Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 04:18 AM EDT

PDB ID	:	1YO6
Title	:	Crystal Structure of the putative Carbonyl Reductase Sniffer of Caenorhabditis elegans
Authors	:	Southeast Collaboratory for Structural Genomics (SECSG)
Deposited on	:	2005-01-26
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

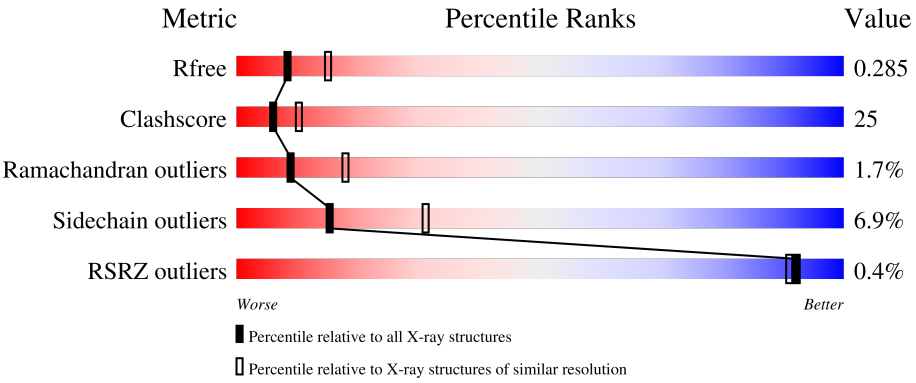
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	250	60% 28% 6% • 5%
1	B	250	59% 30% 5% 6%
1	C	250	58% 31% 7% •
1	D	250	% 52% 36% 6% 6%
1	E	250	51% 39% • 6%

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Mol	Chain	Length	Quality of chain
1	F	250	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10878 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 Putative Carbonyl Reductase Sniffer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1786	1121	311	348	6			
1	B	235	Total	C	N	O	S	0	0	0
			1765	1105	308	346	6			
1	C	240	Total	C	N	O	S	0	0	0
			1809	1135	315	353	6			
1	D	236	Total	C	N	O	S	0	0	0
			1779	1116	310	347	6			
1	E	235	Total	C	N	O	S	0	0	0
			1764	1105	308	346	5			
1	F	230	Total	C	N	O	S	0	0	0
			1739	1091	303	340	5			

- Molecule 2 is water.

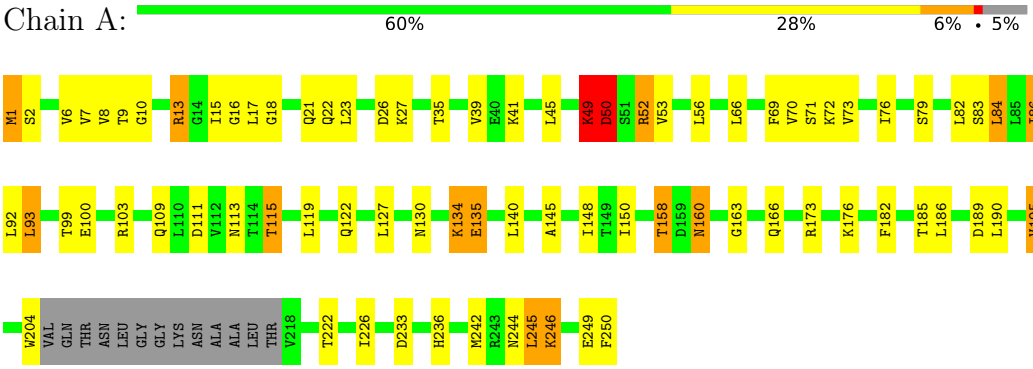
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	B	40	Total	O	0	0
			40	40		
2	C	50	Total	O	0	0
			50	50		
2	D	35	Total	O	0	0
			35	35		
2	E	31	Total	O	0	0
			31	31		
2	F	29	Total	O	0	0
			29	29		

3 Residue-property plots (i)

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

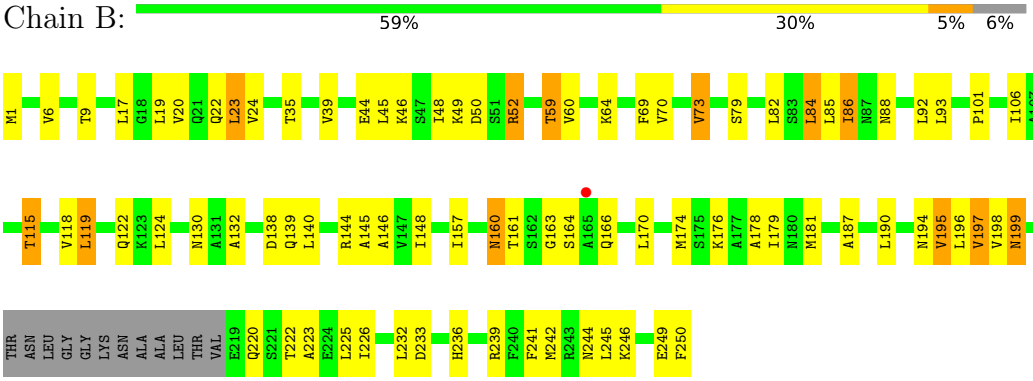
• Molecule 1: Putative Carbonyl Reductase Sniffer

Chain A:



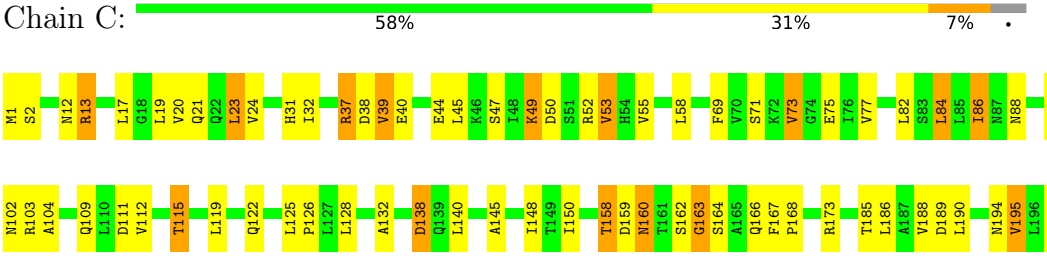
• Molecule 1: Putative Carbonyl Reductase Sniffer

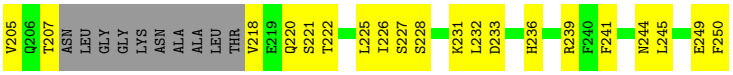
Chain B:



• Molecule 1: Putative Carbonyl Reductase Sniffer

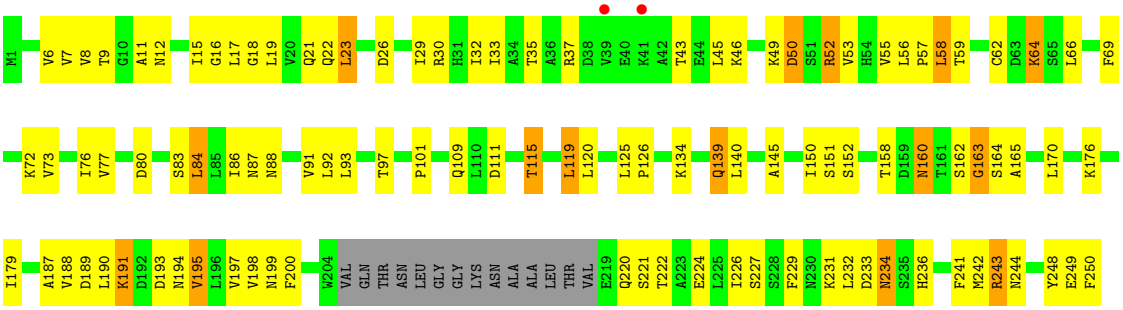
Chain C:





