



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:55 am GMT

PDB ID : 1DCN
Title : INACTIVE MUTANT H162N OF DELTA 2 CRYSTALLIN WITH BOUND ARGININOSUCCINATE
Authors : Vallee, F.; Turner, M.A.; Lindley, P.; Howell, P.L.
Deposited on : 1998-10-29
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

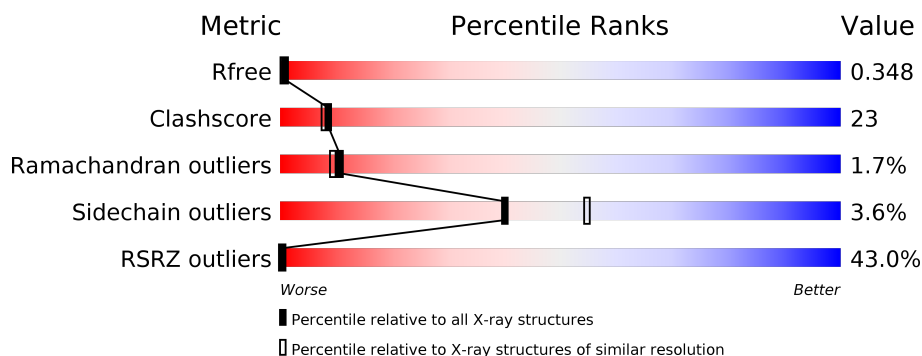
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	<div> <div>48%</div> <div>57%</div> <div>34%</div> <div>5%</div> </div>
1	B	447	<div> <div>29%</div> <div>58%</div> <div>34%</div> <div>6%</div> </div>
1	C	447	<div> <div>60%</div> <div>52%</div> <div>42%</div> <div>• •</div> </div>
1	D	447	<div> <div>28%</div> <div>60%</div> <div>34%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AS1	D	0	X	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13754 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.

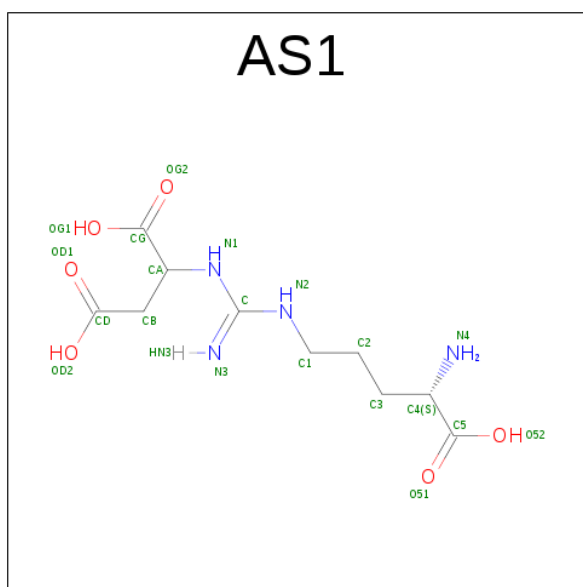
- Molecule 1 is a protein called DELTA 2 CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3287	2080	557	640	10			
1	B	418	Total	C	N	O	S	0	0	0
			3239	2050	549	629	11			
1	C	434	Total	C	N	O	S	0	0	0
			3360	2127	568	654	11			
1	D	436	Total	C	N	O	S	0	0	0
			3377	2139	571	656	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ASN	HIS	CONFLICT	UNP P24058
A	162	ASN	HIS	ENGINEERED	UNP P24058
A	302	SER	ALA	CONFLICT	UNP P24058
A	409	ASN	LYS	CONFLICT	UNP P24058
B	110	ASN	HIS	CONFLICT	UNP P24058
B	162	ASN	HIS	ENGINEERED	UNP P24058
B	302	SER	ALA	CONFLICT	UNP P24058
B	409	ASN	LYS	CONFLICT	UNP P24058
C	110	ASN	HIS	CONFLICT	UNP P24058
C	162	ASN	HIS	ENGINEERED	UNP P24058
C	302	SER	ALA	CONFLICT	UNP P24058
C	409	ASN	LYS	CONFLICT	UNP P24058
D	110	ASN	HIS	CONFLICT	UNP P24058
D	162	ASN	HIS	ENGINEERED	UNP P24058
D	302	SER	ALA	CONFLICT	UNP P24058
D	409	ASN	LYS	CONFLICT	UNP P24058

- Molecule 2 is ARGININOSUCCINATE (three-letter code: AS1) (formula: C₁₀H₁₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			20	10	4	6		

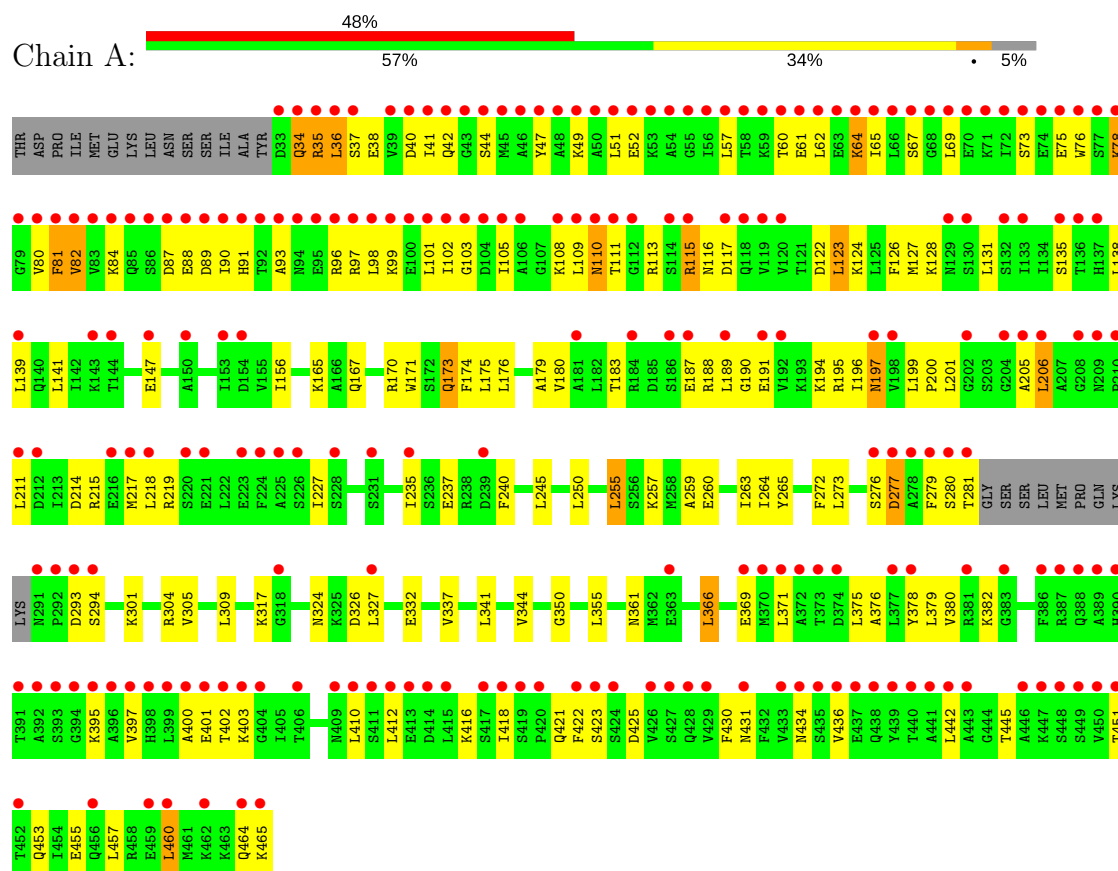
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total	O	0	0
			123	123		
3	B	126	Total	O	0	0
			126	126		
3	C	110	Total	O	0	0
			110	110		
3	D	112	Total	O	0	0
			112	112		

