Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:57 am BST

PDB ID	:	1I0A
Title	:	CRYSTAL STRUCTURE OF WILD TYPE TURKEY DELTA 1 CRYSTALLIN (EYE LENS PROTEIN)
Authors	:	Sampaleanu, L.M.; Vallee, F.; Slingsby, C.; Howell, P.L.
Deposited on	:	2001-01-29
Resolution	:	2.50 Å(reported)

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

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

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

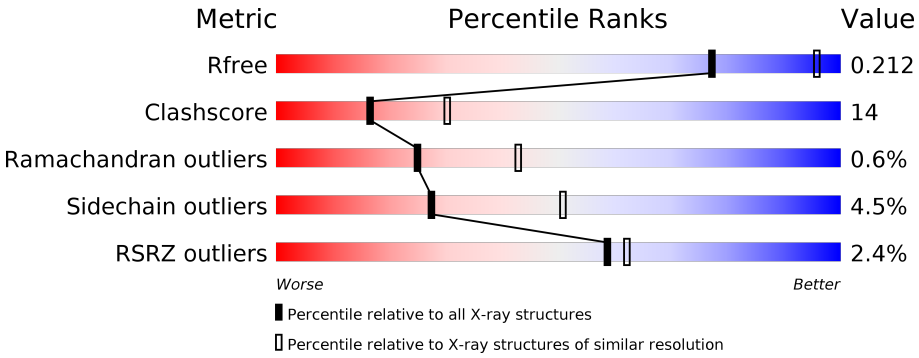
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	466	2% 68% 27% • •
1	B	466	2% 65% 29% • 5%
1	C	466	2% 69% 24% • 5%
1	D	466	2% 70% 23% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14263 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 DELTA CRYSTALLIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3461	2192	581	679	9			
1	B	444	Total	C	N	O	S	0	0	0
			3407	2156	572	670	9			
1	C	445	Total	C	N	O	S	0	0	0
			3413	2159	572	673	9			
1	D	443	Total	C	N	O	S	0	0	0
			3394	2148	569	668	9			

- Molecule 2 is water.

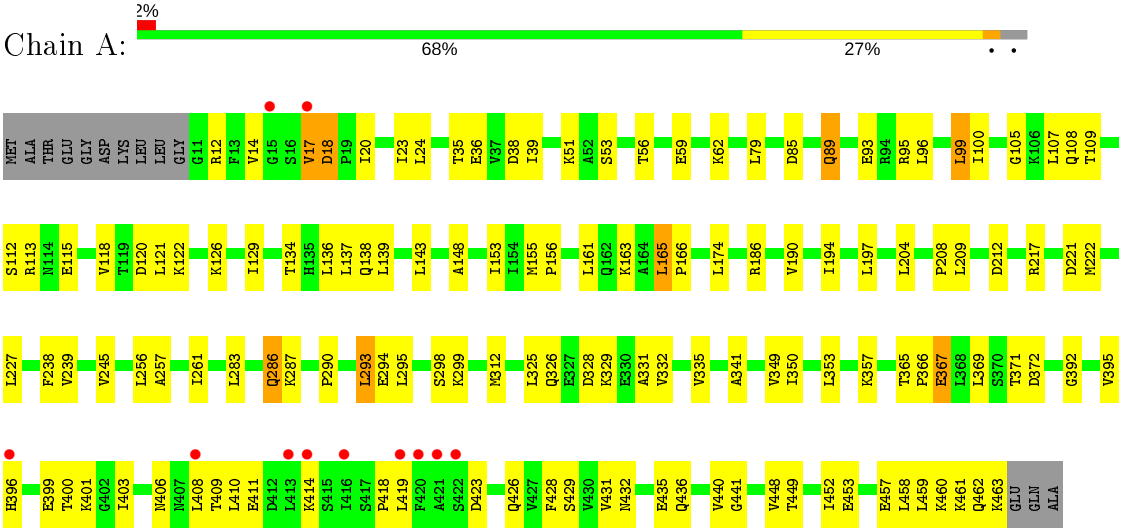
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	156	Total	O	0	0
			156	156		
2	C	142	Total	O	0	0
			142	142		
2	D	144	Total	O	0	0
			144	144		

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 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.

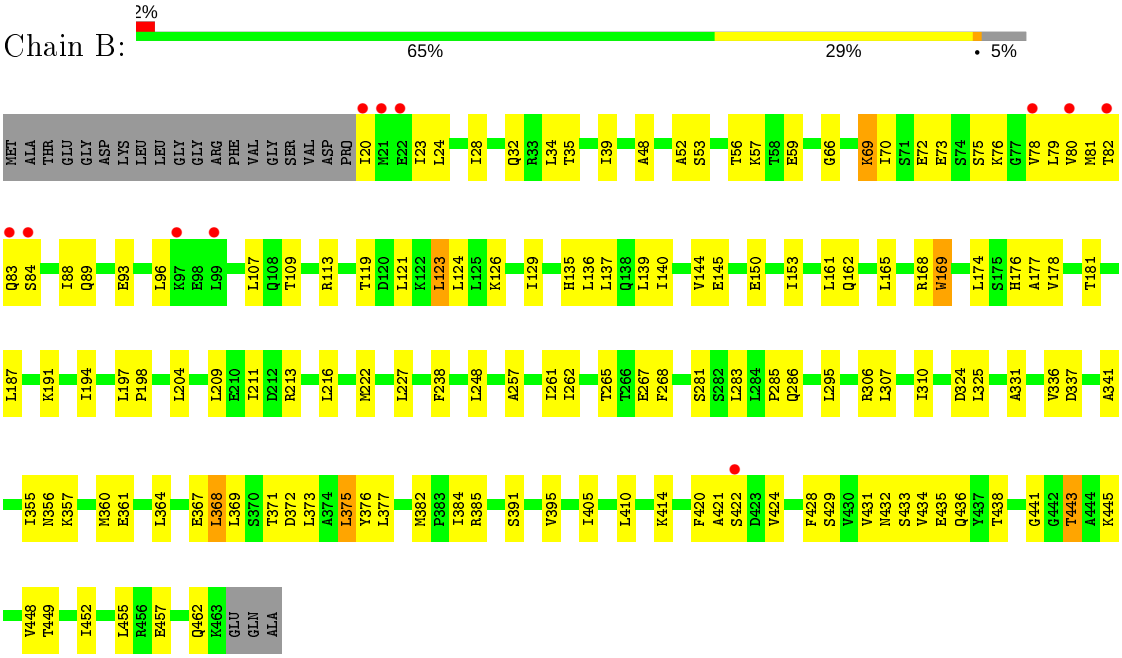
- Molecule 1: DELTA CRYSTALLIN I

Chain A:



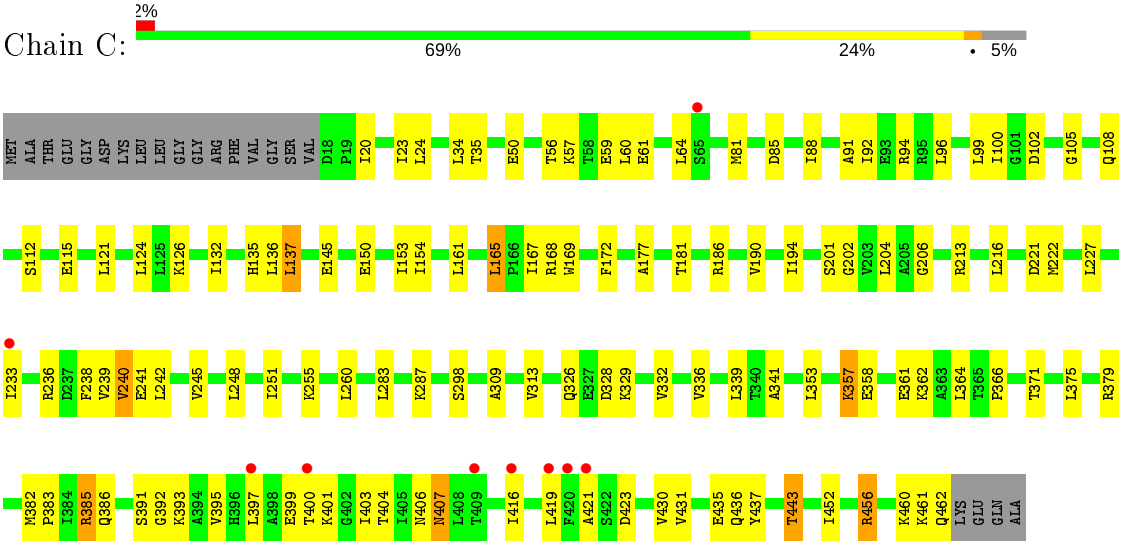
- Molecule 1: DELTA CRYSTALLIN I

Chain B:



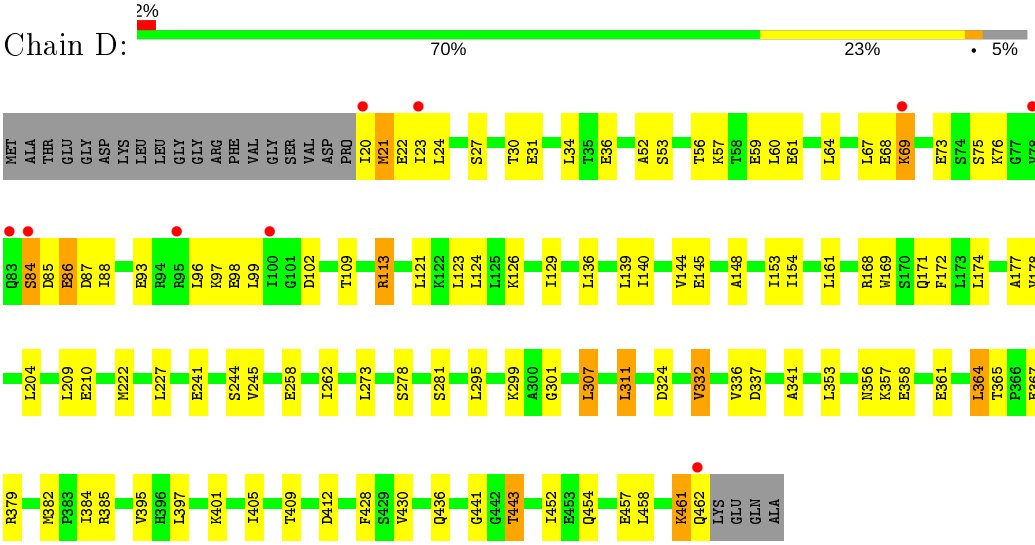
- Molecule 1: DELTA CRYSTALLIN I

Chain C:



- Molecule 1: DELTA CRYSTALLIN I

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.42Å 146.55Å 152.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 2.50 35.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (19.78-2.50) 95.2 (35.27-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	7.09 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.156 , 0.213 0.156 , 0.212	Depositor DCC
R_{free} test set	6641 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14263	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.30	0/3493	0.55	1/4722 (0.0%)
1	B	0.34	0/3437	0.56	0/4644
1	C	0.31	0/3444	0.57	1/4656 (0.0%)
1	D	0.31	0/3424	0.56	0/4628
All	All	0.32	0/13798	0.56	2/18650 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	ASP	N-CA-C	-6.86	92.48	111.00
1	A	85	ASP	N-CA-C	-5.49	96.17	111.00