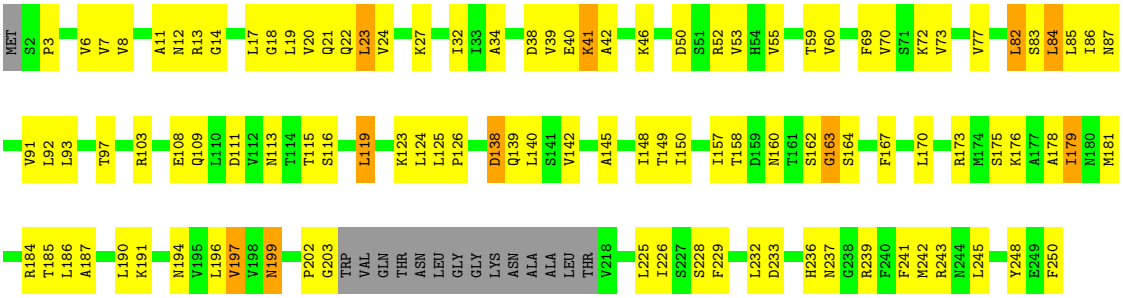
• Molecule 1: Putative Carbonyl Reductase Sniffer

Chain D:



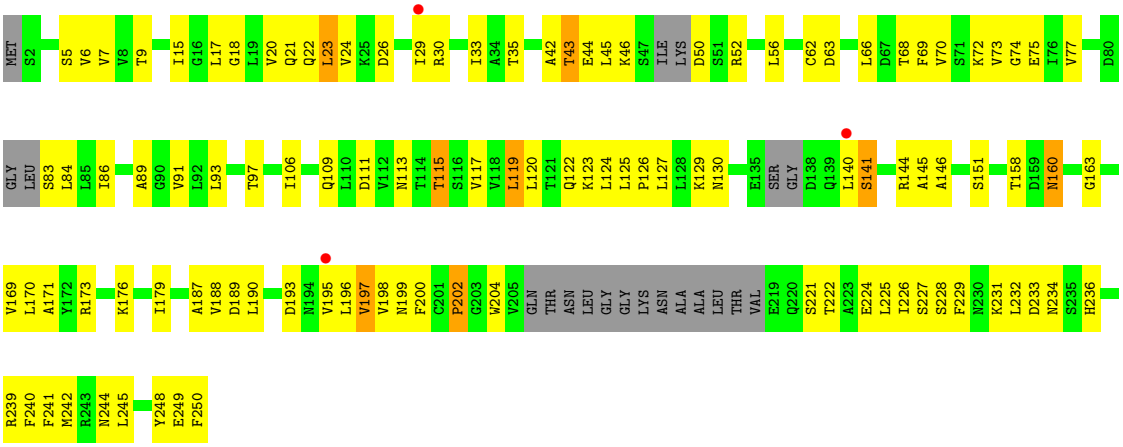
• Molecule 1: Putative Carbonyl Reductase Sniffer

Chain E:



• Molecule 1: Putative Carbonyl Reductase Sniffer

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.87Å 86.32Å 242.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 2.60 47.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (47.12-2.60) 93.5 (47.12-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	7.56 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.286 0.218 , 0.285	Depositor DCC
R_{free} test set	2307 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10878	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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, 0.333 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	0.39	0/1807	0.66	0/2446
1	B	0.40	0/1784	0.63	0/2413
1	C	0.39	0/1830	0.65	0/2478
1	D	0.37	0/1800	0.63	0/2436
1	E	0.36	0/1783	0.61	0/2413
1	F	0.37	0/1757	0.60	1/2376 (0.0%)
All	All	0.38	0/10761	0.63	1/14562 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	202	PRO	N-CA-C	-5.70	97.28	112.10

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	1786	0	1840	82	0
1	B	1765	0	1821	78	0
1	C	1809	0	1864	95	0
1	D	1779	0	1831	112	0
1	E	1764	0	1818	91	0
1	F	1739	0	1779	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	51	0	0	3	0
2	B	40	0	0	4	0
2	C	50	0	0	3	0
2	D	35	0	0	1	0
2	E	31	0	0	0	0
2	F	29	0	0	0	0
All	All	10878	0	10953	535	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 25.