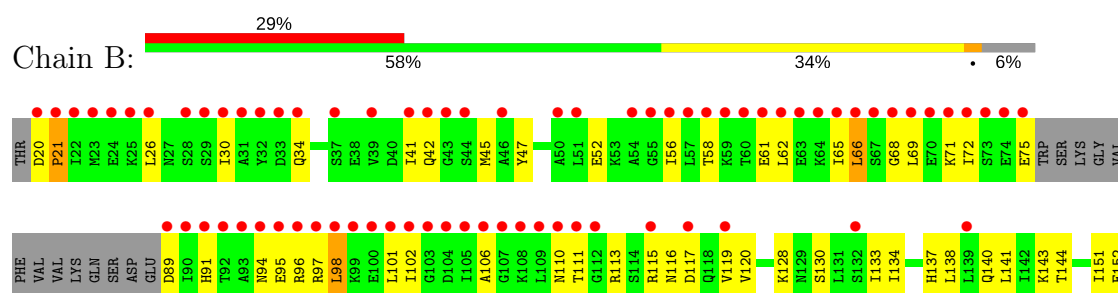
3 Residue-property plots

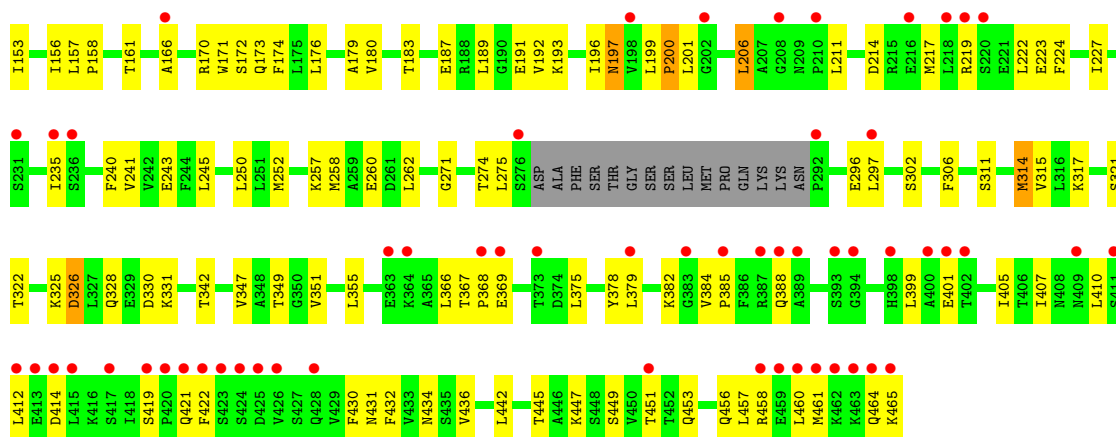
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 2 CRYSTALLIN

