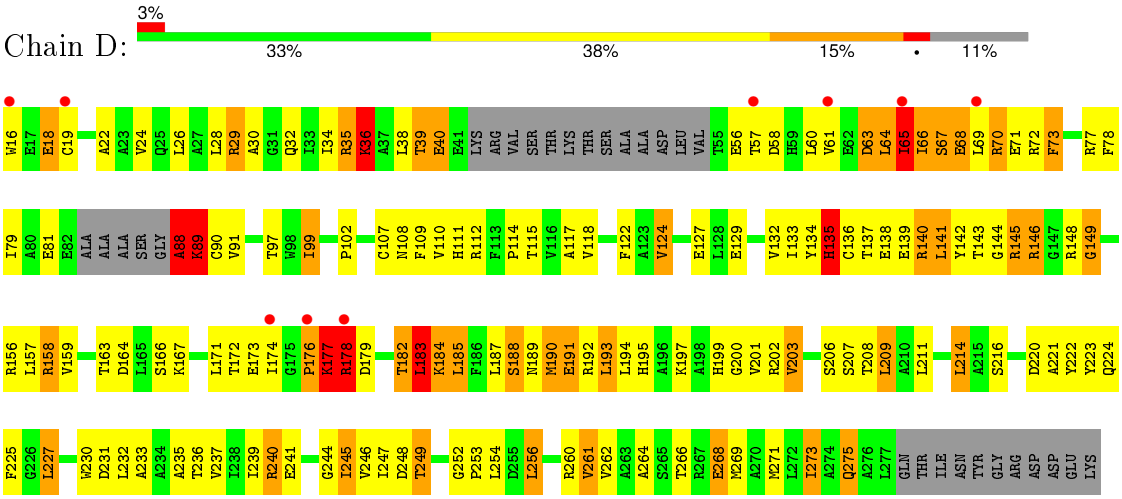
- Molecule 1: Inositol monophosphatase 2

Chain C:



• Molecule 1: Inositol monophosphatase 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.03Å 96.95Å 106.97Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 28.94 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-2.40) 97.6 (28.94-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.95 (at 2.36Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.211 , 0.297 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.0	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 201030 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7516	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.39	0/1911	0.53	0/2587
1	B	0.64	4/1911 (0.2%)	0.56	1/2587 (0.0%)
1	C	0.48	1/1915 (0.1%)	0.53	0/2591
1	D	1.42	5/1911 (0.3%)	0.86	5/2587 (0.2%)
All	All	0.84	10/7648 (0.1%)	0.64	6/10352 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	3
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	LYS	C-O	50.90	2.20	1.23
1	D	88	ALA	C-N	-25.68	0.74	1.34
1	B	71	GLU	CD-OE2	16.85	1.44	1.25
1	D	178	ARG	C-N	-10.74	1.09	1.34
1	B	71	GLU	CD-OE1	10.71	1.37	1.25
1	B	71	GLU	CB-CG	7.54	1.66	1.52
1	D	65	ILE	CG1-CD1	7.44	2.01	1.50
1	D	68	GLU	CD-OE1	6.46	1.32	1.25
1	C	175	GLY	N-CA	5.88	1.54	1.46
1	B	71	GLU	CG-CD	5.67	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	89	LYS	O-C-N	-26.75	79.89	122.70
1	D	88	ALA	O-C-N	-13.42	101.22	122.70
1	D	88	ALA	C-N-CA	12.65	153.34	121.70
1	D	178	ARG	O-C-N	-9.19	108.00	122.70
1	D	88	ALA	CA-C-N	6.40	131.28	117.20
1	B	71	GLU	CG-CD-OE2	-5.18	107.94	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	88	ALA	Peptide
1	D	178	ARG	Mainchain
1	D	88	ALA	Mainchain
1	D	89	LYS	Mainchain

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	1878	0	1871	141	0
1	B	1878	0	1871	158	0
1	C	1882	0	1882	176	0
1	D	1878	0	1869	163	0
All	All	7516	0	7493	611	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 41.

All (611) 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:65:ILE:CD1	1:D:65:ILE:CG1	2.01	1.37
1:D:89:LYS:O	1:D:91:VAL:N	1.69	1.26
1:C:88:ALA:HA	1:C:89:LYS:HB3	1.32	1.11
1:C:88:ALA:HB1	1:C:89:LYS:HG2	1.07	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HB2	1:C:39:THR:HG21	1.39	1.04
1:C:165:LEU:HB2	1:C:272:LEU:HD13	1.39	1.03
1:C:88:ALA:HB1	1:C:89:LYS:CG	1.94	0.96
1:C:165:LEU:HD12	1:C:272:LEU:HB3	1.47	0.96
1:D:178:ARG:HB3	1:D:183:LEU:CD2	1.95	0.96
1:C:88:ALA:CB	1:C:89:LYS:HG2	1.96	0.94
1:D:190:MET:HE3	1:D:201:VAL:HG21	1.47	0.93
1:C:161:GLY:H	1:C:265:SER:HB2	1.35	0.90
1:B:159:VAL:HG23	1:B:161:GLY:H	1.32	0.90
1:D:26:LEU:HB3	1:D:65:ILE:HD12	1.54	0.88
1:C:179:ASP:O	1:C:179:ASP:OD1	1.91	0.87
1:B:267:ARG:O	1:B:271:MET:HG2	1.74	0.86
1:C:102:PRO:O	1:C:118:VAL:HG13	1.77	0.85
1:C:224:GLN:HG2	1:C:227:LEU:HB3	1.58	0.85
1:C:88:ALA:HA	1:C:89:LYS:CB	2.07	0.83
1:C:227:LEU:HD11	1:C:232:LEU:HD13	1.59	0.83
1:C:168:ALA:HB2	1:C:269:MET:HE1	1.60	0.81
1:A:34:ILE:HG23	1:A:109:PHE:HE1	1.44	0.81
1:A:68:GLU:O	1:A:72:ARG:HB2	1.80	0.81
1:B:249:THR:HB	1:B:260:ARG:HD2	1.60	0.81
1:D:178:ARG:HB3	1:D:183:LEU:HD22	1.62	0.81
1:D:134:TYR:HB2	1:D:141:LEU:HD23	1.62	0.81
1:A:211:LEU:HB3	1:A:239:ILE:HD11	1.62	0.81
1:C:190:MET:HE3	1:C:201:VAL:HG21	1.62	0.81
1:C:183:LEU:O	1:C:187:LEU:HD12	1.81	0.80
1:D:89:LYS:O	1:D:89:LYS:C	2.20	0.80
1:C:38:LEU:HD23	1:C:112:ARG:HD2	1.63	0.79
1:B:159:VAL:HG13	1:B:242:ALA:O	1.83	0.78
1:C:254:LEU:HD21	1:C:256:LEU:HD13	1.64	0.78
1:D:102:PRO:O	1:D:118:VAL:HG22	1.83	0.78
1:D:60:LEU:O	1:D:64:LEU:HB2	1.83	0.78
1:D:26:LEU:HB3	1:D:65:ILE:CD1	2.14	0.78
1:C:63:ASP:O	1:C:67:SER:HB3	1.83	0.78
1:A:244:GLY:O	1:A:245:ILE:HD13	1.84	0.77
1:A:107:CYS:O	1:A:110:VAL:HG22	1.84	0.76
1:C:164:ASP:HB3	1:C:167:LYS:HB2	1.66	0.76
1:B:218:ALA:HA	1:C:111:HIS:O	1.84	0.76
1:D:178:ARG:HB3	1:D:183:LEU:HD21	1.66	0.76
1:D:61:VAL:HB	1:D:102:PRO:HB3	1.67	0.75
1:C:61:VAL:O	1:C:65:ILE:HG13	1.84	0.75
1:A:195:HIS:O	1:A:197:LYS:HE3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ALA:O	1:A:239:ILE:HG13	1.86	0.75
1:C:245:ILE:HD13	1:C:267:ARG:HA	1.69	0.75
1:A:246:VAL:HG12	1:A:254:LEU:HD13	1.68	0.75