All (535) 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:C:158:THR:HG21	1:C:249:GLU:HB3	1.45	0.93
1:E:111:ASP:HA	1:E:115:THR:HG22	1.52	0.92
1:F:231:LYS:HE2	1:F:231:LYS:HA	1.52	0.91
1:A:50:ASP:OD1	1:A:52:ARG:HG2	1.71	0.91
1:C:163:GLY:HA2	1:C:173:ARG:HE	1.37	0.90
1:B:93:LEU:H	1:B:109:GLN:NE2	1.71	0.89
1:E:111:ASP:HA	1:E:115:THR:CG2	2.03	0.88
1:D:15:ILE:HD12	1:D:15:ILE:H	1.38	0.87
1:B:160:ASN:HD21	1:B:163:GLY:H	1.23	0.87
1:B:233:ASP:H	1:B:236:HIS:HD2	1.20	0.85
1:A:111:ASP:HA	1:A:115:THR:HG23	1.59	0.85
1:D:158:THR:HG23	1:D:250:PHE:O	1.78	0.84
1:F:127:LEU:HD12	1:F:127:LEU:H	1.41	0.84
1:C:158:THR:HG22	1:C:250:PHE:OXT	1.77	0.84
1:C:233:ASP:H	1:C:236:HIS:HD2	1.22	0.83
1:B:111:ASP:HA	1:B:115:THR:HG23	1.60	0.83
1:B:93:LEU:H	1:B:109:GLN:HE22	1.22	0.82
1:E:19:LEU:O	1:E:23:LEU:HD22	1.78	0.81
1:E:163:GLY:HA2	1:E:173:ARG:HE	1.44	0.81
1:E:138:ASP:HA	1:E:194:ASN:ND2	1.96	0.81
1:C:93:LEU:H	1:C:109:GLN:HE22	1.27	0.81
1:A:15:ILE:HD12	1:A:15:ILE:H	1.45	0.81
1:E:138:ASP:HA	1:E:194:ASN:HD21	1.47	0.80
1:A:166:GLN:HG3	1:C:205:VAL:HG23	1.63	0.80
1:D:50:ASP:OD1	1:D:52:ARG:HG2	1.83	0.78
1:C:218:VAL:N	1:C:221:SER:HG	1.81	0.78
1:B:111:ASP:HA	1:B:115:THR:CG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLY:HA2	1:E:173:ARG:NE	1.99	0.77
1:B:17:LEU:HD21	1:B:44:GLU:OE2	1.85	0.77
1:D:6:VAL:HG13	1:D:84:LEU:HD13	1.66	0.77
1:E:158:THR:HG22	1:F:250:PHE:HD2	1.50	0.76
1:B:50:ASP:OD1	1:B:52:ARG:HG2	1.84	0.76
1:C:239:ARG:HD2	2:C:276:HOH:O	1.86	0.76
1:D:232:LEU:HA	1:D:236:HIS:CD2	2.21	0.75
1:C:93:LEU:H	1:C:109:GLN:NE2	1.85	0.74
1:F:6:VAL:HG13	1:F:84:LEU:HD22	1.68	0.74
1:D:26:ASP:OD2	1:D:29:ILE:HG13	1.86	0.74
1:D:233:ASP:H	1:D:236:HIS:HD2	1.35	0.74
1:A:158:THR:HG22	1:A:250:PHE:OXT	1.88	0.74
1:A:160:ASN:HD21	1:A:163:GLY:H	1.33	0.73
1:D:190:LEU:HB3	1:D:195:VAL:HG13	1.71	0.73
1:D:111:ASP:HA	1:D:115:THR:HG23	1.70	0.72
1:F:233:ASP:H	1:F:236:HIS:HD2	1.37	0.72
1:A:6:VAL:HG13	1:A:84:LEU:HB3	1.71	0.72
1:E:12:ASN:ND2	1:E:13:ARG:HG2	2.04	0.72
1:A:245:LEU:O	1:A:246:LYS:HB3	1.90	0.72
1:D:64:LYS:HE3	1:D:64:LYS:HA	1.71	0.71
1:F:127:LEU:HD12	1:F:127:LEU:N	2.05	0.71
1:D:115:THR:HG21	2:D:271:HOH:O	1.89	0.71
1:F:187:ALA:HA	1:F:197:VAL:HG11	1.71	0.71
1:C:158:THR:CG2	1:C:249:GLU:HB3	2.19	0.71
1:C:13:ARG:NH2	1:C:88:ASN:HD21	1.89	0.71
1:C:50:ASP:HB3	1:C:53:VAL:CG1	2.21	0.70
1:F:111:ASP:HA	1:F:115:THR:HG23	1.74	0.70
1:D:200:PHE:HA	1:D:241:PHE:O	1.91	0.70
1:A:93:LEU:H	1:A:109:GLN:HE22	1.38	0.70
1:C:103:ARG:HB2	1:D:119:LEU:HD21	1.72	0.70
1:E:32:ILE:HB	1:E:53:VAL:HG12	1.73	0.70
1:F:42:ALA:HB1	1:F:45:LEU:HB3	1.73	0.70
1:B:115:THR:HG21	2:B:277:HOH:O	1.92	0.70
1:C:233:ASP:H	1:C:236:HIS:CD2	2.09	0.70
1:A:249:GLU:O	1:A:250:PHE:HB2	1.92	0.69
1:B:6:VAL:HG11	1:B:23:LEU:HD21	1.74	0.69
1:B:69:PHE:O	1:B:73:VAL:HG12	1.92	0.69
1:C:163:GLY:HA2	1:C:173:ARG:NE	2.07	0.69
1:F:158:THR:HG21	1:F:249:GLU:CB	2.23	0.69
1:C:164:SER:HB3	1:D:189:ASP:OD2	1.93	0.68
1:F:190:LEU:HD13	1:F:195:VAL:HG11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ALA:O	1:E:191:LYS:HE3	1.94	0.68
1:A:93:LEU:H	1:A:109:GLN:NE2	1.92	0.68
1:D:73:VAL:O	1:D:77:VAL:HG22	1.94	0.68
1:D:221:SER:HB3	1:D:243:ARG:HH11	1.58	0.68
1:B:6:VAL:HG13	1:B:84:LEU:HD13	1.76	0.67
1:A:111:ASP:HA	1:A:115:THR:CG2	2.24	0.67
1:C:138:ASP:HA	1:C:194:ASN:ND2	2.08	0.67
1:C:91:VAL:HG12	1:C:112:VAL:HG11	1.75	0.67
1:E:19:LEU:HD13	1:E:86:ILE:HD13	1.76	0.67
1:F:33:ILE:HD13	1:F:73:VAL:HG12	1.77	0.67
1:E:187:ALA:HB2	1:E:197:VAL:HG22	1.76	0.67
1:B:139:GLN:HB2	2:B:251:HOH:O	1.94	0.66
1:C:13:ARG:HH22	1:C:88:ASN:HD21	1.40	0.66
1:E:164:SER:HA	1:E:167:PHE:O	1.95	0.66
1:F:66:LEU:O	1:F:70:VAL:HG23	1.94	0.66
1:F:187:ALA:HA	1:F:197:VAL:CG1	2.25	0.66
1:A:173:ARG:HH22	1:C:166:GLN:NE2	1.94	0.66
1:B:242:MET:SD	1:B:246:LYS:HD3	2.36	0.66
1:D:249:GLU:O	1:D:250:PHE:HB2	1.96	0.66
1:F:70:VAL:O	1:F:73:VAL:HG22	1.96	0.66
1:A:103:ARG:HB2	1:B:119:LEU:HD21	1.77	0.65
1:B:249:GLU:O	1:B:250:PHE:HB2	1.94	0.65
1:C:19:LEU:HD13	1:C:86:ILE:HD13	1.78	0.65
1:D:162:SER:O	1:D:163:GLY:O	2.14	0.65
1:E:228:SER:HB3	1:E:245:LEU:HG	1.78	0.65
1:A:7:VAL:O	1:A:86:ILE:HG22	1.97	0.65
1:F:84:LEU:HD23	1:F:84:LEU:C	2.17	0.65
1:F:93:LEU:H	1:F:109:GLN:NE2	1.95	0.65
1:B:233:ASP:H	1:B:236:HIS:CD2	2.11	0.65
1:D:187:ALA:HB2	1:D:197:VAL:CG2	2.27	0.64
1:B:160:ASN:ND2	1:B:163:GLY:H	1.94	0.64
1:F:190:LEU:HD13	1:F:195:VAL:CG1	2.27	0.64
1:D:15:ILE:H	1:D:15:ILE:CD1	2.10	0.64
1:F:18:GLY:HA3	1:F:222:THR:HG21	1.78	0.64
1:E:38:ASP:OD2	1:E:41:LYS:HB2	1.97	0.64
1:F:73:VAL:O	1:F:77:VAL:HG22	1.96	0.64
1:C:250:PHE:HD2	1:D:158:THR:HG22	1.64	0.63
1:D:232:LEU:HA	1:D:236:HIS:HD2	1.63	0.63
1:E:86:ILE:HA	1:E:148:ILE:O	1.99	0.63
1:B:198:VAL:C	1:B:199:ASN:HD22	2.01	0.63
1:F:6:VAL:HG11	1:F:23:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:ASP:H	1:F:236:HIS:CD2	2.16	0.63
1:E:52:ARG:HG3	1:E:52:ARG:HH11	1.64	0.62
1:F:127:LEU:H	1:F:127:LEU:CD1	2.11	0.62
1:F:158:THR:HG21	1:F:249:GLU:HB2	1.80	0.62
1:D:30:ARG:HG3	1:D:30:ARG:HH11	1.64	0.62
1:A:185:THR:HG23	1:B:163:GLY:HA2	1.81	0.62
1:F:18:GLY:O	1:F:22:GLN:HG2	2.00	0.62
1:A:198:VAL:C	1:A:199:ASN:HD22	2.03	0.62
1:D:69:PHE:O	1:D:73:VAL:HG23	1.98	0.62
1:F:63:ASP:O	1:F:66:LEU:HB2	2.00	0.62
1:C:138:ASP:HA	1:C:194:ASN:HD21	1.65	0.61
1:C:13:ARG:HH22	1:C:88:ASN:ND2	1.99	0.61
1:B:160:ASN:HD21	1:B:163:GLY:N	1.97	0.61
1:D:233:ASP:H	1:D:236:HIS:CD2	2.16	0.61
1:D:242:MET:HB3	1:D:248:TYR:CE2	2.36	0.61
1:F:158:THR:HG22	1:F:250:PHE:O	2.00	0.61
1:D:125:LEU:N	1:D:126:PRO:HD2	2.16	0.61
1:E:233:ASP:H	1:E:236:HIS:HD2	1.48	0.61
1:D:15:ILE:HD12	1:D:15:ILE:N	2.11	0.60
1:F:52:ARG:HG2	1:F:52:ARG:HH11	1.65	0.60
1:F:63:ASP:HA	1:F:66:LEU:HD12	1.83	0.60
1:C:19:LEU:HD13	1:C:86:ILE:CD1	2.31	0.60
1:E:160:ASN:HD21	1:E:163:GLY:HA3	1.66	0.60
1:C:19:LEU:O	1:C:23:LEU:HD22	2.01	0.60
1:A:26:ASP:O	1:A:52:ARG:NH2	2.34	0.60