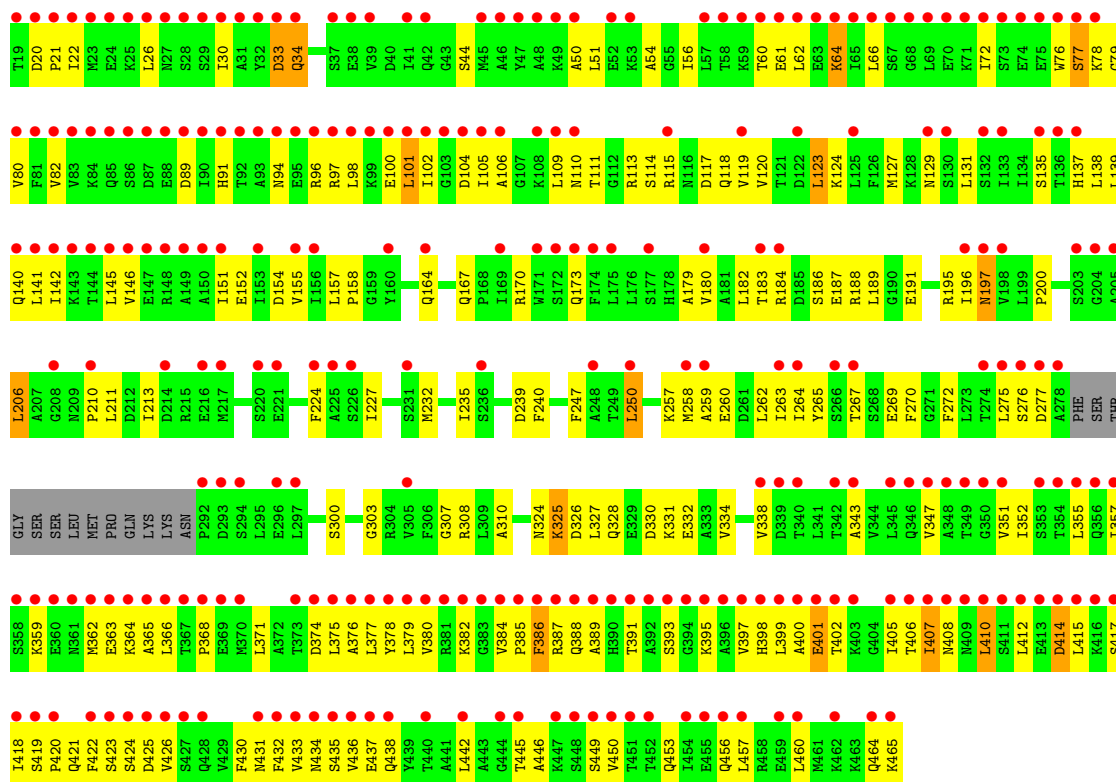


• Molecule 1: DELTA 2 CRYSTALLIN

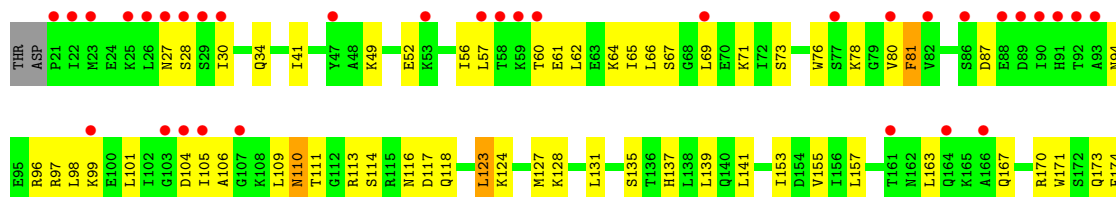


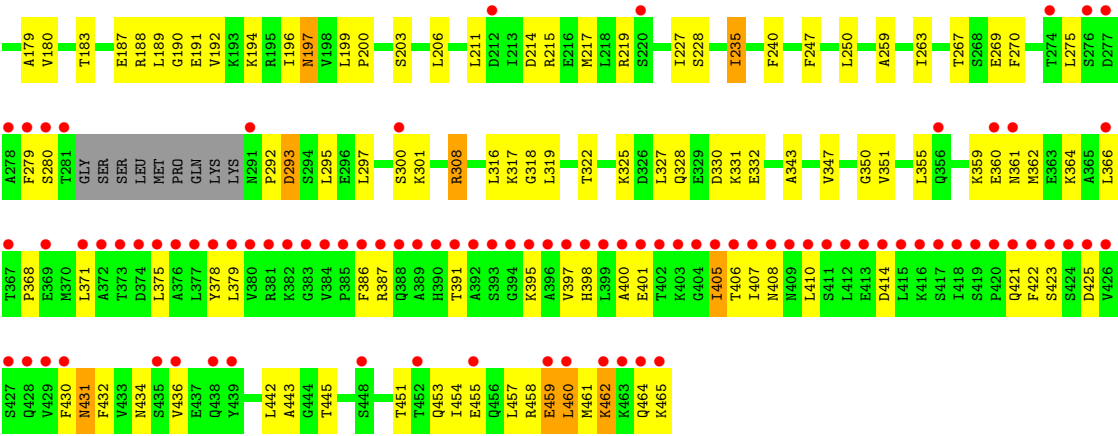


• Molecule 1: DELTA 2 CRYSTALLIN



• Molecule 1: DELTA 2 CRYSTALLIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 99.59Å 107.14Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 8.06 – 2.28	Depositor EDS
% Data completeness (in resolution range)	82.8 (20.00-2.30) 76.1 (8.06-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.229 , 0.290 0.348 , 0.348	Depositor DCC
R_{free} test set	6658 reflections (10.15%)	DCC
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	13754	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AS1

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	0.34	0/3326	0.60	0/4484
1	B	0.35	0/3275	0.59	0/4413
1	C	0.33	0/3400	0.60	0/4584
1	D	0.35	0/3418	0.60	0/4608
All	All	0.34	0/13419	0.60	0/18089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3287	0	3391	165	0
1	B	3239	0	3357	138	0
1	C	3360	0	3470	195	0
1	D	3377	0	3486	145	0
2	D	20	0	13	9	0
3	A	123	0	0	9	0
3	B	126	0	0	10	0
3	C	110	0	0	11	0
3	D	112	0	0	7	0
All	All	13754	0	13717	619	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 23.