1:C:130:PHE:HA	1:C:237:VAL:HG11	1.69	0.75
1:A:93:THR:O	1:A:126:GLN:HG3	1.87	0.74
1:D:108:ASN:ND2	1:D:115:THR:HB	2.03	0.74
1:D:63:ASP:O	1:D:67:SER:HB3	1.90	0.72
1:C:64:LEU:HD22	1:C:64:LEU:O	1.89	0.71
1:A:178:ARG:HA	1:A:183:LEU:HD11	1.71	0.71
1:D:36:LYS:O	1:D:39:THR:HB	1.90	0.71
1:A:17:GLU:O	1:A:21:GLN:HG2	1.89	0.71
1:D:18:GLU:OE2	1:D:72:ARG:NH2	2.24	0.70
1:C:225:PHE:HA	1:C:260:ARG:HB3	1.73	0.70
1:B:20:PHE:O	1:B:23:ALA:HB3	1.92	0.70
1:D:232:LEU:HD11	1:D:261:VAL:HG21	1.74	0.70
1:D:179:ASP:OD2	1:D:182:THR:OG1	2.09	0.69
1:D:24:VAL:O	1:D:28:LEU:HG	1.93	0.69
1:A:74:PRO:CB	1:C:39:THR:HG21	2.20	0.69
1:B:165:LEU:O	1:B:198:ALA:HA	1.93	0.69
1:A:62:GLU:OE2	1:A:82:GLU:HB2	1.92	0.69
1:D:61:VAL:O	1:D:65:ILE:HG12	1.92	0.69
1:D:232:LEU:HD21	1:D:254:LEU:HD11	1.75	0.69
1:D:79:ILE:HB	1:D:99:ILE:HG23	1.74	0.69
1:B:174:ILE:HD12	1:B:175:GLY:O	1.92	0.69
1:C:165:LEU:HD23	1:C:165:LEU:O	1.93	0.68
1:A:184:LYS:HD2	1:A:187:LEU:HD12	1.75	0.68
1:D:235:ALA:O	1:D:239:ILE:HG13	1.94	0.68
1:D:166:SER:HA	1:D:197:LYS:O	1.93	0.68
1:C:264:ALA:HB3	1:C:270:ALA:HB2	1.75	0.68
1:A:34:ILE:HG23	1:A:109:PHE:CE1	2.29	0.68
1:B:181:ALA:O	1:B:185:LEU:HB2	1.94	0.68
1:B:159:VAL:HG23	1:B:161:GLY:N	2.07	0.67
1:D:248:ASP:HB2	1:D:253:PRO:O	1.93	0.67
1:B:166:SER:HA	1:B:197:LYS:O	1.94	0.67
1:D:178:ARG:CB	1:D:183:LEU:HD22	2.25	0.67
1:D:182:THR:O	1:D:183:LEU:HD13	1.94	0.67
1:D:146:ARG:HA	1:D:241:GLU:OE2	1.94	0.67
1:B:114:PRO:HB2	1:B:137:THR:HG21	1.75	0.67
1:A:190:MET:HE1	1:A:201:VAL:HG11	1.76	0.67
1:C:88:ALA:CA	1:C:89:LYS:HB3	2.20	0.67
1:C:180:PRO:HA	1:C:183:LEU:HB2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ILE:HG22	1:C:230:TRP:HA	1.77	0.66
1:C:161:GLY:N	1:C:265:SER:HB2	2.10	0.66
1:B:170:VAL:O	1:B:201:VAL:HA	1.97	0.65
1:A:198:ALA:O	1:D:178:ARG:NH1	2.29	0.65
1:D:190:MET:HE1	1:D:201:VAL:HG11	1.77	0.65
1:B:192:ARG:O	1:B:195:HIS:HB3	1.96	0.65
1:B:152:CYS:CB	1:B:157:LEU:HD21	2.27	0.65
1:D:16:TRP:CZ2	1:D:124:VAL:HG11	2.30	0.65
1:C:164:ASP:OD2	1:C:167:LYS:HD3	1.95	0.65
1:D:30:ALA:HB2	1:D:65:ILE:HD11	1.79	0.65
1:D:88:ALA:O	1:D:90:CYS:N	2.30	0.65
1:C:88:ALA:CA	1:C:89:LYS:CB	2.76	0.64
1:C:176:PRO:HD2	1:C:177:LYS:HE2	1.79	0.64
1:A:174:ILE:HD11	1:D:202:ARG:HH12	1.62	0.64
1:A:169:LEU:HD11	1:A:202:ARG:HG2	1.79	0.64
1:A:88:ALA:HB2	1:B:21:GLN:OE1	1.97	0.64
1:C:272:LEU:O	1:C:275:GLN:HB2	1.98	0.64
1:D:134:TYR:HA	1:D:140:ARG:O	1.97	0.64
1:A:188:SER:O	1:A:192:ARG:HG3	1.97	0.64
1:C:255:ASP:HB3	1:C:258:ALA:HB2	1.79	0.64
1:D:184:LYS:HA	1:D:187:LEU:HD12	1.79	0.64
1:B:214:LEU:HD12	1:B:239:ILE:HD13	1.80	0.64
1:A:184:LYS:HA	1:A:187:LEU:HD12	1.80	0.64
1:B:186:PHE:O	1:B:190:MET:HB2	1.98	0.64
1:C:81:GLU:HG2	1:C:82:GLU:HG2	1.81	0.63
1:D:108:ASN:HD22	1:D:115:THR:HB	1.61	0.63
1:D:163:THR:HG22	1:D:268:GLU:HB2	1.80	0.63
1:C:36:LYS:O	1:C:39:THR:HB	1.98	0.63
1:D:249:THR:HB	1:D:260:ARG:HG3	1.80	0.63
1:D:30:ALA:HB1	1:D:61:VAL:HG13	1.80	0.63
1:D:195:HIS:O	1:D:197:LYS:HE3	1.97	0.63
1:C:172:THR:O	1:C:203:VAL:HB	1.98	0.63
1:D:188:SER:HB2	1:D:192:ARG:HH11	1.63	0.63
1:C:34:ILE:HD11	1:C:103:ILE:HG12	1.81	0.63
1:C:190:MET:HE1	1:C:201:VAL:HG11	1.82	0.62
1:B:38:LEU:HD21	1:B:109:PHE:CD1	2.34	0.62
1:D:66:ILE:HD13	1:D:78:PHE:CD1	2.35	0.62
1:A:71:GLU:O	1:A:71:GLU:CG	2.47	0.62
1:A:179:ASP:OD1	1:A:182:THR:HG23	2.00	0.62
1:A:135:HIS:CE1	1:A:137:THR:HB	2.35	0.62
1:A:61:VAL:HG12	1:A:102:PRO:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:HG23	1:B:209:LEU:HD12	1.82	0.61
1:C:24:VAL:O	1:C:28:LEU:HG	2.00	0.61
1:D:134:TYR:CE2	1:D:136:CYS:HA	2.36	0.61
1:C:38:LEU:CD2	1:C:112:ARG:HD2	2.30	0.61
1:D:34:ILE:HD12	1:D:136:CYS:SG	2.40	0.61
1:B:137:THR:HG22	1:B:138:GLU:HG2	1.81	0.61
1:B:191:GLU:O	1:B:195:HIS:HB2	2.01	0.60
1:B:191:GLU:HG3	1:B:192:ARG:N	2.16	0.60
1:C:227:LEU:HD23	1:C:260:ARG:HA	1.84	0.60
1:B:152:CYS:HB2	1:B:157:LEU:HD21	1.84	0.60
1:C:72:ARG:HB3	1:C:73:PHE:CD1	2.37	0.60
1:C:88:ALA:CB	1:C:89:LYS:CG	2.69	0.60
1:A:74:PRO:HB2	1:C:39:THR:CG2	2.25	0.60
1:D:99:ILE:HD12	1:D:233:ALA:HB2	1.83	0.60
1:B:71:GLU:O	1:B:71:GLU:OE2	2.20	0.60
1:B:235:ALA:O	1:B:239:ILE:HG13	2.02	0.59
1:D:24:VAL:HG13	1:D:141:LEU:HD11	1.84	0.59
1:C:225:PHE:CE2	1:C:249:THR:HG21	2.37	0.59