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	3461	0	3651	101	0
1	B	3407	0	3607	121	0
1	C	3413	0	3605	101	0
1	D	3394	0	3588	96	0
2	A	146	0	0	5	0
2	B	156	0	0	6	0
2	C	142	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	144	0	0	6	0
All	All	14263	0	14451	400	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (400) 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:32:GLN:HE21	1:B:81:MET:HG2	1.34	0.92
1:C:194:ILE:HD13	1:C:238:PHE:HB2	1.56	0.88
1:C:153:ILE:HG23	1:C:169:TRP:HB3	1.59	0.84
1:B:35:THR:HG22	1:B:88:ILE:HD11	1.59	0.83
1:C:379:ARG:HH22	1:C:436:GLN:NE2	1.77	0.83
1:D:168:ARG:H	1:D:443:THR:HG21	1.44	0.82
1:C:357:LYS:O	1:C:361:GLU:HG2	1.81	0.80
1:B:429:SER:HB3	1:B:432:ASN:HD22	1.46	0.80
1:A:99:LEU:HD13	1:A:100:ILE:HD13	1.64	0.80
1:B:153:ILE:HD11	1:B:360:MET:SD	2.23	0.79
1:A:143:LEU:HD21	1:A:350:ILE:HD13	1.65	0.79
1:C:168:ARG:H	1:C:443:THR:HG21	1.49	0.78
1:A:429:SER:HB3	1:A:432:ASN:HD22	1.48	0.78
1:B:153:ILE:HD12	1:B:357:LYS:HG2	1.66	0.77
1:A:129:ILE:HD11	1:A:194:ILE:HD12	1.66	0.77
1:B:168:ARG:H	1:B:443:THR:HG21	1.50	0.76
1:A:35:THR:O	1:A:39:ILE:HG12	1.86	0.76
1:C:150:GLU:O	1:C:153:ILE:HG22	1.87	0.75
1:C:177:ALA:O	1:C:181:THR:HG23	1.85	0.75
1:D:75:SER:C	1:D:76:LYS:HD2	2.07	0.73
1:B:265:THR:HG22	1:B:268:PHE:HB2	1.70	0.73
1:C:358:GLU:HG2	1:C:362:LYS:HE2	1.70	0.73
1:B:89:GLN:HB3	1:B:113:ARG:NH1	2.03	0.73
1:D:31:GLU:HG3	1:D:88:ILE:HB	1.70	0.72
1:B:126:LYS:HD2	1:B:222:MET:CE	2.20	0.71
1:B:265:THR:CG2	1:B:268:PHE:H	2.04	0.71
1:C:385:ARG:H	1:C:385:ARG:HD3	1.56	0.71
1:B:174:LEU:O	1:B:178:VAL:HG12	1.91	0.71
1:B:373:LEU:HD22	1:B:405:ILE:HD11	1.71	0.71
1:C:35:THR:HG22	1:C:88:ILE:HD11	1.73	0.71
1:A:341:ALA:HB3	1:D:24:LEU:HD13	1.73	0.70
1:C:357:LYS:HD2	1:C:357:LYS:H	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ILE:HG13	1:D:357:LYS:HE2	1.72	0.70
1:C:379:ARG:HH22	1:C:436:GLN:HE21	1.36	0.70
1:B:109:THR:HG22	1:B:209:LEU:HD11	1.74	0.69
1:A:12:ARG:NH2	1:A:20:ILE:HD12	2.07	0.69
1:B:410:LEU:O	1:B:414:LYS:HG3	1.93	0.69
1:D:57:LYS:O	1:D:61:GLU:HG2	1.93	0.69
1:B:150:GLU:O	1:B:153:ILE:HG22	1.92	0.69
1:B:28:ILE:HD12	1:B:81:MET:HB3	1.73	0.69
1:B:462:GLN:HE21	1:B:462:GLN:HA	1.57	0.69
1:B:295:LEU:HD21	1:C:24:LEU:HB2	1.76	0.68
1:D:109:THR:HG22	1:D:209:LEU:HD11	1.74	0.68
1:B:35:THR:O	1:B:39:ILE:HG12	1.93	0.68
1:A:457:GLU:HG3	1:A:461:LYS:HE3	1.75	0.67
1:B:376:TYR:HD2	1:B:377:LEU:HD12	1.58	0.67
1:D:82:THR:HG23	1:D:84:SER:HB3	1.75	0.67
1:B:129:ILE:HD11	1:B:194:ILE:HD12	1.77	0.67
1:A:20:ILE:O	1:A:23:ILE:HG12	1.95	0.67
1:A:239:VAL:HG13	1:A:332:VAL:CG1	2.26	0.66
1:A:17:VAL:HG13	1:A:18:ASP:H	1.60	0.66
1:A:286:GLN:H	1:A:286:GLN:NE2	1.94	0.66
1:A:93:GLU:CD	1:A:113:ARG:HH22	2.00	0.65
1:A:129:ILE:CD1	1:A:194:ILE:HD12	2.27	0.65
1:B:153:ILE:HD13	1:B:355:ILE:HD12	1.79	0.65
1:B:265:THR:HG23	1:B:268:PHE:H	1.62	0.64
1:B:177:ALA:O	1:B:181:THR:HG23	1.97	0.64
1:B:23:ILE:O	1:B:23:ILE:HG12	1.98	0.64
1:D:154:ILE:HG21	1:D:430:VAL:CG1	2.28	0.64
1:B:20:ILE:O	1:B:23:ILE:HG22	1.98	0.64
1:A:328:ASP:O	1:A:332:VAL:HG22	1.98	0.63
1:D:458:LEU:O	1:D:461:LYS:HD2	1.97	0.63
1:B:89:GLN:HB3	1:B:113:ARG:HH11	1.63	0.63
1:A:126:LYS:HD2	1:A:222:MET:CE	2.29	0.63
1:D:379:ARG:HH22	1:D:436:GLN:HE21	1.46	0.63
1:B:126:LYS:HD2	1:B:222:MET:HE3	1.80	0.62
1:D:168:ARG:H	1:D:443:THR:CG2	2.13	0.62
1:B:153:ILE:HG23	1:B:169:TRP:HB3	1.82	0.62
1:B:385:ARG:HH12	1:D:102:ASP:HB3	1.63	0.62
1:B:32:GLN:NE2	1:B:81:MET:HG2	2.11	0.62
1:B:73:GLU:HG2	1:B:78:VAL:HB	1.80	0.62
1:B:153:ILE:CD1	1:B:355:ILE:HD12	2.30	0.62
1:D:129:ILE:HD11	1:D:194:ILE:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:THR:CG2	1:D:210:GLU:HG2	2.30	0.61