1:B:190:LEU:HB3	1:B:195:VAL:HG13	1.83	0.60
1:F:83:SER:O	1:F:145:ALA:HA	2.01	0.60
1:C:37:ARG:HA	1:C:58:LEU:O	2.02	0.60
1:C:69:PHE:O	1:C:73:VAL:HG12	2.02	0.60
1:A:135:GLU:O	1:A:135:GLU:HG3	2.01	0.60
1:D:152:SER:HB3	1:D:176:LYS:HG3	1.83	0.60
1:A:8:VAL:HG22	1:A:86:ILE:CG2	2.32	0.59
1:A:50:ASP:OD1	1:A:50:ASP:C	2.39	0.59
1:E:42:ALA:O	1:E:46:LYS:HG3	2.02	0.59
1:D:93:LEU:HD23	1:D:109:GLN:CD	2.22	0.59
1:E:21:GLN:O	1:E:24:VAL:HG22	2.02	0.59
1:A:233:ASP:H	1:A:236:HIS:HD2	1.49	0.59
1:C:50:ASP:HB3	1:C:53:VAL:HG13	1.84	0.59
1:C:17:LEU:O	1:C:21:GLN:HG3	2.03	0.59
1:C:44:GLU:O	1:C:47:SER:HB3	2.03	0.59
1:E:3:PRO:HB3	1:E:142:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:VAL:HA	1:E:23:LEU:HD23	1.85	0.59
1:E:38:ASP:OD1	1:E:41:LYS:HD3	2.02	0.59
1:C:71:SER:O	1:C:75:GLU:HG2	2.02	0.58
1:B:86:ILE:HA	1:B:148:ILE:O	2.04	0.58
1:A:158:THR:CG2	1:A:250:PHE:OXT	2.52	0.58
1:D:19:LEU:HD13	1:D:86:ILE:HD11	1.86	0.58
1:C:218:VAL:HG23	1:C:220:GLN:H	1.68	0.58
1:E:232:LEU:HA	1:E:236:HIS:CD2	2.38	0.58
1:F:126:PRO:O	1:F:130:ASN:HB2	2.03	0.58
1:A:190:LEU:HB3	1:A:195:VAL:HG13	1.86	0.58
1:D:18:GLY:O	1:D:22:GLN:HG2	2.03	0.58
1:D:93:LEU:H	1:D:109:GLN:NE2	2.02	0.58
1:F:140:LEU:O	1:F:141:SER:O	2.22	0.58
1:A:244:ASN:O	1:A:245:LEU:HB2	2.02	0.58
1:B:233:ASP:N	1:B:236:HIS:HD2	1.97	0.58
1:A:8:VAL:HG22	1:A:86:ILE:HG21	1.84	0.57
1:E:97:THR:HG22	1:E:170:LEU:HD22	1.85	0.57
1:A:27:LYS:HA	1:A:52:ARG:NH2	2.20	0.57
1:A:50:ASP:O	1:A:53:VAL:HG12	2.03	0.57
1:F:42:ALA:O	1:F:44:GLU:N	2.36	0.57
1:A:134:LYS:O	1:A:135:GLU:HB3	2.04	0.57
1:A:160:ASN:ND2	1:A:163:GLY:H	2.02	0.57
1:E:12:ASN:O	1:E:13:ARG:HD3	2.04	0.57
1:E:186:LEU:HG	1:E:190:LEU:HD12	1.87	0.57
1:A:222:THR:O	1:A:226:ILE:HG12	2.04	0.57
1:F:244:ASN:O	1:F:245:LEU:HB2	2.04	0.57
1:E:17:LEU:O	1:E:21:GLN:HG3	2.05	0.57
1:A:86:ILE:C	1:A:86:ILE:HD13	2.25	0.56
1:B:93:LEU:N	1:B:109:GLN:HE22	2.00	0.56
1:B:190:LEU:HD13	1:B:195:VAL:HG11	1.87	0.56
1:C:13:ARG:HE	1:C:13:ARG:C	2.07	0.56
1:F:239:ARG:HB2	1:F:241:PHE:CE2	2.41	0.56
1:A:189:ASP:OD2	1:B:164:SER:HB2	2.05	0.56
1:B:92:LEU:C	1:B:92:LEU:HD23	2.26	0.56
1:B:220:GLN:CD	1:B:220:GLN:H	2.09	0.56
1:A:140:LEU:HB3	1:A:196:LEU:HD13	1.88	0.56
1:A:199:ASN:HD22	1:A:199:ASN:N	2.03	0.56
1:A:86:ILE:HD11	1:A:150:ILE:CG1	2.36	0.56
1:C:199:ASN:N	1:C:199:ASN:HD22	2.02	0.56
1:F:226:ILE:HD12	1:F:229:PHE:HB2	1.88	0.56
1:E:93:LEU:HD21	1:E:108:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASN:HD22	1:B:199:ASN:N	2.03	0.55
1:D:220:GLN:HA	1:D:220:GLN:OE1	2.05	0.55
1:E:73:VAL:O	1:E:77:VAL:HG22	2.06	0.55
1:E:50:ASP:O	1:E:53:VAL:HG22	2.06	0.55
1:E:86:ILE:HD11	1:E:150:ILE:HD11	1.88	0.55
1:F:190:LEU:HB3	1:F:195:VAL:CG1	2.35	0.55
1:A:1:MET:HA	1:A:1:MET:CE	2.37	0.55
1:E:158:THR:HG22	1:F:250:PHE:CD2	2.37	0.55
1:E:164:SER:HB3	1:F:189:ASP:OD2	2.06	0.55
1:D:93:LEU:N	1:D:93:LEU:HD22	2.22	0.55
1:F:7:VAL:HG22	1:F:33:ILE:HB	1.88	0.55
1:F:35:THR:HA	1:F:56:LEU:O	2.05	0.55
1:B:190:LEU:HB3	1:B:195:VAL:CG1	2.36	0.55
1:C:199:ASN:ND2	2:C:256:HOH:O	2.39	0.55
1:E:7:VAL:O	1:E:86:ILE:HG22	2.06	0.55
1:C:163:GLY:H	1:C:173:ARG:NH2	2.04	0.55
1:E:199:ASN:N	1:E:199:ASN:HD22	2.05	0.55
1:F:249:GLU:O	1:F:250:PHE:HB2	2.07	0.55
1:C:12:ASN:ND2	1:C:13:ARG:HG3	2.21	0.54
1:C:91:VAL:HG22	1:C:92:LEU:N	2.22	0.54
1:D:22:GLN:HE21	1:D:22:GLN:HA	1.73	0.54
1:F:42:ALA:HB3	1:F:46:LYS:HG2	1.90	0.54
1:D:59:THR:HG1	1:D:62:CYS:HB3	1.72	0.54
1:F:93:LEU:H	1:F:109:GLN:HE22	1.54	0.54
1:C:111:ASP:HA	1:C:115:THR:HG23	1.88	0.54
1:A:49:LYS:HE3	1:A:49:LYS:HA	1.89	0.54
1:C:163:GLY:H	1:C:173:ARG:HH21	1.55	0.54
1:D:72:LYS:O	1:D:76:ILE:HG12	2.08	0.54
1:F:84:LEU:CD2	1:F:86:ILE:HG13	2.38	0.54
1:F:160:ASN:HD21	1:F:163:GLY:H	1.55	0.54
1:B:244:ASN:O	1:B:245:LEU:HB2	2.07	0.54
1:D:243:ARG:O	1:D:244:ASN:CG	2.45	0.54
1:D:18:GLY:HA3	1:D:222:THR:HG21	1.89	0.53
1:B:232:LEU:HA	1:B:236:HIS:CD2	2.43	0.53
1:D:190:LEU:HD13	1:D:195:VAL:HG11	1.90	0.53
1:F:122:GLN:HA	1:F:125:LEU:HG	1.90	0.53
1:E:158:THR:HG23	1:E:250:PHE:O	2.07	0.53
1:A:186:LEU:HD11	1:A:190:LEU:HD11	1.91	0.53
1:C:189:ASP:OD2	1:D:97:THR:HG23	2.07	0.53
1:F:129:LYS:HD2	1:F:193:ASP:OD2	2.09	0.53
1:E:69:PHE:O	1:E:73:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:VAL:O	1:B:46:LYS:HD2	2.08	0.53
1:C:86:ILE:HD12	1:C:150:ILE:HD11	1.90	0.53
1:B:59:THR:HA	2:B:279:HOH:O	2.09	0.53
1:B:86:ILE:HD13	1:B:86:ILE:C	2.28	0.53
1:C:39:VAL:HG22	1:C:39:VAL:O	2.09	0.53
1:C:198:VAL:C	1:C:199:ASN:HD22	2.12	0.53
1:A:13:ARG:HB2	2:A:264:HOH:O	2.09	0.52
1:D:57:PRO:O	1:D:58:LEU:HB2	2.09	0.52
1:A:86:ILE:HG23	1:A:86:ILE:O	2.10	0.52
1:B:160:ASN:C	1:B:160:ASN:HD22	2.12	0.52
1:C:13:ARG:NH2	1:C:88:ASN:ND2	2.55	0.52
1:F:176:LYS:O	1:F:179:ILE:HG22	2.09	0.52
1:D:12:ASN:HA	1:D:45:LEU:HD12	1.91	0.52
1:C:228:SER:O	1:C:232:LEU:HG	2.08	0.52
1:D:45:LEU:HD22	1:D:55:VAL:HG22	1.91	0.52
1:B:239:ARG:HB2	1:B:241:PHE:CZ	2.45	0.52
1:C:122:GLN:HE21	1:D:97:THR:HA	1.74	0.52
1:D:92:LEU:HD23	1:D:93:LEU:O	2.10	0.52
1:C:92:LEU:CD2	1:C:92:LEU:C	2.78	0.52
1:D:7:VAL:HG22	1:D:33:ILE:HB	1.92	0.52
1:A:86:ILE:HD11	1:A:150:ILE:HG12	1.91	0.52
1:F:97:THR:HG22	1:F:170:LEU:HD22	1.91	0.52
1:B:222:THR:O	1:B:226:ILE:HG12	2.10	0.52
1:F:62:CYS:O	1:F:66:LEU:HG	2.10	0.52
1:F:233:ASP:N	1:F:236:HIS:HD2	2.06	0.52
1:C:32:ILE:O	1:C:53:VAL:HA	2.10	0.51
1:E:202:PRO:HG2	1:E:203:GLY:H	1.75	0.51
1:F:15:ILE:N	1:F:15:ILE:HD12	2.25	0.51
1:B:222:THR:HA	1:B:225:LEU:HD12	1.91	0.51
1:C:244:ASN:O	1:C:245:LEU:HB2	2.11	0.51
1:E:103:ARG:NH1	1:F:111:ASP:OD1	2.43	0.51
1:E:93:LEU:H	1:E:109:GLN:NE2	2.08	0.51
1:B:86:ILE:HD13	1:B:86:ILE:O	2.11	0.51
1:C:20:VAL:O	1:C:24:VAL:HG13	2.11	0.51
1:E:39:VAL:HG13	1:E:40:GLU:N	2.26	0.51
1:F:198:VAL:C	1:F:199:ASN:HD22	2.14	0.51
1:F:224:GLU:O	1:F:227:SER:HB3	2.11	0.51
1:E:113:ASN:HB2	1:E:175:SER:HB2	1.92	0.51
1:F:43:THR:HA	1:F:46:LYS:HB2	1.92	0.51