1:A:178:ARG:HD2	1:A:183:LEU:HD11	1.83	0.59
1:C:34:ILE:CD1	1:C:103:ILE:HG12	2.32	0.59
1:B:245:ILE:HD13	1:B:267:ARG:HA	1.84	0.59
1:D:236:THR:O	1:D:240:ARG:HG3	2.02	0.59
1:D:81:GLU:HA	1:D:230:TRP:CH2	2.37	0.59
1:D:135:HIS:CD2	1:D:138:GLU:HB2	2.37	0.59
1:A:249:THR:HG22	1:A:260:ARG:NE	2.17	0.59
1:C:72:ARG:HB3	1:C:73:PHE:CE1	2.38	0.59
1:B:163:THR:HG23	1:B:266:THR:HG21	1.83	0.59
1:D:89:LYS:O	1:D:90:CYS:N	2.36	0.59
1:A:192:ARG:HD2	1:A:277:LEU:HA	1.85	0.59
1:A:190:MET:CE	1:A:201:VAL:HG11	2.33	0.59
1:A:24:VAL:O	1:A:28:LEU:HG	2.03	0.59
1:C:40:GLU:O	1:C:41:GLU:OE2	2.21	0.58
1:D:178:ARG:CA	1:D:183:LEU:HD22	2.32	0.58
1:B:108:ASN:ND2	1:B:115:THR:HB	2.18	0.58
1:C:185:LEU:HD22	1:C:189:ASN:ND2	2.18	0.58
1:B:129:GLU:OE1	1:B:129:GLU:HA	2.03	0.58
1:C:189:ASN:HA	1:C:192:ARG:HG3	1.83	0.58
1:C:234:ALA:O	1:C:238:ILE:HG13	2.04	0.58
1:D:122:PHE:CE1	1:D:124:VAL:HG22	2.39	0.58
1:B:105:GLY:O	1:B:108:ASN:HB2	2.04	0.57
1:B:99:ILE:HG22	1:B:230:TRP:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:THR:HB	1:C:260:ARG:NE	2.19	0.57
1:D:188:SER:HB2	1:D:192:ARG:NH1	2.19	0.57
1:B:65:ILE:HG21	1:B:100:ILE:HD13	1.85	0.57
1:A:169:LEU:HD12	1:A:200:GLY:O	2.05	0.57
1:B:107:CYS:O	1:B:111:HIS:HD2	1.88	0.57
1:B:214:LEU:CD1	1:B:239:ILE:HD13	2.34	0.56
1:B:174:ILE:HD13	1:B:178:ARG:NH1	2.20	0.56
1:B:33:ILE:HG21	1:B:60:LEU:HD12	1.86	0.56
1:D:19:CYS:O	1:D:22:ALA:HB3	2.05	0.56
1:C:269:MET:O	1:C:272:LEU:HB2	2.04	0.56
1:C:141:LEU:O	1:C:152:CYS:HA	2.05	0.56
1:C:227:LEU:HD11	1:C:232:LEU:CD1	2.32	0.56
1:C:267:ARG:O	1:C:271:MET:HG2	2.05	0.56
1:A:174:ILE:HA	1:A:186:PHE:CE2	2.40	0.56
1:C:227:LEU:HD21	1:C:232:LEU:HD21	1.88	0.56
1:C:255:ASP:HB3	1:C:258:ALA:CB	2.36	0.56
1:C:104:ASP:O	1:C:116:VAL:HG13	2.04	0.56
1:B:38:LEU:HA	1:B:112:ARG:NH2	2.21	0.56
1:D:146:ARG:O	1:D:146:ARG:HG3	2.05	0.56
1:D:57:THR:O	1:D:61:VAL:HG23	2.06	0.56
1:D:39:THR:O	1:D:40:GLU:O	2.23	0.56
1:D:132:VAL:HG22	1:D:143:THR:HG22	1.88	0.56
1:D:191:GLU:O	1:D:195:HIS:HB2	2.06	0.55
1:A:135:HIS:CE1	1:A:138:GLU:HG2	2.41	0.55
1:C:188:SER:HB2	1:C:192:ARG:HH12	1.71	0.55
1:C:265:SER:O	1:C:266:THR:HG23	2.07	0.55
1:D:178:ARG:CB	1:D:183:LEU:CD2	2.76	0.55
1:C:140:ARG:HA	1:C:153:ASN:HD21	1.71	0.55
1:D:208:THR:HG22	1:D:231:ASP:O	2.06	0.55
1:B:127:GLU:HG2	1:B:146:ARG:NH2	2.21	0.55
1:A:157:LEU:HD22	1:A:216:SER:HB2	1.87	0.55
1:A:108:ASN:ND2	1:A:115:THR:HB	2.21	0.55
1:C:134:TYR:OH	1:C:139:GLU:HB3	2.07	0.55
1:B:225:PHE:CE2	1:B:249:THR:HG21	2.42	0.55
1:D:135:HIS:HD2	1:D:140:ARG:NH1	2.05	0.55
1:A:169:LEU:HD11	1:A:202:ARG:CG	2.36	0.55
1:B:167:LYS:NZ	1:B:167:LYS:HB3	2.21	0.55
1:A:88:ALA:HB2	1:B:21:GLN:NE2	2.21	0.55
1:D:134:TYR:HB2	1:D:141:LEU:CD2	2.35	0.55
1:C:16:TRP:CZ2	1:C:124:VAL:HG11	2.42	0.55
1:B:137:THR:CG2	1:B:138:GLU:HG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:HD21	1:C:256:LEU:CD1	2.36	0.55
1:D:188:SER:O	1:D:192:ARG:HD2	2.07	0.54
1:D:26:LEU:CB	1:D:65:ILE:HD12	2.33	0.54
1:D:79:ILE:HG13	1:D:97:THR:CG2	2.38	0.54
1:D:225:PHE:CE2	1:D:249:THR:HG21	2.43	0.54
1:C:24:VAL:HG13	1:C:141:LEU:HD11	1.89	0.54
1:C:170:VAL:HG11	1:C:193:LEU:HD11	1.88	0.54
1:A:264:ALA:HB3	1:A:270:ALA:HB2	1.88	0.54
1:A:214:LEU:HD12	1:A:239:ILE:HG23	1.90	0.54
1:A:179:ASP:OD2	1:A:181:ALA:HB3	2.08	0.54
1:A:81:GLU:HA	1:A:230:TRP:CH2	2.41	0.54
1:C:123:ALA:HB2	1:C:128:LEU:HD23	1.89	0.54
1:C:134:TYR:CZ	1:C:139:GLU:HA	2.43	0.54
1:D:157:LEU:HD22	1:D:216:SER:HA	1.89	0.54
1:C:38:LEU:HD23	1:C:112:ARG:CD	2.37	0.54
1:D:65:ILE:CD1	1:D:65:ILE:CB	2.83	0.54
1:A:71:GLU:O	1:A:71:GLU:CD	2.47	0.54
1:C:273:ILE:O	1:C:276:ALA:HB3	2.08	0.54
1:B:228:HIS:CD2	1:B:228:HIS:H	2.24	0.54
1:B:110:VAL:HG23	1:B:111:HIS:CD2	2.43	0.54
1:B:135:HIS:HB3	1:B:140:ARG:HB2	1.90	0.53
1:B:111:HIS:O	1:B:112:ARG:HB2	2.07	0.53
1:A:249:THR:HA	1:A:262:VAL:HG23	1.90	0.53
1:D:61:VAL:CB	1:D:102:PRO:HB3	2.38	0.53
1:B:164:ASP:OD2	1:B:167:LYS:HD3	2.09	0.53
1:D:190:MET:CE	1:D:201:VAL:HG11	2.39	0.53
1:A:99:ILE:HG22	1:A:230:TRP:HA	1.90	0.53
1:C:99:ILE:CG2	1:C:230:TRP:HA	2.37	0.53
1:C:192:ARG:HD3	1:C:277:LEU:N	2.23	0.53
1:D:227:LEU:O	1:D:227:LEU:HG	2.08	0.53
1:D:79:ILE:O	1:D:99:ILE:HA	2.09	0.53
1:D:69:LEU:HD22	1:D:73:PHE:HE1	1.73	0.53