1:D:356:ASN:HB3	2:D:607:HOH:O	1.99	0.61
1:B:356:ASN:HB3	2:B:622:HOH:O	1.98	0.61
1:B:429:SER:HB3	1:B:432:ASN:ND2	2.15	0.60
1:B:56:THR:OG1	1:B:59:GLU:HG3	2.01	0.60
1:C:366:PRO:HB3	1:C:406:ASN:HD22	1.66	0.60
1:C:50:GLU:HG3	1:C:60:LEU:HD22	1.81	0.60
1:D:113:ARG:HD2	2:D:576:HOH:O	2.01	0.60
1:A:126:LYS:HD2	1:A:222:MET:HE1	1.83	0.60
1:B:72:GLU:O	1:B:75:SER:HB3	2.02	0.60
1:D:20:ILE:O	1:D:20:ILE:HD12	2.01	0.60
1:B:20:ILE:N	1:B:20:ILE:HD12	2.17	0.59
1:C:88:ILE:O	1:C:92:ILE:HG12	2.01	0.59
1:D:177:ALA:O	1:D:181:THR:HG23	2.01	0.59
1:D:307:LEU:HD22	1:D:311:LEU:HD22	1.83	0.59
1:A:392:GLY:O	1:A:395:VAL:HG22	2.03	0.59
1:A:197:LEU:HB2	1:A:222:MET:HG3	1.84	0.59
1:C:379:ARG:NH2	1:C:436:GLN:HE21	2.01	0.59
1:C:126:LYS:HD2	1:C:222:MET:CE	2.32	0.59
1:B:109:THR:HG22	1:B:209:LEU:CD1	2.33	0.58
1:C:154:ILE:HG21	1:C:430:VAL:HG12	1.85	0.58
1:B:371:THR:O	1:B:375:LEU:HD22	2.03	0.58
1:C:60:LEU:O	1:C:64:LEU:HD13	2.03	0.58
1:D:64:LEU:O	1:D:68:GLU:HG3	2.04	0.58
1:A:163:LYS:HE3	1:B:267:GLU:OE2	2.04	0.58
1:C:194:ILE:CD1	1:C:238:PHE:HB2	2.32	0.58
1:C:56:THR:OG1	1:C:59:GLU:HG3	2.05	0.57
1:D:462:GLN:HE21	1:D:462:GLN:HA	1.69	0.57
1:A:460:LYS:NZ	1:A:463:LYS:NZ	2.53	0.57
1:A:341:ALA:CB	1:D:24:LEU:HD13	2.34	0.57
1:C:154:ILE:HG21	1:C:430:VAL:CG1	2.35	0.57
1:A:395:VAL:O	1:A:399:GLU:HB2	2.05	0.56
1:B:377:LEU:HD11	1:B:420:PHE:CE1	2.40	0.56
1:C:239:VAL:HG13	1:C:332:VAL:CG1	2.35	0.56
1:D:82:THR:CG2	1:D:84:SER:HB3	2.35	0.56
1:D:21:MET:SD	1:D:21:MET:N	2.77	0.56
1:C:34:LEU:HD23	1:C:124:LEU:HD22	1.85	0.56
1:A:190:VAL:HG21	1:A:245:VAL:HG21	1.88	0.56
1:B:433:SER:O	1:B:436:GLN:HG3	2.06	0.56
1:A:396:HIS:O	1:A:400:THR:HG23	2.06	0.56
1:C:383:PRO:HB2	1:C:386:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ASP:HA	1:C:298:SER:HB3	1.87	0.55
1:C:213:ARG:HA	1:C:216:LEU:HD12	1.88	0.55
1:A:239:VAL:HG13	1:A:332:VAL:HG13	1.88	0.55
1:B:32:GLN:HE22	1:B:79:LEU:HD22	1.71	0.55
1:B:441:GLY:HA2	1:D:227:LEU:O	2.06	0.55
1:C:105:GLY:O	1:C:108:GLN:HG2	2.06	0.55
1:D:126:LYS:HD2	1:D:222:MET:CE	2.37	0.55
1:C:392:GLY:O	1:C:395:VAL:HG22	2.06	0.55
1:B:168:ARG:H	1:B:443:THR:CG2	2.17	0.55
1:D:357:LYS:NZ	1:D:357:LYS:HB3	2.22	0.55
1:A:153:ILE:HD12	1:A:357:LYS:HG2	1.89	0.55
1:A:353:LEU:C	1:A:353:LEU:HD12	2.28	0.55
1:A:418:PRO:HG2	1:A:419:LEU:HD22	1.87	0.54
1:B:76:LYS:HB2	1:B:78:VAL:HG23	1.90	0.54
1:C:153:ILE:CG2	1:C:169:TRP:HB3	2.36	0.54
1:A:24:LEU:HD21	1:D:341:ALA:HB3	1.89	0.54
1:B:140:ILE:O	1:B:144:VAL:HG13	2.07	0.54
1:D:56:THR:OG1	1:D:59:GLU:HG3	2.08	0.54
1:B:181:THR:HG21	1:B:455:LEU:HD22	1.90	0.54
1:B:20:ILE:HA	1:B:23:ILE:HG22	1.89	0.54
1:D:86:GLU:HG2	1:D:87:ASP:N	2.22	0.54
1:B:165:LEU:HD12	1:B:165:LEU:O	2.07	0.54
1:B:168:ARG:HB2	1:B:443:THR:HG22	1.88	0.54
1:B:283:LEU:N	1:B:283:LEU:HD22	2.23	0.54
1:C:375:LEU:O	1:C:379:ARG:HG3	2.08	0.54
1:B:32:GLN:HE21	1:B:81:MET:CG	2.15	0.54
1:B:341:ALA:HB3	1:C:24:LEU:HD21	1.89	0.54
1:C:407:ASN:H	1:C:407:ASN:HD22	1.55	0.54
1:D:20:ILE:HD13	1:D:22:GLU:HB2	1.89	0.54
1:A:14:VAL:HG11	1:A:18:ASP:HA	1.89	0.53
1:B:35:THR:HG22	1:B:88:ILE:CD1	2.36	0.53
1:D:365:THR:O	1:D:368:LEU:HB2	2.08	0.53
1:B:281:SER:HB2	2:B:589:HOH:O	2.08	0.53
1:A:17:VAL:HG13	1:A:18:ASP:N	2.21	0.53
1:D:395:VAL:HA	1:D:405:ILE:HD13	1.89	0.53
1:A:129:ILE:HD11	1:A:194:ILE:CD1	2.38	0.53
1:C:94:ARG:HG2	1:C:94:ARG:HH11	1.74	0.53
1:B:32:GLN:O	1:B:35:THR:HG23	2.08	0.52
1:A:365:THR:HB	1:A:366:PRO:HD2	1.90	0.52
1:D:148:ALA:HB2	1:D:452:ILE:HD13	1.91	0.52
1:D:154:ILE:HG22	1:D:364:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLU:HG3	1:B:368:LEU:HD13	1.90	0.52
1:B:371:THR:HB	2:B:619:HOH:O	2.09	0.52
1:A:99:LEU:CD1	1:A:100:ILE:HD13	2.38	0.52