1:C:132:ALA:HB2	1:C:145:ALA:CB	2.41	0.51
1:D:8:VAL:HA	1:D:86:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:SER:HB3	1:D:243:ARG:NH1	2.25	0.50
1:F:140:LEU:HD22	1:F:234:ASN:HA	1.93	0.50
1:B:93:LEU:CD1	1:B:108:GLU:HB3	2.41	0.50
1:F:69:PHE:O	1:F:73:VAL:HG13	2.12	0.50
1:F:115:THR:O	1:F:119:LEU:HD22	2.12	0.50
1:C:185:THR:HG21	1:D:170:LEU:HD13	1.93	0.50
1:C:190:LEU:HB3	1:C:195:VAL:HG13	1.94	0.50
1:F:50:ASP:OD2	1:F:52:ARG:NH1	2.43	0.50
1:F:120:LEU:O	1:F:124:LEU:HG	2.11	0.50
1:A:245:LEU:O	1:A:246:LYS:CB	2.59	0.50
1:C:186:LEU:HD11	1:C:190:LEU:HD11	1.93	0.50
1:D:50:ASP:O	1:D:53:VAL:HG12	2.12	0.50
1:B:1:MET:CE	1:B:1:MET:HA	2.42	0.50
1:B:93:LEU:HD11	1:B:108:GLU:HB3	1.92	0.50
1:C:188:VAL:HG11	1:D:163:GLY:H	1.77	0.50
1:D:222:THR:O	1:D:226:ILE:HG12	2.12	0.50
1:D:19:LEU:HD13	1:D:86:ILE:CD1	2.42	0.50
1:B:249:GLU:O	1:B:250:PHE:CB	2.60	0.49
1:A:72:LYS:O	1:A:76:ILE:HG13	2.11	0.49
1:A:160:ASN:C	1:A:160:ASN:HD22	2.15	0.49
1:D:30:ARG:HG3	1:D:30:ARG:NH1	2.27	0.49
1:A:204:TRP:CD1	1:C:168:PRO:HD3	2.48	0.49
1:C:86:ILE:CD1	1:C:150:ILE:HD11	2.43	0.49
1:F:5:SER:OG	1:F:83:SER:HB3	2.12	0.49
1:F:222:THR:HA	1:F:225:LEU:HD12	1.93	0.49
1:D:35:THR:HA	1:D:56:LEU:O	2.13	0.49
1:D:193:ASP:O	1:D:194:ASN:HB2	2.12	0.49
1:F:140:LEU:HD13	1:F:234:ASN:ND2	2.27	0.49
1:A:35:THR:HA	1:A:56:LEU:O	2.11	0.49
1:B:45:LEU:HD23	1:B:48:ILE:HD12	1.94	0.49
1:C:21:GLN:O	1:C:24:VAL:HG22	2.13	0.49
1:D:11:ALA:HA	1:D:16:GLY:HA3	1.95	0.49
1:D:140:LEU:O	1:D:233:ASP:HA	2.13	0.49
1:F:21:GLN:O	1:F:24:VAL:HG22	2.13	0.49
1:A:17:LEU:O	1:A:21:GLN:HG3	2.13	0.49
1:C:249:GLU:O	1:C:250:PHE:HB2	2.13	0.49
1:B:118:VAL:O	1:B:122:GLN:HG3	2.13	0.48
1:D:187:ALA:HB2	1:D:197:VAL:HG21	1.95	0.48
1:A:49:LYS:O	1:A:50:ASP:O	2.31	0.48
1:D:224:GLU:CD	1:D:243:ARG:HD2	2.34	0.48
1:E:92:LEU:C	1:E:92:LEU:HD23	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ASN:HD21	1:E:163:GLY:CA	2.25	0.48
1:D:233:ASP:N	1:D:236:HIS:HD2	2.08	0.48
1:E:92:LEU:HD23	1:E:92:LEU:O	2.14	0.48
1:F:125:LEU:HB2	1:F:126:PRO:HD3	1.94	0.48
1:F:187:ALA:CA	1:F:197:VAL:HG11	2.42	0.48
1:C:227:SER:O	1:C:231:LYS:HG3	2.13	0.48
1:D:59:THR:OG1	1:D:62:CYS:HB3	2.13	0.48
1:D:80:ASP:HA	1:D:134:LYS:HE3	1.94	0.48
1:A:242:MET:O	1:A:245:LEU:N	2.45	0.48
1:A:249:GLU:O	1:A:250:PHE:CB	2.60	0.48
1:E:50:ASP:OD1	1:E:52:ARG:HG3	2.14	0.48
1:E:92:LEU:HA	1:E:109:GLN:HE22	1.78	0.48
1:F:113:ASN:ND2	1:F:176:LYS:HE2	2.28	0.48
1:D:190:LEU:HB3	1:D:195:VAL:CG1	2.42	0.48
1:E:11:ALA:HB3	1:E:34:ALA:HB1	1.94	0.48
1:C:82:LEU:HD12	1:C:128:LEU:HD21	1.96	0.48
1:C:84:LEU:HD22	1:C:86:ILE:HG22	1.94	0.48
1:A:185:THR:HG23	1:B:163:GLY:CA	2.44	0.48
1:D:86:ILE:HD12	1:D:229:PHE:HE2	1.78	0.48
1:B:20:VAL:O	1:B:24:VAL:HG13	2.14	0.48
1:F:73:VAL:HG23	1:F:74:GLY:N	2.29	0.47
1:A:15:ILE:HD12	1:A:15:ILE:N	2.23	0.47
1:D:64:LYS:HA	1:D:64:LYS:CE	2.40	0.47
1:D:92:LEU:HD23	1:D:92:LEU:C	2.35	0.47
1:E:83:SER:O	1:E:145:ALA:HA	2.13	0.47
1:F:84:LEU:HD21	1:F:86:ILE:HG13	1.94	0.47
1:F:232:LEU:HA	1:F:236:HIS:CD2	2.48	0.47
1:E:185:THR:HG21	1:F:170:LEU:HD13	1.95	0.47
1:E:50:ASP:OD2	1:E:52:ARG:NH1	2.46	0.47
1:E:87:ASN:HB2	1:E:149:THR:HG23	1.96	0.47
1:C:86:ILE:HA	1:C:148:ILE:O	2.15	0.47
1:D:83:SER:O	1:D:145:ALA:HA	2.15	0.47
1:A:15:ILE:H	1:A:15:ILE:CD1	2.22	0.47
1:A:70:VAL:O	1:A:73:VAL:HG22	2.15	0.47
1:A:83:SER:O	1:A:145:ALA:HA	2.15	0.47
1:D:22:GLN:HA	1:D:22:GLN:NE2	2.29	0.47
1:F:196:LEU:HD21	1:F:232:LEU:HB3	1.96	0.47
1:A:86:ILE:HA	1:A:148:ILE:O	2.15	0.47
1:A:113:ASN:ND2	1:A:176:LYS:HE2	2.30	0.47
1:A:115:THR:HB	1:B:106:ILE:HG21	1.96	0.47
1:F:91:VAL:HG13	1:F:93:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ALA:O	1:D:191:LYS:HE3	2.15	0.47
1:B:190:LEU:HD13	1:B:195:VAL:CG1	2.44	0.47
1:A:22:GLN:HE21	1:A:22:GLN:HA	1.80	0.46
1:D:160:ASN:C	1:D:160:ASN:HD22	2.18	0.46
1:E:196:LEU:HD12	1:E:237:ASN:OD1	2.15	0.46
1:D:45:LEU:O	1:D:45:LEU:HD23	2.16	0.46
1:F:158:THR:HG21	1:F:249:GLU:HB3	1.96	0.46
1:A:140:LEU:O	1:A:233:ASP:HA	2.15	0.46
1:D:188:VAL:O	1:D:191:LYS:HB2	2.16	0.46
1:C:102:ASN:OD1	1:C:104:ALA:HB3	2.16	0.46
1:C:31:HIS:HD2	2:C:265:HOH:O	1.97	0.46
1:C:73:VAL:O	1:C:77:VAL:HG22	2.16	0.46
1:E:125:LEU:N	1:E:126:PRO:CD	2.79	0.46
1:B:9:THR:HA	1:B:35:THR:OG1	2.16	0.46
1:D:23:LEU:HB3	1:D:32:ILE:HD13	1.96	0.46
1:D:66:LEU:CD2	1:D:120:LEU:HD13	2.45	0.46
1:F:123:LYS:O	1:F:124:LEU:HD23	2.15	0.46
1:F:199:ASN:HD22	1:F:199:ASN:N	2.11	0.46
1:A:50:ASP:OD2	1:A:52:ARG:NH1	2.48	0.46
1:E:113:ASN:ND2	1:E:176:LYS:HE2	2.31	0.46
1:C:1:MET:HG3	1:C:2:SER:H	1.81	0.45
1:B:22:GLN:OE1	1:B:223:ALA:HB2	2.16	0.45
1:C:189:ASP:OD2	1:D:97:THR:CG2	2.64	0.45
1:E:162:SER:O	1:F:188:VAL:HG11	2.16	0.45
1:E:40:GLU:C	1:E:41:LYS:HD2	2.37	0.45
1:E:91:VAL:HG22	1:E:92:LEU:N	2.31	0.45
1:B:19:LEU:O	1:B:23:LEU:HB2	2.17	0.45
1:B:170:LEU:O	1:B:174:MET:HG3	2.17	0.45
1:D:249:GLU:O	1:D:250:PHE:CB	2.64	0.45
1:F:140:LEU:HD23	1:F:196:LEU:HD13	1.99	0.45
1:A:22:GLN:HB3	1:A:226:ILE:HG13	1.97	0.45
1:D:17:LEU:O	1:D:21:GLN:HG3	2.16	0.45
1:D:37:ARG:HG3	1:D:59:THR:HG22	1.99	0.45
1:E:11:ALA:O	1:E:17:LEU:HB2	2.14	0.45
1:A:66:LEU:O	1:A:70:VAL:HG23	2.17	0.45
1:E:12:ASN:HD22	1:E:13:ARG:HG2	1.78	0.45
1:E:242:MET:HG2	1:E:248:TYR:CE2	2.51	0.45
1:F:228:SER:HB2	1:F:245:LEU:HG	1.99	0.45
1:A:79:SER:O	1:A:134:LYS:HE2	2.16	0.45
1:E:178:ALA:O	1:E:181:MET:HB3	2.17	0.45
1:A:10:GLY:O	1:A:16:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LEU:HD23	1:C:93:LEU:N	2.31	0.45
1:E:84:LEU:CD2	1:E:85:LEU:N	2.80	0.45
1:C:164:SER:HA	1:C:167:PHE:O	2.17	0.44
1:E:6:VAL:HG12	1:E:7:VAL:N	2.31	0.44
1:E:12:ASN:HD22	1:E:13:ARG:NE	2.15	0.44
1:F:68:THR:HG22	1:F:72:LYS:HE3	1.99	0.44
1:F:113:ASN:HD22	1:F:176:LYS:HE2	1.82	0.44
1:C:222:THR:O	1:C:226:ILE:HG12	2.17	0.44
1:B:49:LYS:HB2	1:B:49:LYS:NZ	2.32	0.44
1:C:198:VAL:HG22	1:C:236:HIS:O	2.18	0.44
1:D:176:LYS:O	1:D:179:ILE:HG22	2.17	0.44
1:D:242:MET:O	1:D:243:ARG:O	2.35	0.44