1:D:99:ILE:HD12	1:D:233:ALA:CB	2.39	0.53
1:D:159:VAL:HG11	1:D:244:GLY:CA	2.38	0.53
1:D:164:ASP:OD2	1:D:167:LYS:HD2	2.08	0.53
1:B:192:ARG:NH2	1:B:277:LEU:HA	2.24	0.53
1:A:71:GLU:O	1:A:71:GLU:HG2	2.09	0.53
1:D:26:LEU:HD13	1:D:65:ILE:HG23	1.90	0.53
1:A:88:ALA:HB2	1:B:21:GLN:HE22	1.74	0.53
1:A:25:GLN:HA	1:A:28:LEU:HD11	1.91	0.53
1:B:104:ASP:O	1:B:116:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:O	1:B:135:HIS:HE1	1.91	0.53
1:B:99:ILE:CG2	1:B:230:TRP:HA	2.39	0.52
1:A:69:LEU:HD22	1:A:98:TRP:CZ2	2.44	0.52
1:B:16:TRP:CZ2	1:B:124:VAL:HG11	2.44	0.52
1:A:32:GLN:HG2	1:A:33:ILE:N	2.22	0.52
1:D:163:THR:HG21	1:D:268:GLU:OE1	2.09	0.52
1:B:210:ALA:O	1:B:213:HIS:HB2	2.09	0.52
1:C:108:ASN:ND2	1:C:115:THR:HB	2.25	0.52
1:A:183:LEU:O	1:A:187:LEU:HG	2.10	0.52
1:B:81:GLU:O	1:B:82:GLU:HG3	2.09	0.52
1:D:67:SER:O	1:D:70:ARG:HB2	2.09	0.52
1:B:247:ILE:CD1	1:B:251:GLY:HA2	2.39	0.52
1:C:164:ASP:CG	1:C:167:LYS:HD3	2.30	0.52
1:B:138:GLU:OE2	1:C:138:GLU:OE2	2.27	0.52
1:D:171:LEU:CD1	1:D:202:ARG:HB2	2.40	0.52
1:D:236:THR:HG23	1:D:246:VAL:HG11	1.91	0.52
1:B:267:ARG:O	1:B:271:MET:CG	2.54	0.52
1:B:115:THR:CG2	1:B:209:LEU:HD12	2.39	0.52
1:A:25:GLN:O	1:A:28:LEU:HD12	2.10	0.52
1:C:189:ASN:HA	1:C:192:ARG:HD2	1.91	0.52
1:D:184:LYS:O	1:D:184:LYS:HD2	2.10	0.52
1:D:171:LEU:HG	1:D:202:ARG:HB2	1.91	0.52
1:B:169:LEU:HB2	1:C:111:HIS:ND1	2.25	0.52
1:A:184:LYS:O	1:A:188:SER:OG	2.25	0.52
1:C:249:THR:HB	1:C:260:ARG:HD2	1.93	0.52
1:D:79:ILE:HG13	1:D:97:THR:HG21	1.93	0.51
1:D:148:ARG:O	1:D:149:GLY:O	2.28	0.51
1:B:192:ARG:CZ	1:B:277:LEU:HA	2.39	0.51
1:A:79:ILE:HG22	1:A:79:ILE:O	2.10	0.51
1:D:91:VAL:O	1:D:91:VAL:HG12	2.10	0.51
1:B:111:HIS:CE1	1:C:169:LEU:HB2	2.45	0.51
1:B:163:THR:CA	1:B:269:MET:HE2	2.41	0.51
1:B:271:MET:CE	1:B:271:MET:HA	2.41	0.51
1:C:145:ARG:HB2	1:C:148:ARG:HB2	1.91	0.51
1:A:91:VAL:HG12	1:A:91:VAL:O	2.11	0.51
1:C:91:VAL:O	1:C:91:VAL:HG12	2.10	0.51
1:B:101:ASP:OD2	1:B:231:ASP:OD1	2.28	0.51
1:C:254:LEU:HD12	1:C:261:VAL:HG23	1.92	0.51
1:B:248:ASP:HB2	1:B:253:PRO:O	2.11	0.51
1:A:29:ARG:HG2	1:A:64:LEU:HD11	1.92	0.51
1:D:185:LEU:HD22	1:D:189:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ALA:O	1:B:112:ARG:NH2	2.44	0.51
1:C:248:ASP:CG	1:C:260:ARG:HH21	2.14	0.51
1:A:179:ASP:OD2	1:A:181:ALA:N	2.44	0.51
1:D:32:GLN:O	1:D:36:LYS:HB2	2.11	0.51
1:C:138:GLU:HB2	1:C:140:ARG:HG3	1.93	0.51
1:B:152:CYS:HB3	1:B:157:LEU:HD21	1.92	0.51
1:A:101:ASP:OD2	1:A:231:ASP:OD1	2.29	0.51
1:B:175:GLY:O	1:B:176:PRO:O	2.29	0.51
1:C:174:ILE:O	1:C:175:GLY:O	2.29	0.51
1:D:28:LEU:HD21	1:D:141:LEU:HG	1.93	0.50
1:D:122:PHE:HE1	1:D:124:VAL:HG22	1.76	0.50
1:B:162:GLU:HG3	1:B:269:MET:CE	2.40	0.50
1:A:111:HIS:HE1	1:D:220:ASP:OD2	1.95	0.50
1:A:190:MET:HE2	1:A:194:LEU:CD2	2.42	0.50
1:C:81:GLU:HB2	1:C:230:TRP:CZ2	2.46	0.50
1:D:163:THR:HG22	1:D:266:THR:OG1	2.12	0.50
1:B:163:THR:HG22	1:B:266:THR:OG1	2.11	0.50
1:C:170:VAL:HG21	1:C:193:LEU:CD1	2.42	0.50
1:B:173:GLU:HA	1:B:173:GLU:OE1	2.11	0.50
1:B:232:LEU:O	1:B:232:LEU:HG	2.11	0.50
1:A:273:ILE:O	1:A:276:ALA:O	2.30	0.50
1:A:88:ALA:HB2	1:B:21:GLN:CD	2.33	0.50
1:D:222:TYR:OH	1:D:224:GLN:NE2	2.45	0.50
1:C:101:ASP:OD2	1:C:231:ASP:OD1	2.30	0.50
1:D:115:THR:HG23	1:D:209:LEU:HD12	1.94	0.50
1:B:206:SER:HB3	1:B:209:LEU:HB2	1.93	0.50
1:D:22:ALA:O	1:D:26:LEU:HG	2.12	0.50
1:A:224:GLN:NE2	1:A:227:LEU:HD13	2.27	0.49
1:A:211:LEU:HD21	1:A:222:TYR:CD1	2.47	0.49
1:B:247:ILE:HD12	1:B:248:ASP:O	2.12	0.49
1:A:66:ILE:O	1:A:70:ARG:HG3	2.13	0.49
1:C:211:LEU:HD22	1:C:239:ILE:HD11	1.94	0.49
1:A:17:GLU:CD	1:A:145:ARG:HH22	2.15	0.49
1:D:163:THR:HG23	1:D:266:THR:HG21	1.93	0.49
1:D:24:VAL:HG13	1:D:141:LEU:CD1	2.42	0.49
1:D:245:ILE:HG13	1:D:245:ILE:O	2.12	0.49
1:C:111:HIS:O	1:C:112:ARG:HB2	2.11	0.49
1:A:104:ASP:OD2	1:A:208:THR:HG23	2.12	0.49
1:C:179:ASP:OD1	1:C:182:THR:N	2.37	0.49
1:A:188:SER:HB2	1:A:192:ARG:NH1	2.27	0.49
1:D:111:HIS:O	1:D:112:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:HG2	1:D:64:LEU:HD11	1.95	0.49
1:A:191:GLU:OE2	1:A:195:HIS:ND1	2.46	0.49
1:A:269:MET:O	1:A:273:ILE:HD12	2.13	0.49
1:D:149:GLY:HA3	1:D:156:ARG:NH2	2.28	0.49
1:C:135:HIS:CD2	1:C:138:GLU:HG3	2.48	0.49
1:C:81:GLU:HG3	1:C:81:GLU:O	2.13	0.49