1:C:364:LEU:HD13	1:C:430:VAL:HG11	1.91	0.52
1:B:48:ALA:HB1	1:B:211:ILE:HG12	1.92	0.52
1:D:76:LYS:HD2	1:D:76:LYS:N	2.25	0.51
1:D:154:ILE:HG21	1:D:430:VAL:HG12	1.92	0.51
1:C:190:VAL:HG21	1:C:245:VAL:HG21	1.92	0.51
1:A:99:LEU:O	1:A:100:ILE:HD12	2.10	0.51
1:B:168:ARG:HB2	1:B:443:THR:CG2	2.40	0.51
1:C:407:ASN:ND2	1:C:407:ASN:H	2.09	0.51
1:C:20:ILE:HG23	1:C:23:ILE:HD12	1.93	0.51
1:B:391:SER:O	1:B:395:VAL:HG23	2.10	0.51
1:C:168:ARG:H	1:C:443:THR:CG2	2.20	0.51
1:D:34:LEU:HD23	1:D:124:LEU:HD22	1.91	0.51
1:B:82:THR:C	1:B:84:SER:H	2.14	0.51
1:D:397:LEU:O	1:D:401:LYS:HG3	2.12	0.50
1:C:57:LYS:O	1:C:61:GLU:HG2	2.11	0.50
1:D:20:ILE:HD13	1:D:22:GLU:CB	2.41	0.50
1:D:405:ILE:HG23	1:D:428:PHE:HE2	1.75	0.50
1:C:202:GLY:O	1:C:233:ILE:HD11	2.11	0.50
1:C:357:LYS:H	1:C:357:LYS:CD	2.23	0.50
1:C:236:ARG:O	1:C:240:VAL:HG12	2.12	0.50
1:C:385:ARG:HH11	1:C:385:ARG:HG2	1.77	0.50
1:B:89:GLN:O	1:B:93:GLU:HG3	2.12	0.50
1:A:109:THR:HG22	1:A:209:LEU:CD1	2.42	0.50
1:A:51:LYS:HE2	1:A:212:ASP:OD1	2.12	0.50
1:B:79:LEU:C	1:B:79:LEU:HD23	2.32	0.50
1:A:410:LEU:O	1:A:414:LYS:HB2	2.12	0.49
1:B:377:LEU:HD11	1:B:420:PHE:CZ	2.48	0.49
1:C:391:SER:O	1:C:395:VAL:HG13	2.12	0.49
1:D:244:SER:HB3	2:D:610:HOH:O	2.11	0.49
1:A:283:LEU:N	1:A:283:LEU:HD12	2.28	0.49
1:A:367:GLU:HG2	2:A:607:HOH:O	2.12	0.49
1:A:419:LEU:HD22	1:A:419:LEU:N	2.28	0.49
1:A:109:THR:HG22	1:A:209:LEU:HD11	1.95	0.49
1:C:112:SER:O	1:C:115:GLU:HG2	2.13	0.49
1:B:197:LEU:HD12	1:B:198:PRO:HD2	1.95	0.49
1:B:361:GLU:HA	1:B:364:LEU:HD23	1.95	0.49
1:B:168:ARG:HD2	1:B:443:THR:O	2.12	0.49
1:D:361:GLU:O	1:D:364:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ARG:O	1:B:310:ILE:HG12	2.11	0.49
1:B:79:LEU:HD23	1:B:80:VAL:N	2.27	0.49
1:C:20:ILE:HA	1:C:23:ILE:HD12	1.94	0.49
1:C:168:ARG:HB2	1:C:443:THR:HG22	1.94	0.49
1:C:399:GLU:C	1:C:401:LYS:H	2.16	0.49
1:A:208:PRO:HB3	1:C:437:TYR:CE2	2.47	0.49
1:A:137:LEU:HD22	1:A:459:LEU:HD22	1.94	0.49
1:B:69:LYS:O	1:B:73:GLU:HB2	2.13	0.49
1:C:242:LEU:O	1:C:242:LEU:HD23	2.12	0.49
1:A:143:LEU:CD2	1:A:350:ILE:HD13	2.39	0.48
1:B:410:LEU:HD21	1:B:422:SER:HA	1.95	0.48
1:C:383:PRO:HD2	1:C:386:GLN:HG3	1.93	0.48
1:D:332:VAL:O	1:D:336:VAL:HG13	2.13	0.48
1:B:126:LYS:HD2	1:B:222:MET:HE1	1.93	0.48
1:D:129:ILE:CD1	1:D:194:ILE:HD12	2.42	0.48
1:D:140:ILE:O	1:D:144:VAL:HG13	2.13	0.48
1:D:405:ILE:HG23	1:D:428:PHE:CE2	2.48	0.48
1:C:165:LEU:HD12	1:C:165:LEU:O	2.14	0.48
1:A:12:ARG:HA	2:A:554:HOH:O	2.13	0.48
1:B:48:ALA:HB3	1:B:211:ILE:HD11	1.96	0.48
1:B:445:LYS:O	1:B:449:THR:HG23	2.14	0.48
1:B:462:GLN:HA	1:B:462:GLN:NE2	2.26	0.48
1:C:251:ILE:O	1:C:255:LYS:HG3	2.14	0.48
1:B:119:THR:HG22	1:B:123:LEU:CD2	2.43	0.48
1:B:168:ARG:NH1	1:B:434:VAL:HG21	2.28	0.48
1:D:23:ILE:HG13	1:D:23:ILE:O	2.13	0.48
1:C:135:HIS:HE1	2:C:593:HOH:O	1.97	0.48
1:A:165:LEU:HB2	1:A:166:PRO:HD2	1.96	0.48
1:C:332:VAL:O	1:C:336:VAL:HG13	2.14	0.48
1:A:293:LEU:HD11	1:A:349:VAL:HG11	1.95	0.47
1:B:34:LEU:HD23	1:B:124:LEU:HD22	1.96	0.47
1:C:407:ASN:ND2	1:C:407:ASN:N	2.62	0.47
1:A:256:LEU:HD21	1:A:350:ILE:HD11	1.96	0.47
1:A:369:LEU:HD13	1:A:428:PHE:HA	1.96	0.47
1:C:242:LEU:C	1:C:242:LEU:HD23	2.34	0.47
1:C:283:LEU:N	1:C:283:LEU:HD12	2.28	0.47
1:A:122:LYS:HE3	1:A:238:PHE:CD2	2.49	0.47
1:D:241:GLU:O	1:D:245:VAL:HG23	2.14	0.47
1:B:369:LEU:HD13	1:B:428:PHE:HA	1.96	0.47
1:B:265:THR:HG21	1:B:268:PHE:HD1	1.80	0.47
1:A:35:THR:HG23	1:A:36:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:HB3	1:A:432:ASN:ND2	2.21	0.47
1:A:56:THR:OG1	1:A:59:GLU:HG3	2.15	0.47
1:B:283:LEU:O	1:B:285:PRO:HD3	2.14	0.47
1:C:126:LYS:HD2	1:C:222:MET:HE3	1.97	0.47
1:D:20:ILE:HD13	1:D:22:GLU:CG	2.45	0.47