1:E:19:LEU:HD13	1:E:86:ILE:CD1	2.45	0.44
1:E:60:VAL:HB	1:E:116:SER:HB3	1.98	0.44
1:A:160:ASN:ND2	1:A:160:ASN:C	2.71	0.44
1:E:184:ARG:HG2	1:F:160:ASN:HB3	2.00	0.44
1:F:17:LEU:O	1:F:21:GLN:HG3	2.18	0.44
1:A:91:VAL:HG22	1:A:92:LEU:N	2.33	0.44
1:B:187:ALA:HA	1:B:197:VAL:HG13	2.00	0.44
1:C:163:GLY:N	1:C:173:ARG:HH21	2.13	0.44
1:C:222:THR:HA	1:C:225:LEU:HD12	1.99	0.44
1:D:57:PRO:O	1:D:58:LEU:CB	2.66	0.44
1:D:7:VAL:O	1:D:86:ILE:HG23	2.17	0.44
1:D:92:LEU:HA	1:D:109:GLN:HE22	1.83	0.44
1:E:139:GLN:O	1:E:139:GLN:HG2	2.18	0.44
1:B:85:LEU:HD22	1:B:124:LEU:HD12	2.00	0.44
1:C:160:ASN:C	1:C:160:ASN:HD22	2.21	0.44
1:A:242:MET:HB2	1:A:245:LEU:O	2.18	0.44
1:B:160:ASN:ND2	1:B:160:ASN:C	2.71	0.44
1:C:239:ARG:HB2	1:C:241:PHE:CZ	2.53	0.44
1:C:122:GLN:HA	1:C:125:LEU:HG	2.00	0.43
1:D:45:LEU:HD22	1:D:55:VAL:CG2	2.48	0.43
1:D:227:SER:O	1:D:231:LYS:HG3	2.18	0.43
1:E:233:ASP:N	1:E:236:HIS:HD2	2.16	0.43
1:F:9:THR:HB	1:F:89:ALA:HB2	1.99	0.43
1:F:30:ARG:O	1:F:52:ARG:HB2	2.18	0.43
1:C:207:THR:O	1:C:207:THR:CG2	2.66	0.43
1:E:113:ASN:O	1:E:179:ILE:HG13	2.19	0.43
1:A:9:THR:O	1:A:88:ASN:HB3	2.18	0.43
1:A:122:GLN:HB3	1:B:101:PRO:HG3	2.00	0.43
1:B:146:ALA:HA	1:B:196:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLY:O	1:D:189:ASP:OD1	2.36	0.43
1:F:151:SER:HB3	1:F:240:PHE:CE1	2.53	0.43
1:F:169:VAL:O	1:F:173:ARG:HG3	2.19	0.43
1:B:178:ALA:O	1:B:181:MET:HB3	2.18	0.43
1:C:1:MET:HG3	1:C:2:SER:N	2.34	0.43
1:E:52:ARG:HG3	1:E:52:ARG:NH1	2.31	0.43
1:B:160:ASN:HD22	1:B:161:THR:N	2.17	0.43
1:D:43:THR:HA	1:D:46:LYS:HD3	2.01	0.43
1:E:70:VAL:HG21	1:E:123:LYS:HB3	2.00	0.43
1:E:140:LEU:HB3	1:E:196:LEU:HB2	1.99	0.43
1:A:22:GLN:HA	1:A:22:GLN:NE2	2.33	0.43
1:A:69:PHE:O	1:A:73:VAL:HG13	2.19	0.43
1:C:162:SER:OG	1:C:163:GLY:N	2.52	0.43
1:D:88:ASN:HA	1:D:150:ILE:HD13	2.01	0.43
1:A:18:GLY:O	1:A:22:GLN:HG2	2.18	0.43
1:B:70:VAL:HA	1:B:73:VAL:CG1	2.48	0.43
1:C:207:THR:O	1:C:207:THR:HG22	2.18	0.43
1:D:86:ILE:HD12	1:D:229:PHE:CE2	2.54	0.43
1:D:91:VAL:HG13	1:D:93:LEU:HD22	2.00	0.43
1:B:50:ASP:OD2	1:B:52:ARG:NH1	2.52	0.43
1:C:125:LEU:N	1:C:126:PRO:CD	2.82	0.42
1:D:8:VAL:HG22	1:D:86:ILE:HG21	2.01	0.42
1:E:157:ILE:O	1:E:160:ASN:HB3	2.18	0.42
1:F:20:VAL:O	1:F:24:VAL:HG13	2.19	0.42
1:B:157:ILE:N	1:B:250:PHE:O	2.40	0.42
1:D:9:THR:O	1:D:88:ASN:HB3	2.19	0.42
1:D:97:THR:HG23	1:D:164:SER:OG	2.19	0.42
1:F:15:ILE:HG12	1:F:202:PRO:HG3	2.00	0.42
1:F:200:PHE:HZ	1:F:232:LEU:HD21	1.85	0.42
1:A:50:ASP:HA	2:A:293:HOH:O	2.20	0.42
1:E:119:LEU:HD13	1:F:106:ILE:HD12	2.01	0.42
1:A:127:LEU:HG	2:A:262:HOH:O	2.20	0.42
1:D:87:ASN:O	1:D:150:ILE:HD13	2.19	0.42
1:B:187:ALA:HA	1:B:197:VAL:CG1	2.49	0.42
1:C:49:LYS:HD3	1:C:49:LYS:N	2.34	0.42
1:B:64:LYS:HD3	1:B:64:LYS:HA	1.76	0.42
1:D:7:VAL:O	1:D:7:VAL:HG12	2.19	0.42
1:D:198:VAL:C	1:D:199:ASN:HD22	2.22	0.42
1:E:8:VAL:HG22	1:E:86:ILE:CG2	2.49	0.42
1:F:151:SER:HB3	1:F:240:PHE:HE1	1.84	0.42
1:F:231:LYS:HE2	1:F:231:LYS:CA	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:VAL:O	1:D:197:VAL:HG23	2.20	0.42
1:D:49:LYS:O	1:D:50:ASP:C	2.58	0.42
1:E:18:GLY:O	1:E:22:GLN:HG2	2.20	0.42
1:E:82:LEU:HD12	1:E:124:LEU:HD22	2.02	0.42
1:E:160:ASN:HD21	1:E:163:GLY:N	2.18	0.42
1:E:239:ARG:HB2	1:E:241:PHE:CE1	2.55	0.42
1:E:39:VAL:HG23	1:E:55:VAL:HG11	2.02	0.42
1:F:26:ASP:OD1	1:F:29:ILE:HG13	2.19	0.41
1:B:23:LEU:HD13	1:B:226:ILE:HD12	2.02	0.41
1:C:82:LEU:HD12	1:C:128:LEU:CD2	2.50	0.41
1:E:225:LEU:HD23	1:E:243:ARG:HA	2.03	0.41
1:F:93:LEU:N	1:F:93:LEU:HD22	2.35	0.41
1:F:140:LEU:HD23	1:F:196:LEU:CD1	2.49	0.41
1:B:132:ALA:HB2	1:B:145:ALA:CB	2.50	0.41
1:B:176:LYS:O	1:B:179:ILE:HG22	2.20	0.41
1:C:160:ASN:C	1:C:160:ASN:ND2	2.73	0.41
1:C:189:ASP:OD1	1:D:163:GLY:HA3	2.20	0.41
1:D:19:LEU:HD22	1:D:226:ILE:HD11	2.02	0.41
1:B:138:ASP:HA	1:B:194:ASN:ND2	2.35	0.41
1:C:12:ASN:CG	1:C:13:ARG:HG3	2.40	0.41
1:C:190:LEU:HB3	1:C:195:VAL:CG1	2.50	0.41
1:B:23:LEU:HD12	1:B:23:LEU:HA	1.93	0.41
1:C:39:VAL:HG23	1:C:55:VAL:HG12	2.02	0.41
1:E:179:ILE:HD13	1:E:179:ILE:HA	1.88	0.41
1:A:233:ASP:H	1:A:236:HIS:CD2	2.34	0.41
1:C:38:ASP:C	1:C:40:GLU:H	2.24	0.41
1:C:50:ASP:OD1	1:C:52:ARG:HG3	2.20	0.41
1:C:164:SER:HB3	1:D:189:ASP:CG	2.41	0.41
1:F:50:ASP:OD1	1:F:52:ARG:HG2	2.20	0.41
1:A:99:THR:O	1:A:100:GLU:C	2.58	0.41
1:D:32:ILE:O	1:D:53:VAL:HA	2.21	0.41
1:E:93:LEU:CD2	1:E:108:GLU:HB3	2.50	0.41
1:F:117:VAL:HG11	1:F:179:ILE:HD11	2.03	0.41
1:D:190:LEU:HD13	1:D:195:VAL:CG1	2.50	0.41
1:D:227:SER:O	1:D:231:LYS:HE3	2.21	0.41
1:A:39:VAL:O	1:A:41:LYS:N	2.53	0.41
1:B:9:THR:O	1:B:88:ASN:HB3	2.21	0.41
1:E:84:LEU:HD21	1:E:148:ILE:HD13	2.02	0.41
1:E:32:ILE:O	1:E:53:VAL:HA	2.20	0.41
1:F:242:MET:HG2	1:F:248:TYR:CE2	2.56	0.41
1:B:144:ARG:HB3	2:B:289:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LYS:HE3	1:D:64:LYS:CA	2.47	0.40
1:D:176:LYS:HA	1:D:176:LYS:HD3	1.87	0.40
1:F:221:SER:O	1:F:225:LEU:HG	2.20	0.40
1:A:49:LYS:HA	1:A:49:LYS:CE	2.52	0.40
1:A:135:GLU:O	1:A:135:GLU:CG	2.68	0.40
1:D:140:LEU:HB2	1:D:234:ASN:OD1	2.21	0.40
1:E:226:ILE:HA	1:E:229:PHE:CD2	2.55	0.40
1:F:109:GLN:HG2	1:F:171:ALA:CB	2.51	0.40
1:F:146:ALA:HA	1:F:196:LEU:O	2.22	0.40
1:D:151:SER:HA	1:D:176:LYS:HD2	2.03	0.40
1:F:52:ARG:HH11	1:F:52:ARG:CG	2.29	0.40
1:A:182:PHE:HD1	1:B:170:LEU:HD11	1.85	0.40
1:B:79:SER:O	1:B:130:ASN:ND2	2.53	0.40
1:F:91:VAL:HG13	1:F:93:LEU:HD21	2.03	0.40
1:B:92:LEU:C	1:B:92:LEU:CD2	2.90	0.40
1:D:52:ARG:HG2	1:D:52:ARG:H	1.77	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	233/250 (93%)	214 (92%)	13 (6%)	6 (3%)	5 9
1	B	231/250 (92%)	211 (91%)	18 (8%)	2 (1%)	17 35
1	C	236/250 (94%)	224 (95%)	10 (4%)	2 (1%)	19 39
1	D	232/250 (93%)	209 (90%)	15 (6%)	8 (3%)	3 5
1	E	231/250 (92%)	212 (92%)	16 (7%)	3 (1%)	12 24
1	F	220/250 (88%)	194 (88%)	23 (10%)	3 (1%)	11 22
All	All	1383/1500 (92%)	1264 (91%)	95 (7%)	24 (2%)	9 18