1:D:30:ALA:CB	1:D:61:VAL:HG13	2.42	0.48
1:D:179:ASP:OD2	1:D:179:ASP:O	2.31	0.48
1:A:177:LYS:O	1:A:178:ARG:HD3	2.12	0.48
1:D:249:THR:HA	1:D:262:VAL:HG23	1.95	0.48
1:A:24:VAL:HG13	1:A:141:LEU:HD11	1.94	0.48
1:C:269:MET:O	1:C:272:LEU:N	2.46	0.48
1:B:214:LEU:HD11	1:B:264:ALA:N	2.28	0.48
1:C:190:MET:CE	1:C:201:VAL:HG11	2.43	0.48
1:A:179:ASP:O	1:A:183:LEU:HD13	2.12	0.48
1:D:184:LYS:O	1:D:188:SER:OG	2.30	0.48
1:D:26:LEU:HD13	1:D:65:ILE:CG2	2.43	0.48
1:D:183:LEU:HD12	1:D:183:LEU:HA	1.70	0.48
1:B:146:ARG:HG2	1:B:146:ARG:O	2.12	0.48
1:C:258:ALA:O	1:C:260:ARG:HG2	2.13	0.48
1:D:134:TYR:OH	1:D:139:GLU:HG2	2.13	0.48
1:C:29:ARG:NH2	1:C:68:GLU:OE2	2.47	0.48
1:C:34:ILE:HG23	1:C:109:PHE:HE1	1.77	0.48
1:B:38:LEU:HA	1:B:112:ARG:CZ	2.44	0.48
1:A:108:ASN:O	1:A:113:PHE:N	2.47	0.48
1:A:65:ILE:HG21	1:A:100:ILE:HD13	1.96	0.48
1:A:161:GLY:H	1:A:265:SER:HB2	1.77	0.48
1:B:130:PHE:HB2	1:B:144:GLY:O	2.14	0.48
1:C:249:THR:HB	1:C:260:ARG:CD	2.44	0.48
1:A:275:GLN:O	1:A:277:LEU:O	2.32	0.48
1:B:202:ARG:HH12	1:C:174:ILE:HD11	1.79	0.48
1:C:145:ARG:HH11	1:C:145:ARG:HG3	1.79	0.48
1:D:185:LEU:HD22	1:D:189:ASN:HD21	1.78	0.48
1:B:107:CYS:O	1:B:110:VAL:HG22	2.14	0.47
1:A:247:ILE:HB	1:A:252:GLY:O	2.14	0.47
1:A:192:ARG:HD2	1:A:277:LEU:CA	2.44	0.47
1:B:191:GLU:HA	1:B:194:LEU:HD12	1.95	0.47
1:D:224:GLN:HB3	1:D:227:LEU:HD22	1.96	0.47
1:D:144:GLY:O	1:D:237:VAL:HG11	2.13	0.47
1:B:174:ILE:HD12	1:B:175:GLY:N	2.28	0.47
1:B:185:LEU:HD22	1:B:189:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:MET:HE3	1:B:271:MET:HA	1.96	0.47
1:C:17:GLU:OE2	1:C:145:ARG:NH2	2.47	0.47
1:C:117:ALA:HB2	1:C:209:LEU:HD11	1.96	0.47
1:B:142:TYR:HB3	1:B:238:ILE:HD13	1.97	0.47
1:B:190:MET:O	1:B:190:MET:HE2	2.15	0.47
1:B:142:TYR:CE1	1:B:212:CYS:HB3	2.49	0.47
1:C:170:VAL:HG11	1:C:193:LEU:CD1	2.43	0.47
1:C:162:GLU:OE1	1:C:164:ASP:HB2	2.14	0.47
1:A:188:SER:HB2	1:A:192:ARG:HH12	1.79	0.47
1:A:165:LEU:CD2	1:A:196:ALA:HB1	2.45	0.47
1:B:188:SER:O	1:B:191:GLU:N	2.45	0.47
1:B:236:THR:O	1:B:240:ARG:HG3	2.15	0.47
1:A:172:THR:OG1	1:A:173:GLU:N	2.48	0.47
1:A:114:PRO:HB2	1:A:137:THR:HG21	1.95	0.47
1:B:208:THR:HG22	1:B:231:ASP:O	2.15	0.47
1:C:164:ASP:CB	1:C:167:LYS:HD3	2.45	0.46
1:A:185:LEU:CD2	1:A:189:ASN:HD21	2.26	0.46
1:D:149:GLY:HA3	1:D:156:ARG:CZ	2.45	0.46
1:B:159:VAL:HG11	1:B:244:GLY:N	2.29	0.46
1:A:185:LEU:O	1:A:188:SER:OG	2.33	0.46
1:B:192:ARG:NE	1:B:277:LEU:HA	2.30	0.46
1:A:40:GLU:C	1:A:112:ARG:HH21	2.19	0.46
1:B:256:LEU:HA	1:B:256:LEU:HD12	1.80	0.46
1:B:174:ILE:HD13	1:B:178:ARG:CZ	2.45	0.46
1:C:189:ASN:CA	1:C:192:ARG:HG3	2.46	0.46
1:B:167:LYS:NZ	1:B:167:LYS:CB	2.76	0.46
1:C:179:ASP:OD1	1:C:182:THR:HG23	2.16	0.46
1:A:138:GLU:HG3	1:A:140:ARG:NH2	2.31	0.46
1:A:122:PHE:CE1	1:A:124:VAL:HG22	2.50	0.46
1:B:165:LEU:HD12	1:B:165:LEU:O	2.16	0.46
1:D:149:GLY:C	1:D:241:GLU:HB3	2.36	0.46
1:B:157:LEU:O	1:B:158:ARG:HG3	2.15	0.46
1:A:140:ARG:HA	1:A:153:ASN:HD21	1.80	0.46
1:D:135:HIS:N	1:D:140:ARG:O	2.49	0.46
1:D:32:GLN:HA	1:D:35:ARG:NH2	2.31	0.46
1:A:29:ARG:NH2	1:A:64:LEU:HD21	2.30	0.46
1:A:161:GLY:HA2	1:A:266:THR:HG23	1.96	0.46
1:D:247:ILE:HB	1:D:252:GLY:O	2.16	0.46
1:A:111:HIS:CE1	1:D:220:ASP:OD2	2.69	0.46
1:B:179:ASP:O	1:B:181:ALA:N	2.48	0.46
1:D:211:LEU:HD21	1:D:222:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:ILE:HB	1:C:252:GLY:O	2.16	0.46
1:B:179:ASP:N	1:B:182:THR:OG1	2.49	0.46
1:A:165:LEU:HA	1:A:269:MET:HE1	1.98	0.46
1:A:225:PHE:CE2	1:A:249:THR:HG21	2.51	0.46
1:B:79:ILE:HD12	1:B:99:ILE:HG12	1.98	0.46
1:B:151:PHE:CE2	1:B:156:ARG:HD3	2.51	0.46
1:B:169:LEU:HB2	1:C:111:HIS:CE1	2.51	0.45
1:B:179:ASP:O	1:B:182:THR:N	2.49	0.45
1:A:174:ILE:HD13	1:D:200:GLY:HA2	1.98	0.45
1:A:79:ILE:N	1:A:98:TRP:O	2.49	0.45
1:C:122:PHE:O	1:C:129:GLU:HB3	2.16	0.45
1:C:213:HIS:O	1:C:218:ALA:N	2.49	0.45
1:C:168:ALA:HB2	1:C:269:MET:CE	2.40	0.45
1:A:227:LEU:HD23	1:A:227:LEU:O	2.15	0.45
1:A:184:LYS:HZ2	1:A:187:LEU:HB2	1.82	0.45
1:B:115:THR:O	1:B:115:THR:HG22	2.14	0.45
1:C:41:GLU:OE2	1:C:41:GLU:HA	2.17	0.45
1:C:185:LEU:HD22	1:C:189:ASN:HD21	1.80	0.45
1:A:38:LEU:HA	1:A:38:LEU:HD23	1.79	0.45
1:C:57:THR:O	1:C:61:VAL:HG23	2.17	0.45