1:D:461:LYS:HG2	1:D:461:LYS:O	2.14	0.47
1:B:360:MET:O	1:B:364:LEU:HD22	2.15	0.47
1:D:174:LEU:O	1:D:178:VAL:HG13	2.15	0.47
1:C:169:TRP:O	1:C:172:PHE:HB3	2.15	0.46
1:D:144:VAL:HG23	1:D:145:GLU:N	2.30	0.46
1:D:80:VAL:O	1:D:81:MET:HG3	2.15	0.46
1:A:287:LYS:HG3	1:B:162:GLN:HB3	1.98	0.46
1:C:382:MET:CE	1:C:419:LEU:HD12	2.45	0.46
1:D:385:ARG:HH11	1:D:385:ARG:HG2	1.80	0.46
1:D:93:GLU:OE1	1:D:113:ARG:NH2	2.48	0.46
1:D:126:LYS:HD2	1:D:222:MET:HE1	1.97	0.46
1:D:273:LEU:HB2	1:D:278:SER:OG	2.16	0.46
1:A:35:THR:HG21	2:A:568:HOH:O	2.15	0.45
1:A:148:ALA:HB2	1:A:452:ILE:HD13	1.98	0.45
1:B:257:ALA:O	1:B:261:ILE:HG13	2.15	0.45
1:A:441:GLY:HA2	1:C:227:LEU:O	2.16	0.45
1:D:153:ILE:N	1:D:153:ILE:HD12	2.30	0.45
1:A:134:THR:HG22	1:A:138:GLN:HE21	1.81	0.45
1:C:353:LEU:C	1:C:353:LEU:HD12	2.36	0.45
1:D:52:ALA:O	1:D:53:SER:HB2	2.16	0.45
1:C:397:LEU:O	1:C:401:LYS:HG2	2.17	0.45
1:A:460:LYS:HZ1	1:A:463:LYS:HZ1	1.65	0.45
1:A:460:LYS:HZ3	1:A:463:LYS:NZ	2.14	0.45
1:D:82:THR:HG23	1:D:84:SER:CB	2.44	0.45
1:A:89:GLN:O	1:A:93:GLU:HG3	2.16	0.45
1:B:227:LEU:O	1:D:441:GLY:HA2	2.17	0.45
1:B:28:ILE:HG23	1:B:81:MET:HB2	1.98	0.45
1:C:404:THR:O	1:C:407:ASN:ND2	2.50	0.45
1:D:20:ILE:HD12	1:D:23:ILE:HG22	1.98	0.45
1:A:431:VAL:O	1:A:435:GLU:HG2	2.17	0.45
1:A:62:LYS:HE2	1:A:62:LYS:HB3	1.84	0.45
1:C:382:MET:HG2	1:C:386:GLN:HB2	1.98	0.45
1:A:290:PRO:O	1:A:294:GLU:HG3	2.16	0.45
1:C:421:ALA:HB3	1:C:423:ASP:OD1	2.17	0.45
1:D:27:SER:OG	1:D:30:THR:HG23	2.15	0.45
1:A:174:LEU:HD11	1:A:448:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ASN:N	1:C:407:ASN:HD22	2.13	0.44
1:B:153:ILE:CD1	1:B:360:MET:SD	3.00	0.44
1:C:287:LYS:HE3	2:C:578:HOH:O	2.17	0.44
1:C:309:ALA:O	1:C:313:VAL:HG23	2.17	0.44
1:B:24:LEU:HD21	1:C:341:ALA:HB3	1.98	0.44
1:D:109:THR:HG22	1:D:209:LEU:CD1	2.45	0.44
1:B:283:LEU:C	1:B:285:PRO:HD3	2.37	0.44
1:C:431:VAL:O	1:C:435:GLU:HG2	2.17	0.44
1:A:155:MET:HB2	1:A:156:PRO:HD2	2.00	0.44
1:A:186:ARG:HD3	1:C:241:GLU:OE2	2.17	0.44
1:D:258:GLU:O	1:D:262:ILE:HG12	2.17	0.44
1:B:129:ILE:CD1	1:B:194:ILE:HD12	2.45	0.44
1:C:190:VAL:HG22	1:C:241:GLU:HG2	2.00	0.44
1:C:460:LYS:C	1:C:462:GLN:H	2.21	0.44
1:D:20:ILE:O	1:D:24:LEU:HB2	2.17	0.44
1:A:186:ARG:O	1:A:190:VAL:HG23	2.18	0.44
1:A:295:LEU:O	1:A:299:LYS:HG2	2.18	0.44
1:B:310:ILE:HD11	1:B:331:ALA:CB	2.48	0.44
1:A:298:SER:HB3	1:D:324:ASP:HA	1.98	0.44
1:C:328:ASP:O	1:C:332:VAL:HG22	2.18	0.44
1:C:401:LYS:HB2	1:C:403:ILE:HG12	1.99	0.44
1:A:312:MET:HG2	1:D:301:GLY:HA2	1.98	0.43
1:A:460:LYS:NZ	1:A:463:LYS:HZ3	2.14	0.43
1:C:328:ASP:OD2	1:C:329:LYS:N	2.51	0.43
1:A:12:ARG:HH22	1:A:20:ILE:HD12	1.81	0.43
1:B:80:VAL:HG13	1:B:80:VAL:O	2.18	0.43
1:D:161:LEU:HA	1:D:161:LEU:HD23	1.80	0.43
1:A:38:ASP:OD2	1:A:120:ASP:OD1	2.35	0.43
1:A:449:THR:O	1:A:453:GLU:HG2	2.19	0.43
1:A:457:GLU:CG	1:A:461:LYS:HE3	2.45	0.43
1:D:409:THR:O	1:D:412:ASP:HB2	2.17	0.43
1:A:53:SER:HB2	2:A:564:HOH:O	2.18	0.43
1:A:105:GLY:O	1:A:108:GLN:HG2	2.19	0.43
1:A:165:LEU:O	1:A:165:LEU:HD12	2.18	0.43
1:B:135:HIS:HE1	2:B:500:HOH:O	2.01	0.43
1:C:99:LEU:O	1:C:100:ILE:HD12	2.18	0.43
1:D:60:LEU:O	1:D:64:LEU:HB2	2.19	0.43
1:A:112:SER:O	1:A:115:GLU:HG2	2.19	0.43
1:A:153:ILE:CD1	1:A:357:LYS:HD3	2.49	0.43
1:C:167:ILE:CG1	1:C:443:THR:HG21	2.49	0.43
1:D:384:ILE:HG23	1:D:385:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LYS:HZ1	1:A:463:LYS:NZ	2.16	0.43
1:A:89:GLN:H	1:A:89:GLN:NE2	2.16	0.43
1:D:169:TRP:O	1:D:172:PHE:HB3	2.19	0.43
1:C:326:GLN:HG2	1:C:326:GLN:O	2.19	0.42
1:D:462:GLN:HA	1:D:462:GLN:NE2	2.32	0.42
1:B:161:LEU:HD11	1:B:262:ILE:HD13	1.99	0.42
1:B:52:ALA:O	1:B:53:SER:HB2	2.19	0.42