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	50	ASP
1	A	135	GLU
1	C	163	GLY
1	D	58	LEU
1	D	163	GLY
1	E	163	GLY
1	F	43	THR
1	F	141	SER
1	B	60	VAL
1	C	39	VAL
1	D	50	ASP
1	D	139	GLN
1	D	243	ARG
1	E	27	LYS
1	F	144	ARG
1	A	246	LYS
1	B	166	GLN
1	D	234	ASN
1	A	134	LYS
1	A	245	LEU
1	E	14	GLY
1	D	165	ALA
1	D	101	PRO

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	203/212 (96%)	182 (90%)	21 (10%)	7 13
1	B	201/212 (95%)	187 (93%)	14 (7%)	15 30
1	C	206/212 (97%)	186 (90%)	20 (10%)	8 15
1	D	202/212 (95%)	192 (95%)	10 (5%)	24 47
1	E	201/212 (95%)	190 (94%)	11 (6%)	21 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	198/212 (93%)	191 (96%)	7 (4%)	36 62
All	All	1211/1272 (95%)	1128 (93%)	83 (7%)	15 31

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	13	ARG
1	A	23	LEU
1	A	45	LEU
1	A	49	LYS
1	A	50	ASP
1	A	52	ARG
1	A	71	SER
1	A	82	LEU
1	A	84	LEU
1	A	86	ILE
1	A	93	LEU
1	A	115	THR
1	A	119	LEU
1	A	130	ASN
1	A	158	THR
1	A	160	ASN
1	A	195	VAL
1	A	197	VAL
1	A	199	ASN
1	B	23	LEU
1	B	52	ARG
1	B	59	THR
1	B	73	VAL
1	B	82	LEU
1	B	84	LEU
1	B	86	ILE
1	B	115	THR
1	B	119	LEU
1	B	140	LEU
1	B	160	ASN
1	B	195	VAL
1	B	197	VAL
1	B	199	ASN
1	C	13	ARG