1:A:81:GLU:HG2	1:A:82:GLU:OE2	2.16	0.45
1:C:93:THR:O	1:C:126:GLN:HA	2.16	0.45
1:D:214:LEU:HD12	1:D:239:ILE:HD13	1.97	0.45
1:B:194:LEU:HD21	1:B:201:VAL:HG11	1.97	0.45
1:B:222:TYR:OH	1:B:224:GLN:NE2	2.49	0.45
1:D:141:LEU:HA	1:D:141:LEU:HD23	1.84	0.45
1:A:222:TYR:OH	1:A:224:GLN:NE2	2.50	0.45
1:D:66:ILE:O	1:D:70:ARG:HB2	2.17	0.45
1:C:189:ASN:O	1:C:192:ARG:HG3	2.17	0.45
1:B:65:ILE:HG22	1:B:69:LEU:HD12	1.97	0.45
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.82	0.45
1:C:179:ASP:O	1:C:181:ALA:N	2.50	0.45
1:B:176:PRO:HB2	1:B:177:LYS:H	1.55	0.45
1:D:135:HIS:NE2	1:D:138:GLU:HG2	2.30	0.45
1:B:178:ARG:NH2	1:C:199:HIS:O	2.50	0.45
1:A:190:MET:O	1:A:194:LEU:HB2	2.16	0.45
1:B:127:GLU:HG2	1:B:146:ARG:CZ	2.47	0.45
1:C:123:ALA:HB1	1:C:127:GLU:O	2.17	0.45
1:B:160:SER:OG	1:B:220:ASP:OD1	2.30	0.44
1:B:184:LYS:HE2	1:B:188:SER:HB2	1.98	0.44
1:A:138:GLU:HB2	1:A:140:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:CE1	1:D:111:HIS:HE2	2.35	0.44
1:B:140:ARG:HA	1:B:153:ASN:ND2	2.32	0.44
1:B:163:THR:N	1:B:269:MET:HE2	2.33	0.44
1:C:273:ILE:O	1:C:276:ALA:N	2.50	0.44
1:C:254:LEU:CD2	1:C:256:LEU:HD13	2.42	0.44
1:A:110:VAL:HG23	1:A:111:HIS:CD2	2.53	0.44
1:C:146:ARG:HG3	1:C:146:ARG:HH11	1.83	0.44
1:D:158:ARG:HB2	1:D:158:ARG:CZ	2.48	0.44
1:C:110:VAL:HG22	1:C:111:HIS:CD2	2.52	0.44
1:C:246:VAL:HG12	1:C:254:LEU:HD13	1.98	0.44
1:B:128:LEU:O	1:B:146:ARG:NH1	2.50	0.44
1:B:172:THR:OG1	1:B:173:GLU:N	2.50	0.44
1:D:107:CYS:O	1:D:111:HIS:HD2	2.00	0.44
1:D:38:LEU:HG	1:D:109:PHE:CE1	2.53	0.44
1:D:249:THR:HB	1:D:260:ARG:CG	2.46	0.44
1:C:142:TYR:CD1	1:C:152:CYS:HB2	2.53	0.44
1:D:193:LEU:HD23	1:D:223:TYR:CE1	2.52	0.44
1:C:222:TYR:OH	1:C:224:GLN:NE2	2.50	0.44
1:C:227:LEU:HD21	1:C:232:LEU:CD2	2.48	0.44
1:C:261:VAL:HG22	1:C:262:VAL:N	2.33	0.44
1:B:179:ASP:OD1	1:B:182:THR:HG23	2.18	0.44
1:B:276:ALA:O	1:B:277:LEU:CB	2.65	0.44
1:A:41:GLU:OE2	1:A:41:GLU:O	2.35	0.44
1:B:245:ILE:HD11	1:B:270:ALA:HB3	2.00	0.44
1:C:188:SER:HB2	1:C:192:ARG:NH1	2.33	0.44
1:D:172:THR:OG1	1:D:173:GLU:N	2.50	0.44
1:D:63:ASP:OD1	1:D:64:LEU:N	2.50	0.44
1:D:66:ILE:HA	1:D:78:PHE:CE1	2.53	0.44
1:D:269:MET:HG3	1:D:273:ILE:CD1	2.47	0.44
1:A:38:LEU:O	1:A:112:ARG:NE	2.49	0.43
1:C:152:CYS:HB3	1:C:157:LEU:HD21	2.00	0.43
1:C:276:ALA:O	1:C:277:LEU:CB	2.66	0.43
1:C:94:HIS:CE1	1:C:126:GLN:OE1	2.70	0.43
1:C:178:ARG:HA	1:C:178:ARG:HD3	1.66	0.43
1:B:255:ASP:HB3	1:B:258:ALA:CB	2.48	0.43
1:A:249:THR:O	1:A:274:ALA:HB1	2.18	0.43
1:B:255:ASP:HB3	1:B:258:ALA:HB3	2.00	0.43
1:C:245:ILE:CD1	1:C:267:ARG:HA	2.45	0.43
1:B:140:ARG:HA	1:B:153:ASN:HD21	1.84	0.43
1:A:203:VAL:HG22	1:A:203:VAL:O	2.19	0.43
1:B:164:ASP:O	1:B:167:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LYS:HA	1:C:184:LYS:HD2	1.55	0.43
1:A:191:GLU:O	1:A:195:HIS:HB2	2.19	0.43
1:D:137:THR:HG22	1:D:138:GLU:OE1	2.19	0.43
1:C:180:PRO:HA	1:C:183:LEU:HD23	2.00	0.43
1:C:35:ARG:O	1:C:38:LEU:N	2.52	0.43
1:A:203:VAL:HG13	1:D:203:VAL:HG13	1.99	0.43
1:B:99:ILE:HG21	1:B:233:ALA:HB2	1.99	0.43
1:C:174:ILE:H	1:C:174:ILE:HG13	1.67	0.43
1:C:225:PHE:CZ	1:C:249:THR:HG21	2.54	0.43
1:C:190:MET:HE3	1:C:201:VAL:CG2	2.42	0.43
1:A:196:ALA:O	1:A:197:LYS:HB2	2.19	0.43
1:B:228:HIS:HB2	1:B:230:TRP:CE2	2.53	0.43
1:C:124:VAL:N	1:C:127:GLU:O	2.50	0.43
1:D:133:ILE:O	1:D:142:TYR:N	2.49	0.43
1:B:55:THR:HG22	1:B:56:GLU:N	2.34	0.43
1:B:218:ALA:O	1:C:111:HIS:HB3	2.18	0.43
1:A:106:THR:HG22	1:A:107:CYS:N	2.34	0.43
1:C:65:ILE:HG22	1:C:69:LEU:HD12	2.01	0.43
1:C:148:ARG:NH1	1:C:148:ARG:HG2	2.34	0.43
1:C:106:THR:HG22	1:C:107:CYS:N	2.33	0.43
1:A:38:LEU:HD21	1:A:109:PHE:CD1	2.54	0.43
1:A:248:ASP:OD2	1:A:260:ARG:NE	2.48	0.43
1:B:264:ALA:HB3	1:B:270:ALA:HB2	2.00	0.42
1:D:159:VAL:HG11	1:D:244:GLY:HA3	2.00	0.42
1:A:173:GLU:OE2	1:A:206:SER:N	2.48	0.42
1:C:148:ARG:HH11	1:C:148:ARG:HG2	1.84	0.42
1:D:61:VAL:CG1	1:D:102:PRO:HB3	2.49	0.42
1:B:111:HIS:ND1	1:C:169:LEU:HB2	2.35	0.42
1:C:20:PHE:O	1:C:24:VAL:HG23	2.19	0.42
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.19	0.42
1:D:26:LEU:CD1	1:D:69:LEU:HD21	2.49	0.42
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.83	0.42
1:A:165:LEU:HD12	1:A:269:MET:SD	2.60	0.42
1:A:140:ARG:HB3	1:A:152:CYS:SG	2.59	0.42