1:C:395:VAL:O	1:C:399:GLU:HG3	2.18	0.42
1:D:97:LYS:C	1:D:99:LEU:H	2.22	0.42
1:B:213:ARG:HA	1:B:216:LEU:HD12	2.01	0.42
1:C:201:SER:HA	1:C:206:GLY:HA2	2.01	0.42
1:C:167:ILE:HG12	1:C:443:THR:HG21	2.00	0.42
1:C:452:ILE:O	1:C:456:ARG:HB2	2.19	0.42
1:C:135:HIS:HD2	2:C:607:HOH:O	2.02	0.42
1:A:401:LYS:O	1:A:403:ILE:HG23	2.19	0.42
1:A:406:ASN:HA	1:A:428:PHE:CE2	2.54	0.42
1:D:281:SER:HB3	2:D:590:HOH:O	2.19	0.42
1:D:336:VAL:HG23	1:D:337:ASP:N	2.35	0.42
1:A:403:ILE:HD11	1:A:408:LEU:HD23	2.02	0.42
1:B:372:ASP:HA	1:B:375:LEU:HD23	2.01	0.42
1:C:393:LYS:HB3	1:C:416:ILE:HD12	2.01	0.42
1:C:366:PRO:CB	1:C:406:ASN:HD22	2.32	0.42
1:D:129:ILE:HD11	1:D:194:ILE:CD1	2.50	0.42
1:A:372:ASP:CG	1:A:436:GLN:HE22	2.23	0.42
1:A:406:ASN:HA	1:A:428:PHE:CD2	2.55	0.42
1:B:176:HIS:HD2	2:B:576:HOH:O	2.03	0.42
1:D:353:LEU:C	1:D:353:LEU:HD12	2.40	0.42
1:D:365:THR:HB	1:D:367:GLU:OE1	2.20	0.42
1:D:454:GLN:O	1:D:457:GLU:HB3	2.20	0.42
1:C:385:ARG:H	1:C:385:ARG:CD	2.28	0.42
1:A:409:THR:C	1:A:411:GLU:H	2.23	0.41
1:A:423:ASP:HB2	1:A:426:GLN:HE21	1.84	0.41
1:A:458:LEU:O	1:A:462:GLN:HG2	2.20	0.41
1:B:377:LEU:HD23	1:B:382:MET:SD	2.60	0.41
1:C:35:THR:HG22	1:C:88:ILE:CD1	2.47	0.41
1:C:371:THR:HB	2:C:602:HOH:O	2.19	0.41
1:D:369:LEU:N	1:D:369:LEU:HD22	2.35	0.41
1:A:331:ALA:O	1:A:335:VAL:HG23	2.21	0.41
1:A:126:LYS:HD2	1:A:222:MET:HE3	2.00	0.41
1:A:95:ARG:O	1:A:99:LEU:HG	2.20	0.41
1:B:165:LEU:HD12	1:B:165:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:HG12	1:B:238:PHE:HB2	2.01	0.41
1:B:267:GLU:CD	1:B:267:GLU:H	2.22	0.41
1:B:431:VAL:O	1:B:435:GLU:HG2	2.21	0.41
1:B:429:SER:CB	1:B:432:ASN:HD22	2.22	0.41
1:D:168:ARG:HB2	1:D:443:THR:HG22	2.03	0.41
1:B:144:VAL:CG2	1:B:145:GLU:N	2.83	0.41
1:B:373:LEU:O	1:B:377:LEU:HD13	2.20	0.41
1:C:137:LEU:HD12	1:C:137:LEU:HA	1.92	0.41
1:C:20:ILE:HA	1:C:23:ILE:CD1	2.51	0.41
1:A:326:GLN:HG2	1:A:326:GLN:O	2.21	0.41
1:A:371:THR:HB	2:A:579:HOH:O	2.21	0.41
1:B:144:VAL:HG23	1:B:145:GLU:N	2.35	0.41
1:B:448:VAL:O	1:B:452:ILE:HG13	2.20	0.41
1:D:82:THR:HG23	1:D:84:SER:H	1.86	0.41
1:B:384:ILE:HG23	1:B:385:ARG:N	2.36	0.41
1:B:283:LEU:H	1:B:283:LEU:HD22	1.85	0.41
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.89	0.41
1:D:144:VAL:CG2	1:D:145:GLU:N	2.83	0.41
1:D:295:LEU:O	1:D:299:LYS:HG2	2.21	0.41
1:B:421:ALA:O	1:B:424:VAL:HG12	2.21	0.41
1:C:132:ILE:HD13	1:C:339:LEU:HD23	2.02	0.41
1:C:393:LYS:CB	1:C:416:ILE:HD12	2.51	0.41
1:A:257:ALA:O	1:A:261:ILE:HG13	2.21	0.40
1:B:161:LEU:HA	1:B:161:LEU:HD23	1.78	0.40
1:B:28:ILE:HD11	1:B:83:GLN:HA	2.04	0.40
1:D:378:VAL:HA	1:D:382:MET:O	2.21	0.40
1:A:328:ASP:OD2	1:A:329:LYS:N	2.54	0.40
1:C:186:ARG:O	1:C:190:VAL:HG23	2.21	0.40
1:C:382:MET:HE3	1:C:419:LEU:HD12	2.03	0.40
1:D:171:GLN:HB2	1:D:443:THR:HG23	2.03	0.40
1:B:191:LYS:HE2	2:B:596:HOH:O	2.21	0.40
1:B:66:GLY:O	1:B:70:ILE:HG13	2.22	0.40
1:C:81:MET:HG3	1:C:91:ALA:HB2	2.03	0.40
1:D:34:LEU:CD2	1:D:124:LEU:HD22	2.51	0.40
1:D:69:LYS:HZ1	1:D:73:GLU:CD	2.24	0.40
1:B:336:VAL:HG23	1:B:337:ASP:N	2.37	0.40
1:A:24:LEU:HD21	1:D:341:ALA:CB	2.51	0.40
1:D:245:VAL:HG23	2:D:610:HOH:O	2.21	0.40
1:D:358:GLU:HB2	2:D:607:HOH:O	2.21	0.40
1:D:82:THR:O	1:D:85:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	451/466 (97%)	435 (96%)	12 (3%)	4 (1%)	17	31
1	B	442/466 (95%)	427 (97%)	14 (3%)	1 (0%)	47	68
1	C	443/466 (95%)	427 (96%)	12 (3%)	4 (1%)	17	31
1	D	441/466 (95%)	426 (97%)	13 (3%)	2 (0%)	29	48
All	All	1777/1864 (95%)	1715 (96%)	51 (3%)	11 (1%)	25	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	LEU
1	D	204	LEU
1	C	204	LEU
1	C	400	THR
1	A	204	LEU
1	C	461	LYS
1	A	17	VAL
1	C	102	ASP
1	D	98	GLU
1	A	18	ASP
1	A	440	VAL