All (619) 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)
2:D:0:AS1:CA	2:D:0:AS1:CB	1.79	1.60
2:D:0:AS1:N2	2:D:0:AS1:C1	1.69	1.53
1:B:456:GLN:O	1:B:460:LEU:HD23	1.66	0.95
1:A:403:LYS:HA	1:A:403:LYS:HE2	1.48	0.92
1:C:131:LEU:HD22	1:C:189:LEU:HD11	1.51	0.90
1:C:61:GLU:HG2	1:C:105:ILE:HD11	1.53	0.90
1:A:431:ASN:HB3	1:A:434:ASN:HD22	1.42	0.85
1:D:436:VAL:HG13	1:D:445:THR:HG23	1.60	0.83
1:B:173:GLN:HE22	1:B:453:GLN:HE22	1.24	0.83
1:D:366:LEU:HB3	1:D:432:PHE:CE2	2.14	0.83
1:D:155:VAL:HG22	1:D:359:LYS:HE3	1.59	0.82
1:B:140:GLN:O	1:B:144:THR:HG23	1.81	0.81
1:C:123:LEU:HD12	3:C:514:HOH:O	1.80	0.81
1:D:275:LEU:HB2	1:D:280:SER:HB3	1.61	0.80
1:A:397:VAL:O	1:A:401:GLU:HB2	1.80	0.79
1:C:415:LEU:HD23	1:C:418:ILE:HD12	1.64	0.79
1:B:193:LYS:HE3	3:B:523:HOH:O	1.83	0.78
1:D:464:GLN:O	1:D:465:LYS:HB2	1.83	0.77
1:A:80:VAL:O	1:A:81:PHE:HB2	1.83	0.77
1:D:397:VAL:O	1:D:401:GLU:HB2	1.85	0.77
1:A:379:LEU:HD11	1:A:422:PHE:CE1	2.19	0.76
1:D:215:ARG:HH22	1:D:228:SER:HB2	1.50	0.76
1:C:374:ASP:HA	1:C:377:LEU:HD12	1.66	0.76
1:C:378:TYR:O	1:C:382:LYS:HG2	1.84	0.76
1:B:102:ILE:HD11	1:B:106:ALA:HB2	1.69	0.74
1:B:206:LEU:HD21	1:D:167:GLN:HG2	1.68	0.74
1:A:110:ASN:HD22	1:A:113:ARG:HB3	1.53	0.73
1:D:60:THR:HG22	1:D:64:LYS:HE2	1.70	0.73
1:D:200:PRO:HA	1:D:228:SER:OG	1.87	0.73
1:A:111:THR:HG22	1:A:211:LEU:HD11	1.70	0.73
1:C:131:LEU:HD22	1:C:189:LEU:CD1	2.19	0.72
2:D:0:AS1:H12	2:D:0:AS1:N2	1.99	0.72
1:D:173:GLN:HE22	1:D:453:GLN:HE22	1.35	0.72
1:D:170:ARG:HG3	1:D:436:VAL:HG11	1.72	0.71
1:A:102:ILE:HG13	1:A:103:GLY:H	1.55	0.71
1:B:143:LYS:NZ	1:B:143:LYS:HB2	2.06	0.71
1:A:332:GLU:HG3	3:A:480:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:HG3	3:A:574:HOH:O	1.91	0.71
1:C:405:ILE:HD11	1:C:410:LEU:HD23	1.73	0.71
1:A:199:LEU:HD11	1:A:201:LEU:HB3	1.74	0.70
1:D:196:ILE:HG12	1:D:240:PHE:HB2	1.73	0.70
1:C:400:ALA:HB1	1:C:405:ILE:O	1.91	0.70
1:C:398:HIS:O	1:C:401:GLU:HG3	1.92	0.69
1:C:332:GLU:HG3	3:C:529:HOH:O	1.92	0.69
1:A:78:LYS:HB3	1:A:78:LYS:NZ	2.07	0.69
1:B:314:MET:HG2	1:C:303:GLY:HA2	1.74	0.69
1:B:111:THR:OG1	1:D:386:PHE:HB2	1.93	0.69
1:B:436:VAL:HG13	1:B:445:THR:HG23	1.75	0.69
1:B:144:THR:HG21	1:B:349:THR:HG23	1.74	0.69
1:C:386:PHE:HE2	1:C:387:ARG:HH21	1.41	0.69
1:C:173:GLN:HE22	1:C:453:GLN:HE22	1.40	0.68
1:C:460:LEU:O	1:C:464:GLN:HG2	1.94	0.68
1:A:382:LYS:HE2	1:A:421:GLN:O	1.93	0.68
1:A:395:LYS:HD2	1:A:418:ILE:HG23	1.75	0.68
1:D:135:SER:O	1:D:139:LEU:HD13	1.94	0.68
1:C:257:LYS:HD3	3:C:479:HOH:O	1.93	0.67
1:A:87:ASP:HB3	1:A:96:ARG:HH21	1.59	0.67
1:C:379:LEU:HB3	1:C:384:VAL:HB	1.76	0.67
1:D:131:LEU:HD22	1:D:189:LEU:HD11	1.75	0.67
1:B:179:ALA:O	1:B:183:THR:HG23	1.94	0.67
1:A:127:MET:O	1:A:131:LEU:HG	1.95	0.67
1:B:458:ARG:HA	1:B:461:MET:HE2	1.76	0.67
1:D:398:HIS:O	1:D:401:GLU:HB3	1.94	0.66
1:A:190:GLY:O	1:A:194:LYS:HG2	1.96	0.66
1:A:378:TYR:HD2	1:A:379:LEU:HD12	1.61	0.66
1:C:44:SER:HB3	1:C:109:LEU:HD21	1.77	0.66
1:C:154:ASP:HB2	3:C:558:HOH:O	1.94	0.66
1:A:115:ARG:NH1	1:A:116:ASN:HD21	1.94	0.66
1:B:219:ARG:HH11	1:B:219:ARG:HG2	1.60	0.66
1:D:461:MET:O	1:D:462:LYS:HB3	1.95	0.65
1:B:274:THR:HG23	3:B:568:HOH:O	1.95	0.65
1:A:277:ASP:HA	1:A:280:SER:OG	1.97	0.65
1:C:22:ILE:N	1:C:22:ILE:HD12	2.11	0.65
1:D:400:ALA:HB2	1:D:410:LEU:HD21	1.78	0.65
1:A:173:GLN:HE21	1:A:173:GLN:HA	1.61	0.65
1:B:41:ILE:HD11	1:B:72:ILE:HG22	1.79	0.65
1:C:435:SER:HA	1:C:438:GLN:HE21	1.61	0.64
2:D:0:AS1:CB	2:D:0:AS1:CG	2.72	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ASP:O	1:C:417:SER:N	2.25	0.64
1:B:111:THR:HG22	1:B:211:LEU:HD11	1.79	0.64
1:D:111:THR:HG22	1:D:211:LEU:HD11	1.78	0.64
1:A:101:LEU:HD22	1:A:101:LEU:H	1.60	0.64
1:B:52:GLU:HG3	1:B:62:LEU:HD22	1.80	0.64
1:A:173:GLN:HE22	1:A:453:GLN:HE22	1.46	0.64
1:A:90:ILE:HD12	1:A:93:ALA:HB3	1.79	0.64
1:C:431:ASN:HB3	1:C:434:ASN:HD22	1.61	0.63