1:A:156:ARG:HG3	1:A:157:LEU:N	2.33	0.42
1:A:220:ASP:O	1:A:221:ALA:HB2	2.19	0.42
1:A:229:CYS:HB2	1:A:256:LEU:HG	2.01	0.42
1:C:22:ALA:O	1:C:26:LEU:HD12	2.20	0.42
1:A:31:GLY:HA3	1:A:134:TYR:CD2	2.54	0.42
1:D:64:LEU:HD22	1:D:64:LEU:HA	1.93	0.42
1:D:145:ARG:O	1:D:148:ARG:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:HG22	1:B:206:SER:HB2	2.01	0.42
1:B:224:GLN:NE2	1:B:227:LEU:HB2	2.33	0.42
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.86	0.42
1:C:151:PHE:CD2	1:C:156:ARG:HA	2.55	0.42
1:B:159:VAL:HG23	1:B:160:SER:N	2.34	0.42
1:A:197:LYS:HD3	1:A:197:LYS:HA	1.85	0.42
1:B:140:ARG:HD2	1:B:142:TYR:CE2	2.55	0.42
1:A:108:ASN:HD22	1:A:115:THR:HB	1.84	0.42
1:D:129:GLU:OE2	1:D:146:ARG:HG2	2.20	0.42
1:B:186:PHE:O	1:B:190:MET:N	2.48	0.42
1:B:202:ARG:NH1	1:C:174:ILE:HD11	2.35	0.42
1:B:151:PHE:CZ	1:B:156:ARG:HD3	2.54	0.42
1:D:206:SER:HB3	1:D:209:LEU:HB2	2.01	0.42
1:B:135:HIS:HD2	1:B:140:ARG:NH1	2.18	0.42
1:C:81:GLU:HA	1:C:230:TRP:CH2	2.55	0.42
1:A:268:GLU:N	1:A:268:GLU:OE2	2.50	0.42
1:C:89:LYS:HE2	1:C:91:VAL:HG21	2.02	0.42
1:A:38:LEU:HD23	1:A:109:PHE:CZ	2.55	0.42
1:D:135:HIS:HB3	1:D:140:ARG:HG3	2.02	0.42
1:A:224:GLN:HE21	1:A:227:LEU:HD13	1.85	0.42
1:D:117:ALA:HB2	1:D:209:LEU:HD21	2.02	0.42
1:C:193:LEU:O	1:C:198:ALA:HB2	2.20	0.42
1:A:65:ILE:HG22	1:A:69:LEU:HD12	2.01	0.42
1:B:172:THR:O	1:B:203:VAL:HB	2.20	0.42
1:A:215:ALA:O	1:A:242:ALA:HB1	2.20	0.42
1:C:26:LEU:CD2	1:C:64:LEU:HD13	2.50	0.41
1:A:182:THR:O	1:A:185:LEU:HB3	2.20	0.41
1:C:179:ASP:C	1:C:179:ASP:OD1	2.58	0.41
1:A:187:LEU:CD2	1:D:191:GLU:HA	2.51	0.41
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.76	0.41
1:D:256:LEU:HA	1:D:256:LEU:HD12	1.84	0.41
1:B:261:VAL:HG22	1:B:262:VAL:N	2.35	0.41
1:C:30:ALA:HB1	1:C:61:VAL:CG1	2.49	0.41
1:B:167:LYS:HE3	1:B:167:LYS:HB2	1.78	0.41
1:A:179:ASP:OD1	1:A:182:THR:CG2	2.68	0.41
1:D:187:LEU:O	1:D:191:GLU:HB3	2.21	0.41
1:C:138:GLU:HG3	1:C:140:ARG:NH2	2.35	0.41
1:A:190:MET:HE2	1:A:194:LEU:HD22	2.02	0.41
1:B:194:LEU:HG	1:B:194:LEU:H	1.67	0.41
1:B:214:LEU:HD12	1:B:263:ALA:HB1	2.02	0.41
1:B:135:HIS:HD2	1:B:140:ARG:HH12	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HA	1:D:203:VAL:HG22	2.03	0.41
1:C:28:LEU:HG	1:C:28:LEU:H	1.69	0.41
1:A:249:THR:HG22	1:A:260:ARG:CZ	2.50	0.41
1:B:164:ASP:OD2	1:B:167:LYS:HG3	2.20	0.41
1:D:176:PRO:HB2	1:D:177:LYS:H	1.60	0.41
1:C:69:LEU:HD22	1:C:98:TRP:CE2	2.55	0.41
1:A:180:PRO:O	1:A:184:LYS:HB2	2.20	0.41
1:B:115:THR:HG22	1:B:206:SER:CB	2.51	0.41
1:B:267:ARG:C	1:B:271:MET:HG2	2.41	0.41
1:B:158:ARG:HE	1:B:158:ARG:HB2	1.64	0.41
1:C:20:PHE:CZ	1:C:145:ARG:HD3	2.55	0.41
1:D:178:ARG:C	1:D:183:LEU:HD22	2.40	0.41
1:B:190:MET:HE1	1:B:201:VAL:HG11	2.03	0.41
1:D:189:ASN:HB3	1:D:223:TYR:CE2	2.56	0.41
1:C:92:LEU:O	1:C:126:GLN:NE2	2.53	0.41
1:B:249:THR:CB	1:B:260:ARG:HD2	2.42	0.41
1:D:236:THR:CG2	1:D:246:VAL:HG11	2.51	0.41
1:D:275:GLN:HA	1:D:275:GLN:NE2	2.36	0.41
1:B:267:ARG:CZ	1:B:267:ARG:HB2	2.49	0.40
1:D:114:PRO:HB2	1:D:137:THR:HG21	2.02	0.40
1:C:177:LYS:H	1:C:177:LYS:HG2	1.38	0.40
1:C:124:VAL:CG2	1:C:129:GLU:HB2	2.51	0.40
1:C:124:VAL:HG22	1:C:129:GLU:HB2	2.02	0.40
1:C:196:ALA:O	1:C:197:LYS:HB2	2.20	0.40
1:A:138:GLU:HG3	1:A:140:ARG:CZ	2.51	0.40
1:A:94:HIS:HB2	1:B:139:GLU:OE2	2.20	0.40
1:D:117:ALA:HB2	1:D:209:LEU:CD2	2.52	0.40
1:D:26:LEU:HD11	1:D:69:LEU:HD21	2.03	0.40
1:C:89:LYS:HD2	1:C:91:VAL:HG23	2.02	0.40
1:D:32:GLN:OE1	1:D:36:LYS:NZ	2.49	0.40
1:B:122:PHE:O	1:B:129:GLU:N	2.49	0.40
1:C:161:GLY:HA2	1:C:266:THR:HG23	2.04	0.40
1:D:221:ALA:HA	1:D:264:ALA:HA	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	238/273 (87%)	210 (88%)	20 (8%)	8 (3%)	5 4
1	B	238/273 (87%)	208 (87%)	23 (10%)	7 (3%)	6 5
1	C	238/273 (87%)	208 (87%)	25 (10%)	5 (2%)	9 10
1	D	238/273 (87%)	206 (87%)	24 (10%)	8 (3%)	5 4
All	All	952/1092 (87%)	832 (87%)	92 (10%)	28 (3%)	6 5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	PRO
1	B	229	CYS
1	C	175	GLY
1	D	40	GLU
1	D	89	LYS
1	A	159	VAL
1	B	36	LYS
1	C	181	ALA
1	D	36	LYS
1	D	135	HIS
1	D	149	GLY
1	D	176	PRO
1	D	183	LEU
1	A	70	ARG
1	A	89	LYS
1	B	146	ARG
1	C	276	ALA
1	D	177	LYS
1	A	40	GLU
1	A	93	THR
1	A	176	PRO