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	394/406 (97%)	376 (95%)	18 (5%)	27 50
1	B	390/406 (96%)	371 (95%)	19 (5%)	25 47
1	C	391/406 (96%)	376 (96%)	15 (4%)	33 58
1	D	388/406 (96%)	370 (95%)	18 (5%)	27 50
All	All	1563/1624 (96%)	1493 (96%)	70 (4%)	27 51

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	89	GLN
1	A	96	LEU
1	A	99	LEU
1	A	107	LEU
1	A	118	VAL
1	A	121	LEU
1	A	136	LEU
1	A	139	LEU
1	A	161	LEU
1	A	165	LEU
1	A	217	ARG
1	A	221	ASP
1	A	227	LEU
1	A	286	GLN
1	A	293	LEU
1	A	325	LEU
1	A	367	GLU
1	B	57	LYS
1	B	69	LYS
1	B	96	LEU
1	B	107	LEU
1	B	121	LEU
1	B	123	LEU
1	B	136	LEU
1	B	137	LEU
1	B	139	LEU
1	B	169	TRP
1	B	187	LEU
1	B	248	LEU
1	B	286	GLN
1	B	307	LEU
1	B	325	LEU

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Mol	Chain	Res	Type
1	B	368	LEU
1	B	375	LEU
1	B	443	THR
1	B	457	GLU
1	C	96	LEU
1	C	136	LEU
1	C	137	LEU
1	C	145	GLU
1	C	161	LEU
1	C	165	LEU
1	C	221	ASP
1	C	240	VAL
1	C	248	LEU
1	C	260	LEU
1	C	357	LYS
1	C	385	ARG
1	C	407	ASN
1	C	443	THR
1	C	456	ARG
1	D	21	MET
1	D	36	GLU
1	D	67	LEU
1	D	69	LYS
1	D	84	SER
1	D	86	GLU
1	D	96	LEU
1	D	113	ARG
1	D	121	LEU
1	D	123	LEU
1	D	136	LEU
1	D	139	LEU
1	D	307	LEU
1	D	311	LEU
1	D	332	VAL
1	D	364	LEU
1	D	443	THR
1	D	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	89	GLN
1	A	138	GLN
1	A	286	GLN
1	A	326	GLN
1	A	359	ASN
1	A	426	GLN
1	A	432	ASN
1	B	32	GLN
1	B	135	HIS
1	B	176	HIS
1	B	354	GLN
1	B	359	ASN
1	B	407	ASN
1	B	426	GLN
1	B	432	ASN
1	B	462	GLN
1	C	32	GLN
1	C	40	GLN
1	C	83	GLN
1	C	162	GLN
1	C	176	HIS
1	C	356	ASN
1	C	359	ASN
1	C	388	GLN
1	C	406	ASN
1	C	407	ASN
1	C	432	ASN
1	C	436	GLN
1	D	32	GLN
1	D	108	GLN
1	D	114	ASN
1	D	386	GLN
1	D	388	GLN
1	D	407	ASN
1	D	436	GLN
1	D	462	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	453/466 (97%)	-0.21	11 (2%)	59	62	18, 36, 83, 98	0
1	B	444/466 (95%)	-0.16	11 (2%)	57	61	17, 37, 80, 100	0
1	C	445/466 (95%)	-0.18	9 (2%)	65	68	18, 37, 76, 93	0
1	D	443/466 (95%)	-0.25	11 (2%)	57	61	16, 34, 76, 100	0
All	All	1785/1864 (95%)	-0.20	42 (2%)	59	62	16, 36, 80, 100	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	VAL	6.8
1	D	80	VAL	6.6
1	B	82	THR	6.1
1	D	20	ILE	4.8
1	B	21	MET	4.2
1	A	420	PHE	4.0
1	B	22	GLU	3.6
1	D	83	GLN	3.5
1	D	84	SER	3.5
1	D	23	ILE	3.4
1	B	83	GLN	3.4
1	A	416	ILE	3.4
1	C	421	ALA	3.2
1	B	84	SER	3.1
1	C	400	THR	3.0
1	A	421	ALA	3.0
1	C	420	PHE	2.9
1	A	413	LEU	2.9
1	B	78	VAL	2.8
1	A	422	SER	2.8
1	B	20	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	414	LYS	2.7
1	B	99	LEU	2.7
1	D	78	VAL	2.6
1	C	419	LEU	2.6
1	A	408	LEU	2.5
1	C	416	ILE	2.5
1	D	69	LYS	2.5
1	D	82	THR	2.5
1	D	462	GLN	2.4
1	D	95	ARG	2.4
1	C	65	SER	2.3
1	A	419	LEU	2.3
1	A	396	HIS	2.2
1	C	233	ILE	2.2
1	D	100	ILE	2.2
1	A	17	VAL	2.1
1	B	422	SER	2.1
1	A	15	GLY	2.1
1	C	397	LEU	2.1
1	C	409	THR	2.1
1	B	97	LYS	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.