1:D:461:MET:O	1:D:462:LYS:CB	2.46	0.63
1:D:362:MET:O	1:D:366:LEU:HD13	1.95	0.63
1:B:98:LEU:HD22	1:B:106:ALA:HB2	1.78	0.63
1:D:49:LYS:NZ	1:D:66:LEU:HD21	2.14	0.63
1:D:361:ASN:HA	1:D:364:LYS:HE2	1.81	0.63
1:B:442:LEU:HB3	3:D:498:HOH:O	1.98	0.62
1:C:386:PHE:HE2	1:C:387:ARG:NH2	1.96	0.62
2:D:0:AS1:H11	2:D:0:AS1:N2	1.99	0.62
1:C:363:GLU:HA	1:C:366:LEU:HD13	1.79	0.62
1:C:393:SER:O	1:C:397:VAL:HG23	1.99	0.62
1:A:219:ARG:HG2	1:A:219:ARG:HH11	1.65	0.62
1:B:311:SER:O	1:B:315:VAL:HG23	1.99	0.62
1:A:102:ILE:HG13	1:A:103:GLY:N	2.15	0.61
1:C:374:ASP:CG	1:C:438:GLN:HE22	2.03	0.61
1:A:131:LEU:HD11	1:A:196:ILE:HD12	1.80	0.61
1:A:214:ASP:OD2	1:A:217:MET:HB2	2.01	0.61
1:D:190:GLY:O	1:D:194:LYS:HG2	1.99	0.61
1:D:110:ASN:HD22	1:D:113:ARG:HB3	1.65	0.61
1:B:405:ILE:HD11	1:B:410:LEU:HD23	1.81	0.61
1:A:187:GLU:O	1:A:191:GLU:HG3	2.01	0.61
1:B:214:ASP:OD2	1:B:217:MET:HB2	2.01	0.60
1:B:458:ARG:HA	1:B:461:MET:CE	2.30	0.60
1:B:379:LEU:HB3	1:B:384:VAL:HB	1.83	0.60
1:B:378:TYR:O	1:B:382:LYS:HG2	2.02	0.60
1:A:460:LEU:O	1:A:464:GLN:HG2	2.01	0.60
1:A:170:ARG:HG3	1:A:436:VAL:HG11	1.82	0.60
1:D:49:LYS:HZ3	1:D:66:LEU:HD21	1.65	0.60
1:C:179:ALA:O	1:C:183:THR:HG23	2.02	0.60
1:C:56:ILE:N	1:C:56:ILE:HD12	2.16	0.60
1:A:176:LEU:O	1:A:180:VAL:HG23	2.01	0.60
1:B:173:GLN:HE22	1:B:453:GLN:NE2	1.99	0.60
1:B:98:LEU:HD22	1:B:106:ALA:CB	2.32	0.60
1:C:72:ILE:HD11	1:C:94:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:GLU:OE1	1:D:462:LYS:HD3	2.02	0.60
1:D:173:GLN:HA	1:D:173:GLN:HE21	1.67	0.59
1:A:60:THR:O	1:A:64:LYS:HD3	2.03	0.59
1:A:276:SER:O	1:A:277:ASP:HB2	2.02	0.59
1:B:379:LEU:HD11	1:B:422:PHE:CE1	2.37	0.59
1:C:331:LYS:HD2	3:C:528:HOH:O	2.01	0.59
1:B:258:MET:O	1:B:262:LEU:HD13	2.03	0.59
1:C:456:GLN:O	1:C:460:LEU:HD23	2.02	0.59
1:A:227:ILE:HD11	1:C:442:LEU:HD13	1.84	0.59
1:C:366:LEU:HD23	1:C:432:PHE:CD2	2.37	0.59
1:C:401:GLU:O	1:C:401:GLU:OE1	2.21	0.59
1:C:60:THR:O	1:C:64:LYS:HD3	2.03	0.59
1:D:157:LEU:HA	1:D:366:LEU:HD11	1.84	0.59
1:C:275:LEU:HD22	1:C:351:VAL:HG13	1.84	0.59
1:B:117:ASP:HB3	1:B:235:ILE:HD11	1.85	0.58
1:C:155:VAL:HG22	1:C:359:LYS:HE3	1.86	0.58
1:C:364:LYS:HB2	1:C:364:LYS:NZ	2.18	0.58
1:D:431:ASN:HB3	1:D:434:ASN:ND2	2.18	0.58
1:A:81:PHE:HZ	1:A:93:ALA:O	1.86	0.58
1:B:199:LEU:HD11	1:B:201:LEU:HB3	1.86	0.58
1:D:454:ILE:O	1:D:458:ARG:HB2	2.04	0.58
1:B:399:LEU:HD21	1:B:414:ASP:HB3	1.85	0.58
1:B:297:LEU:HD11	1:C:26:LEU:HD13	1.85	0.58
1:C:387:ARG:O	1:C:391:THR:HG23	2.04	0.58
1:D:60:THR:CG2	1:D:64:LYS:HE2	2.34	0.58
1:A:199:LEU:HD21	1:A:218:LEU:HB2	1.86	0.58
1:D:187:GLU:O	1:D:191:GLU:HG3	2.03	0.57
1:D:360:GLU:O	1:D:364:LYS:HG3	2.04	0.57
1:C:22:ILE:H	1:C:22:ILE:HD12	1.69	0.57
1:C:117:ASP:HB3	1:C:235:ILE:HD11	1.85	0.57
1:A:87:ASP:CB	1:A:96:ARG:HH21	2.17	0.57
1:B:314:MET:HG2	1:C:303:GLY:CA	2.33	0.57
1:B:375:LEU:O	1:B:378:TYR:HB3	2.04	0.57
1:C:20:ASP:OD1	1:C:22:ILE:HD13	2.04	0.57
1:D:421:GLN:HA	1:D:421:GLN:HE21	1.69	0.57
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.69	0.57
1:B:196:ILE:HG12	1:B:240:PHE:HB2	1.87	0.57
1:B:385:PRO:HB2	1:B:388:GLN:HG2	1.85	0.57
1:B:388:GLN:HA	1:B:388:GLN:HE21	1.70	0.57
1:C:366:LEU:HB3	1:C:432:PHE:CE2	2.39	0.57
1:C:422:PHE:CD1	1:C:426:VAL:HG21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLU:O	1:B:191:GLU:HG3	2.06	0.56
3:B:483:HOH:O	1:D:442:LEU:HB3	2.04	0.56
1:B:115:ARG:HH21	1:B:115:ARG:HG3	1.70	0.56
1:C:408:ASN:HB3	1:C:430:PHE:CD2	2.40	0.56
1:A:276:SER:O	1:A:277:ASP:CB	2.54	0.56
1:A:451:THR:O	1:A:455:GLU:HG3	2.05	0.56
1:A:89:ASP:OD2	1:A:91:HIS:HB2	2.05	0.56
1:C:412:LEU:HD12	1:C:412:LEU:N	2.20	0.56
1:C:21:PRO:HG2	1:C:22:ILE:HD12	1.87	0.56
1:A:309:LEU:HD21	3:A:499:HOH:O	2.05	0.56
1:A:324:ASN:O	1:A:327:LEU:HD13	2.06	0.56
1:C:379:LEU:HD12	1:C:379:LEU:N	2.19	0.56
1:B:116:ASN:HB3	1:B:235:ILE:HG23	1.87	0.56