1	A	197	LYS

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Mol	Chain	Res	Type
1	B	159	VAL
1	C	233	ALA
1	B	180	PRO
1	B	237	VAL
1	A	79	ILE
1	C	180	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	195/219 (89%)	157 (80%)	38 (20%)	2 2
1	B	195/219 (89%)	152 (78%)	43 (22%)	1 1
1	C	196/219 (90%)	146 (74%)	50 (26%)	1 0
1	D	195/219 (89%)	142 (73%)	53 (27%)	0 0
All	All	781/876 (89%)	597 (76%)	184 (24%)	1 1

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	28	LEU
1	A	29	ARG
1	A	32	GLN
1	A	35	ARG
1	A	36	LYS
1	A	41	GLU
1	A	55	THR
1	A	60	LEU
1	A	64	LEU
1	A	70	ARG
1	A	72	ARG
1	A	73	PHE
1	A	95	SER
1	A	103	ILE

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Mol	Chain	Res	Type
1	A	124	VAL
1	A	126	GLN
1	A	141	LEU
1	A	158	ARG
1	A	167	LYS
1	A	172	THR
1	A	174	ILE
1	A	178	ARG
1	A	179	ASP
1	A	184	LYS
1	A	187	LEU
1	A	188	SER
1	A	194	LEU
1	A	195	HIS
1	A	197	LYS
1	A	203	VAL
1	A	207	SER
1	A	214	LEU
1	A	216	SER
1	A	227	LEU
1	A	232	LEU
1	A	265	SER
1	A	271	MET
1	B	17	GLU
1	B	29	ARG
1	B	55	THR
1	B	56	GLU
1	B	60	LEU
1	B	64	LEU
1	B	70	ARG
1	B	71	GLU
1	B	75	SER
1	B	77	ARG
1	B	106	THR
1	B	112	ARG
1	B	124	VAL
1	B	127	GLU
1	B	137	THR
1	B	141	LEU
1	B	156	ARG
1	B	158	ARG
1	B	163	THR

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Mol	Chain	Res	Type
1	B	167	LYS
1	B	179	ASP
1	B	184	LYS
1	B	185	LEU
1	B	190	MET
1	B	191	GLU
1	B	192	ARG
1	B	193	LEU
1	B	194	LEU
1	B	201	VAL
1	B	202	ARG
1	B	214	LEU
1	B	216	SER
1	B	228	HIS
1	B	229	CYS
1	B	232	LEU
1	B	245	ILE
1	B	249	THR
1	B	256	LEU
1	B	257	MET
1	B	260	ARG
1	B	267	ARG
1	B	273	ILE
1	B	275	GLN
1	C	25	GLN
1	C	29	ARG
1	C	32	GLN
1	C	39	THR
1	C	41	GLU
1	C	55	THR
1	C	58	ASP
1	C	64	LEU
1	C	67	SER
1	C	71	GLU
1	C	72	ARG
1	C	77	ARG
1	C	95	SER
1	C	110	VAL
1	C	112	ARG
1	C	118	VAL
1	C	124	VAL
1	C	125	ARG

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Mol	Chain	Res	Type
1	C	127	GLU
1	C	137	THR
1	C	138	GLU
1	C	141	LEU
1	C	145	ARG
1	C	155	GLN
1	C	158	ARG
1	C	164	ASP
1	C	174	ILE
1	C	177	LYS
1	C	183	LEU
1	C	184	LYS
1	C	185	LEU
1	C	187	LEU
1	C	188	SER
1	C	190	MET
1	C	191	GLU
1	C	192	ARG
1	C	193	LEU
1	C	194	LEU
1	C	214	LEU
1	C	227	LEU
1	C	232	LEU
1	C	245	ILE
1	C	247	ILE
1	C	249	THR
1	C	254	LEU
1	C	255	ASP
1	C	256	LEU
1	C	260	ARG
1	C	266	THR
1	C	275	GLN
1	D	18	GLU
1	D	29	ARG
1	D	35	ARG
1	D	36	LYS
1	D	39	THR
1	D	56	GLU
1	D	58	ASP
1	D	63	ASP
1	D	64	LEU
1	D	65	ILE

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Mol	Chain	Res	Type
1	D	66	ILE
1	D	67	SER
1	D	68	GLU
1	D	70	ARG
1	D	71	GLU
1	D	73	PHE
1	D	77	ARG
1	D	99	ILE
1	D	110	VAL
1	D	124	VAL
1	D	127	GLU
1	D	135	HIS
1	D	140	ARG
1	D	141	LEU
1	D	145	ARG
1	D	146	ARG
1	D	158	ARG
1	D	174	ILE
1	D	177	LYS
1	D	182	THR
1	D	183	LEU
1	D	184	LYS
1	D	185	LEU
1	D	188	SER
1	D	190	MET
1	D	191	GLU
1	D	193	LEU
1	D	194	LEU
1	D	199	HIS
1	D	203	VAL
1	D	207	SER
1	D	209	LEU
1	D	214	LEU
1	D	227	LEU
1	D	240	ARG
1	D	245	ILE
1	D	249	THR
1	D	256	LEU
1	D	261	VAL
1	D	268	GLU
1	D	271	MET
1	D	273	ILE

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Mol	Chain	Res	Type
1	D	275	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	153	ASN
1	A	189	ASN
1	A	224	GLN
1	B	94	HIS
1	B	135	HIS
1	B	153	ASN
1	B	199	HIS
1	B	224	GLN
1	B	228	HIS
1	B	275	GLN
1	C	25	GLN
1	C	32	GLN
1	C	59	HIS
1	C	94	HIS
1	C	111	HIS
1	C	135	HIS
1	C	153	ASN
1	C	199	HIS
1	C	224	GLN
1	D	21	GLN
1	D	94	HIS
1	D	135	HIS
1	D	224	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	244/273 (89%)	-0.24	2 (0%)	87	87	22, 46, 90, 118	0
1	B	244/273 (89%)	-0.19	3 (1%)	81	81	25, 49, 98, 138	0
1	C	244/273 (89%)	-0.21	6 (2%)	61	60	23, 52, 94, 124	0
1	D	244/273 (89%)	-0.10	9 (3%)	45	46	22, 56, 109, 139	0
All	All	976/1092 (89%)	-0.19	20 (2%)	68	68	22, 51, 100, 139	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	TRP	5.2
1	B	38	LEU	5.1
1	D	178	ARG	4.0
1	C	174	ILE	3.5
1	C	89	LYS	3.3
1	C	61	VAL	3.2
1	D	174	ILE	3.2
1	D	176	PRO	3.0
1	A	277	LEU	3.0
1	D	65	ILE	2.9
1	A	184	LYS	2.6
1	D	69	LEU	2.4
1	D	57	THR	2.4
1	D	61	VAL	2.3
1	D	19	CYS	2.3
1	C	273	ILE	2.2
1	C	193	LEU	2.2
1	B	55	THR	2.1
1	B	150	ALA	2.1
1	C	267	ARG	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.