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Mol	Chain	Res	Type
1	C	23	LEU
1	C	37	ARG
1	C	45	LEU
1	C	49	LYS
1	C	53	VAL
1	C	73	VAL
1	C	84	LEU
1	C	86	ILE
1	C	92	LEU
1	C	115	THR
1	C	119	LEU
1	C	138	ASP
1	C	140	LEU
1	C	158	THR
1	C	159	ASP
1	C	160	ASN
1	C	195	VAL
1	C	197	VAL
1	C	199	ASN
1	D	23	LEU
1	D	52	ARG
1	D	64	LYS
1	D	84	LEU
1	D	115	THR
1	D	119	LEU
1	D	139	GLN
1	D	160	ASN
1	D	191	LYS
1	D	195	VAL
1	E	23	LEU
1	E	41	LYS
1	E	59	THR
1	E	72	LYS
1	E	82	LEU
1	E	84	LEU
1	E	119	LEU
1	E	138	ASP
1	E	179	ILE
1	E	197	VAL
1	E	199	ASN
1	F	23	LEU
1	F	75	GLU

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Mol	Chain	Res	Type
1	F	115	THR
1	F	119	LEU
1	F	160	ASN
1	F	197	VAL
1	F	204	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	109	GLN
1	A	130	ASN
1	A	139	GLN
1	A	160	ASN
1	A	166	GLN
1	A	199	ASN
1	A	236	HIS
1	B	109	GLN
1	B	160	ASN
1	B	194	ASN
1	B	199	ASN
1	B	236	HIS
1	C	31	HIS
1	C	88	ASN
1	C	109	GLN
1	C	122	GLN
1	C	160	ASN
1	C	166	GLN
1	C	194	ASN
1	C	199	ASN
1	C	236	HIS
1	D	22	GLN
1	D	54	HIS
1	D	109	GLN
1	D	160	ASN
1	D	199	ASN
1	D	236	HIS
1	E	12	ASN
1	E	109	GLN
1	E	122	GLN
1	E	160	ASN
1	E	194	ASN

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Mol	Chain	Res	Type
1	E	199	ASN
1	E	220	GLN
1	E	236	HIS
1	F	22	GLN
1	F	31	HIS
1	F	109	GLN
1	F	160	ASN
1	F	199	ASN
1	F	236	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	237/250 (94%)	-0.23	0 100 100	26, 41, 61, 74	0
1	B	235/250 (94%)	-0.29	1 (0%) 92 91	27, 44, 64, 73	0
1	C	240/250 (96%)	-0.34	0 100 100	27, 38, 59, 71	0
1	D	236/250 (94%)	-0.23	2 (0%) 86 84	29, 48, 79, 92	0
1	E	235/250 (94%)	-0.29	0 100 100	33, 50, 69, 82	0
1	F	230/250 (92%)	0.02	3 (1%) 77 73	34, 58, 79, 88	0
All	All	1413/1500 (94%)	-0.23	6 (0%) 92 91	26, 45, 71, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	140	LEU	3.0
1	D	39	VAL	2.9
1	D	41	LYS	2.6
1	B	165	ALA	2.4
1	F	195	VAL	2.1
1	F	29	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.