1:B:133:ILE:HD13	3:B:535:HOH:O	2.05	0.56
1:C:20:ASP:OD2	1:C:22:ILE:HB	2.06	0.56
1:C:399:LEU:O	1:C:402:THR:HB	2.06	0.56
1:A:102:ILE:HD12	1:A:105:ILE:HG23	1.87	0.56
1:C:98:LEU:HD11	1:C:102:ILE:HD11	1.87	0.56
1:A:101:LEU:CD2	1:A:101:LEU:H	2.18	0.56
1:A:110:ASN:ND2	1:A:113:ARG:HB3	2.20	0.56
1:B:378:TYR:CD2	1:B:379:LEU:HD12	2.41	0.55
1:C:137:HIS:HE1	3:C:475:HOH:O	1.90	0.55
1:C:368:PRO:O	1:C:407:ILE:HD11	2.05	0.55
1:C:330:ASP:OD1	1:C:331:LYS:N	2.39	0.55
1:D:297:LEU:O	1:D:297:LEU:HD13	2.06	0.55
1:B:199:LEU:HB3	1:B:227:ILE:HG22	1.88	0.55
1:C:180:VAL:HG12	1:C:184:ARG:HH12	1.72	0.55
1:B:151:ILE:HG13	1:B:152:GLU:HG3	1.88	0.55
1:C:269:GLU:CD	1:C:269:GLU:H	2.10	0.55
1:A:139:LEU:HD21	1:A:464:GLN:CB	2.36	0.55
1:A:52:GLU:HG3	1:A:62:LEU:HD22	1.88	0.55
1:A:99:LYS:HD2	1:A:99:LYS:H	1.71	0.55
1:C:391:THR:O	1:C:395:LYS:HG3	2.07	0.55
1:C:123:LEU:HD22	1:C:127:MET:SD	2.47	0.55
1:D:371:LEU:HD13	1:D:430:PHE:HA	1.89	0.55
1:C:379:LEU:HB3	1:C:384:VAL:CB	2.37	0.54
1:A:101:LEU:HD22	1:A:101:LEU:N	2.21	0.54
1:B:128:LYS:NZ	1:B:197:ASN:ND2	2.55	0.54
1:C:164:GLN:HE22	1:D:267:THR:HA	1.73	0.54
1:B:96:ARG:HH11	1:B:96:ARG:HG2	1.73	0.54
1:D:96:ARG:O	1:D:99:LYS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:GLN:HE22	1:C:453:GLN:NE2	2.05	0.54
1:C:139:LEU:HD11	1:C:186:SER:OG	2.07	0.54
1:A:34:GLN:HG3	1:A:35:ARG:N	2.22	0.54
1:A:81:PHE:HE2	1:A:93:ALA:HB1	1.72	0.54
1:C:412:LEU:HD12	1:C:412:LEU:H	1.72	0.54
1:C:117:ASP:HA	1:C:120:VAL:HG12	1.90	0.54
1:B:326:ASP:HA	1:C:300:SER:HB3	1.89	0.54
1:D:67:SER:O	1:D:71:LYS:HG3	2.08	0.54
1:A:171:TRP:O	1:A:174:PHE:HB3	2.08	0.54
1:A:259:ALA:O	1:A:263:ILE:HG13	2.07	0.54
1:C:119:VAL:HG22	3:C:528:HOH:O	2.07	0.54
1:B:219:ARG:HG2	1:B:219:ARG:NH1	2.23	0.54
1:A:176:LEU:HD22	1:A:457:LEU:CD1	2.38	0.53
1:A:195:ARG:NH1	1:C:187:GLU:OE2	2.41	0.53
1:B:42:GLN:HA	1:B:42:GLN:NE2	2.23	0.53
1:B:170:ARG:HG3	1:B:436:VAL:HG11	1.90	0.53
1:C:366:LEU:HD23	1:C:432:PHE:CG	2.43	0.53
1:B:325:LYS:HE2	1:B:328:GLN:OE1	2.09	0.53
1:C:324:ASN:O	1:C:327:LEU:HD23	2.09	0.53
1:B:41:ILE:O	1:B:45:MET:HG3	2.09	0.53
1:C:98:LEU:HD12	1:C:106:ALA:HB1	1.91	0.53
1:A:317:LYS:C	1:A:317:LYS:HD3	2.28	0.53
1:B:117:ASP:HA	1:B:120:VAL:HG12	1.91	0.53
1:B:192:VAL:HG22	1:B:243:GLU:HB3	1.90	0.53
1:B:378:TYR:HD2	1:B:379:LEU:HD12	1.72	0.53
1:B:41:ILE:HG23	1:B:69:LEU:HB3	1.90	0.53
1:D:292:PRO:HB3	1:D:295:LEU:HD12	1.89	0.53
1:D:279:PHE:CZ	1:D:350:GLY:HA3	2.43	0.53
1:B:137:HIS:CE1	1:B:342:THR:HG23	2.44	0.53
1:B:71:LYS:HD3	1:B:101:LEU:HD21	1.90	0.53
1:C:124:LYS:HE2	1:C:240:PHE:CD2	2.44	0.53
1:B:191:GLU:HA	3:B:511:HOH:O	2.09	0.53
1:B:260:GLU:HG2	1:D:318:GLY:O	2.09	0.53
1:C:431:ASN:CB	1:C:434:ASN:HD22	2.21	0.53
1:A:97:ARG:HH11	1:A:97:ARG:HG2	1.75	0.52
1:C:188:ARG:NH2	1:C:250:LEU:HD13	2.24	0.52
1:C:61:GLU:CG	1:C:105:ILE:HD11	2.33	0.52
1:C:371:LEU:HD13	1:C:430:PHE:HA	1.92	0.52
1:D:297:LEU:O	1:D:301:LYS:HD3	2.09	0.52
1:D:407:ILE:HG13	1:D:430:PHE:HE2	1.74	0.52
1:D:328:GLN:HE21	2:D:0:AS1:HN41	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLU:HG2	1:D:105:ILE:HD11	1.89	0.52
1:A:97:ARG:HG3	1:A:101:LEU:HD21	1.90	0.52
1:A:442:LEU:HD13	1:C:227:ILE:HD11	1.91	0.52
1:D:61:GLU:CG	1:D:105:ILE:HD11	2.39	0.52
1:B:367:THR:OG1	1:B:369:GLU:HG2	2.10	0.52
1:D:116:ASN:ND2	2:D:0:AS1:H11	2.25	0.52
1:A:375:LEU:O	1:A:378:TYR:HB3	2.10	0.52
1:A:403:LYS:CA	1:A:403:LYS:HE2	2.32	0.52
1:C:170:ARG:HG3	1:C:436:VAL:HG11	1.92	0.52
1:A:191:GLU:HB3	1:C:191:GLU:OE2	2.10	0.52
1:A:355:LEU:O	1:A:355:LEU:HD12	2.09	0.52
1:B:65:ILE:O	1:B:65:ILE:HG22	2.10	0.52
1:C:78:LYS:C	1:C:80:VAL:H	2.11	0.52
1:D:214:ASP:OD2	1:D:217:MET:HB2	2.10	0.52
1:C:146:VAL:HG22	1:C:457:LEU:HD13	1.92	0.52
1:D:219:ARG:HH11	1:D:219:ARG:HG2	1.75	0.52
1:A:167:GLN:HG2	3:A:568:HOH:O	2.10	0.51
1:A:219:ARG:HG2	1:A:219:ARG:NH1	2.25	0.51
1:A:337:VAL:O	1:A:341:LEU:HD13	2.10	0.51
1:A:78:LYS:HB3	1:A:78:LYS:HZ2	1.75	0.51
1:B:176:LEU:O	1:B:180:VAL:HG23	2.10	0.51
1:D:387:ARG:HA	1:D:387:ARG:NE	2.25	0.51
1:B:197:ASN:ND2	1:B:224:PHE:HA	2.25	0.51
1:D:110:ASN:ND2	1:D:113:ARG:HB3	2.24	0.51
1:A:36:LEU:HD22	1:A:122:ASP:HB3	1.93	0.51
1:C:334:VAL:O	1:C:338:VAL:HG23	2.11	0.51
1:D:61:GLU:HG2	1:D:105:ILE:CD1	2.41	0.51
1:C:265:TYR:HB3	1:C:272:PHE:HB2	1.93	0.51
1:D:97:ARG:NE	1:D:101:LEU:HD11	2.26	0.51
1:B:56:ILE:N	1:B:56:ILE:HD12	2.26	0.51
1:C:355:LEU:O	1:C:355:LEU:HD12	2.11	0.51
1:D:459:GLU:OE1	1:D:459:GLU:HA	2.11	0.51
1:A:141:LEU:C	1:A:141:LEU:HD23	2.31	0.51
1:A:423:SER:HB3	1:A:425:ASP:OD2	2.11	0.51
1:B:41:ILE:HD11	1:B:72:ILE:CG2	2.41	0.51
1:D:400:ALA:HB2	1:D:410:LEU:CD2	2.40	0.51
1:A:139:LEU:HD21	1:A:464:GLN:HB3	1.92	0.51
1:A:464:GLN:HE21	1:A:464:GLN:HA	1.76	0.51
1:C:77:SER:O	1:C:78:LYS:HD3	2.11	0.51
1:C:78:LYS:HB2	1:C:80:VAL:HG23	1.91	0.51
1:C:91:HIS:CD2	1:C:118:GLN:NE2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ALA:O	1:D:263:ILE:HG13	2.11	0.51
1:C:97:ARG:O	1:C:101:LEU:HB2	2.11	0.51
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.76	0.51
1:B:176:LEU:HD22	1:B:457:LEU:HD12	1.93	0.51
1:C:259:ALA:O	1:C:263:ILE:HG13	2.11	0.51
1:A:327:LEU:N	1:A:327:LEU:HD12	2.25	0.50
1:A:436:VAL:HG13	1:A:445:THR:HG23	1.93	0.50
1:B:143:LYS:HZ2	1:B:143:LYS:HB2	1.74	0.50
1:D:431:ASN:HB3	1:D:434:ASN:HD22	1.74	0.50
1:A:189:LEU:HD23	1:A:189:LEU:C	2.32	0.50
1:A:76:TRP:C	1:A:78:LYS:H	2.15	0.50
1:A:227:ILE:HG12	3:A:472:HOH:O	2.11	0.50
1:A:304:ARG:NH1	3:A:555:HOH:O	2.44	0.50
1:B:119:VAL:HG22	3:B:570:HOH:O	2.10	0.50
1:C:196:ILE:HG12	1:C:240:PHE:HB2	1.92	0.50
1:D:98:LEU:HB3	1:D:106:ALA:HB1	1.94	0.50
1:A:97:ARG:HG3	1:A:101:LEU:CD2	2.41	0.50
1:A:403:LYS:HA	1:A:403:LYS:CE	2.32	0.50
1:C:111:THR:HG22	1:C:211:LEU:HD11	1.94	0.50
1:D:423:SER:HB3	1:D:425:ASP:OD2	2.12	0.50
1:A:188:ARG:CZ	1:A:250:LEU:HD23	2.42	0.50
1:C:33:ASP:OD1	1:C:33:ASP:O	2.30	0.50
1:C:141:LEU:HD22	1:C:182:LEU:HD13	1.93	0.50
1:D:431:ASN:HD22	1:D:432:PHE:N	2.09	0.50
1:A:81:PHE:CE2	1:A:93:ALA:HB1	2.47	0.49
1:B:161:THR:HG21	2:D:0:AS1:HB1	1.93	0.49
1:C:142:ILE:O	1:C:146:VAL:HG23	2.12	0.49
1:C:270:PHE:CE1	1:D:269:GLU:HG2	2.48	0.49
1:B:271:GLY:HA2	3:B:585:HOH:O	2.11	0.49
1:C:141:LEU:HD23	1:C:141:LEU:C	2.33	0.49
1:C:357:ILE:HB	1:C:362:MET:HE3	1.95	0.49
1:C:269:GLU:HG2	1:D:270:PHE:CD2	2.48	0.49
1:D:375:LEU:O	1:D:378:TYR:HB3	2.12	0.49
1:D:408:ASN:HB3	1:D:430:PHE:CD2	2.47	0.49
1:A:257:LYS:HB2	3:C:500:HOH:O	2.13	0.49
1:A:431:ASN:HB3	1:A:434:ASN:ND2	2.19	0.49
1:C:379:LEU:CD1	1:C:379:LEU:H	2.26	0.49
1:D:379:LEU:HD11	1:D:422:PHE:CE1	2.48	0.49
1:C:157:LEU:HB3	1:C:362:MET:HB3	1.93	0.49
1:A:196:ILE:HG12	1:A:240:PHE:HB2	1.95	0.49
1:D:330:ASP:OD1	1:D:331:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:C	1:D:355:LEU:HD12	2.33	0.49
1:D:436:VAL:HG13	1:D:445:THR:CG2	2.36	0.49
1:B:176:LEU:HD22	1:B:457:LEU:CD1	2.43	0.49
1:A:205:ALA:O	1:A:206:LEU:HB3	2.12	0.48
1:A:327:LEU:H	1:A:327:LEU:CD1	2.26	0.48
1:A:47:TYR:O	1:A:51:LEU:HB2	2.13	0.48
1:B:94:ASN:O	1:B:98:LEU:HB2	2.13	0.48
1:A:402:THR:HG22	1:A:403:LYS:HE3	1.94	0.48
1:D:199:LEU:HB3	1:D:227:ILE:HG22	1.95	0.48
1:A:135:SER:O	1:A:139:LEU:HD13	2.14	0.48
1:A:260:GLU:O	1:A:264:ILE:HG13	2.13	0.48
1:C:135:SER:O	1:C:139:LEU:HD13	2.12	0.48
1:C:270:PHE:CD1	1:D:269:GLU:HG2	2.49	0.48
1:D:173:GLN:HA	1:D:173:GLN:NE2	2.27	0.48
1:A:102:ILE:HD12	1:A:105:ILE:CG2	2.44	0.48
1:C:465:LYS:NZ	1:C:465:LYS:HB3	2.29	0.48
1:A:379:LEU:N	1:A:379:LEU:HD12	2.29	0.48
1:A:61:GLU:O	1:A:65:ILE:HG13	2.13	0.48
1:B:66:LEU:O	1:B:66:LEU:HD23	2.13	0.48
1:C:206:LEU:HD12	1:C:232:MET:HG2	1.96	0.48
1:C:50:ALA:CB	1:C:213:ILE:HD11	2.44	0.48
1:A:35:ARG:O	1:A:37:SER:N	2.47	0.48
1:C:362:MET:O	1:C:366:LEU:CD1	2.61	0.48
1:B:464:GLN:O	1:B:465:LYS:HB2	2.14	0.48
1:D:292:PRO:CB	1:D:295:LEU:HD12	2.44	0.48
1:C:343:ALA:O	1:C:347:VAL:HG23	2.14	0.47
1:A:141:LEU:O	1:A:141:LEU:HD23	2.15	0.47
1:B:421:GLN:NE2	1:B:421:GLN:HA	2.30	0.47
1:B:97:ARG:HD3	1:B:97:ARG:O	2.14	0.47
1:A:115:ARG:NH1	1:A:116:ASN:ND2	2.60	0.47
1:B:128:LYS:NZ	1:B:197:ASN:HD21	2.12	0.47
1:C:197:ASN:ND2	1:C:224:PHE:HA	2.29	0.47
1:A:117:ASP:HB3	1:A:235:ILE:HD11	1.97	0.47
1:B:447:LYS:O	1:B:451:THR:HG23	2.14	0.47
1:C:188:ARG:CZ	1:C:250:LEU:HD13	2.45	0.47
1:B:30:ILE:O	1:B:34:GLN:HG3	2.15	0.47
1:B:407:ILE:HG13	1:B:430:PHE:CE2	2.50	0.47
1:C:258:MET:O	1:C:262:LEU:HD13	2.15	0.47
1:C:398:HIS:CG	1:C:398:HIS:O	2.68	0.47
1:C:50:ALA:HB1	1:C:213:ILE:HD11	1.96	0.47
1:C:197:ASN:HD21	1:C:224:PHE:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ILE:HB	1:C:362:MET:CE	2.45	0.47
1:C:78:LYS:O	1:C:80:VAL:N	2.48	0.47
1:D:30:ILE:O	1:D:34:GLN:HG3	2.15	0.47
1:A:82:VAL:HG13	1:A:82:VAL:O	2.15	0.47
1:B:222:LEU:O	1:B:223:GLU:HB2	2.15	0.47
1:B:26:LEU:HD11	1:C:343:ALA:HB1	1.96	0.47
1:C:446:ALA:O	1:C:450:VAL:HG23	2.15	0.47
1:D:61:GLU:CD	1:D:105:ILE:HD11	2.35	0.47
1:C:105:ILE:HG12	1:C:105:ILE:O	2.14	0.46
1:C:415:LEU:C	1:C:417:SER:N	2.69	0.46
1:A:139:LEU:HD21	1:A:464:GLN:HB2	1.98	0.46
1:B:30:ILE:HB	1:B:89:ASP:HA	1.97	0.46
1:C:352:ILE:HG22	1:C:352:ILE:O	2.16	0.46
1:C:419:SER:C	1:C:421:GLN:H	2.16	0.46
1:C:82:VAL:O	1:C:82:VAL:HG13	2.15	0.46
1:D:203:SER:HB2	1:D:235:ILE:HD13	1.98	0.46
1:B:189:LEU:O	1:B:189:LEU:HD23	2.14	0.46
1:C:119:VAL:HG22	1:C:331:LYS:HZ2	1.81	0.46
1:D:131:LEU:HD22	1:D:189:LEU:CD1	2.43	0.46
1:D:366:LEU:HB3	1:D:432:PHE:CD2	2.50	0.46
1:D:421:GLN:HA	1:D:421:GLN:NE2	2.31	0.46
1:D:52:GLU:HG3	1:D:62:LEU:HD22	1.97	0.46
1:A:179:ALA:O	1:A:183:THR:HG23	2.15	0.46
1:B:275:LEU:CD1	1:B:351:VAL:HG13	2.46	0.46
1:B:431:ASN:HB3	1:B:434:ASN:HD22	1.81	0.46
1:B:89:ASP:OD1	1:B:91:HIS:HB2	2.16	0.46
3:A:490:HOH:O	1:C:239:ASP:HB3	2.14	0.46
1:C:384:VAL:HG12	1:C:389:ALA:HB2	1.97	0.46
1:D:124:LYS:NZ	3:D:569:HOH:O	2.48	0.46
1:D:52:GLU:HA	1:D:57:LEU:HB2	1.98	0.46
1:A:376:ALA:O	1:A:380:VAL:HG23	2.16	0.46
1:A:69:LEU:HD23	1:A:98:LEU:HD11	1.97	0.46
1:D:371:LEU:CD1	1:D:430:PHE:HA	2.46	0.46
1:D:117:ASP:HB3	1:D:235:ILE:HD11	1.97	0.46
1:D:316:LEU:HA	1:D:319:LEU:HD12	1.98	0.46
1:A:34:GLN:HG3	1:A:35:ARG:HG3	1.98	0.46
1:C:379:LEU:CD1	1:C:379:LEU:N	2.79	0.46
1:D:368:PRO:O	1:D:407:ILE:HD11	2.16	0.46
1:A:293:ASP:OD1	1:D:325:LYS:HE3	2.16	0.45
1:A:99:LYS:HD2	1:A:99:LYS:N	2.31	0.45
1:C:380:VAL:HA	1:C:384:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:SER:C	1:C:425:ASP:H	2.19	0.45
1:C:76:TRP:C	1:C:78:LYS:H	2.20	0.45
1:D:123:LEU:HD22	1:D:127:MET:SD	2.56	0.45
1:D:179:ALA:O	1:D:183:THR:HG23	2.16	0.45
1:D:203:SER:CB	1:D:235:ILE:HD13	2.46	0.45
1:A:110:ASN:O	1:A:110:ASN:ND2	2.50	0.45
1:A:176:LEU:HD22	1:A:457:LEU:HD12	1.97	0.45
1:D:173:GLN:HE22	1:D:453:GLN:NE2	2.08	0.45
1:A:61:GLU:CD	1:A:105:ILE:HD11	2.36	0.45
1:A:47:TYR:CE2	1:A:113:ARG:HB2	2.51	0.45
1:A:327:LEU:CD1	1:A:327:LEU:N	2.80	0.45
1:B:66:LEU:C	1:B:66:LEU:HD23	2.36	0.45
1:C:180:VAL:HG12	1:C:184:ARG:NH1	2.30	0.45
1:D:219:ARG:NH1	1:D:219:ARG:HG2	2.31	0.45
1:D:41:ILE:CD1	1:D:73:SER:HA	2.46	0.45
1:A:65:ILE:C	1:A:67:SER:H	2.20	0.45
1:B:200:PRO:HB3	3:B:493:HOH:O	2.16	0.45
1:B:297:LEU:C	1:B:297:LEU:HD13	2.37	0.45
1:B:58:THR:OG1	1:B:61:GLU:HG3	2.17	0.45
1:C:119:VAL:HG21	1:C:331:LYS:HZ1	1.82	0.45
1:C:54:ALA:HB3	1:C:56:ILE:HD13	1.97	0.45
1:D:391:THR:O	1:D:395:LYS:HG3	2.16	0.45
1:B:275:LEU:HD11	1:B:351:VAL:HG13	1.99	0.45
1:C:91:HIS:CD2	1:C:115:ARG:HD2	2.51	0.45
1:C:140:GLN:HG2	3:C:544:HOH:O	2.15	0.45
1:D:170:ARG:HB3	3:D:540:HOH:O	2.17	0.45
1:A:165:LYS:HE2	3:B:466:HOH:O	2.17	0.45
1:C:206:LEU:CD1	1:C:232:MET:HG2	2.47	0.45
1:A:124:LYS:HE2	3:A:519:HOH:O	2.17	0.45
1:B:331:LYS:HE3	3:B:570:HOH:O	2.15	0.45
1:D:131:LEU:HD11	1:D:196:ILE:HD12	1.99	0.45
1:D:188:ARG:O	1:D:192:VAL:HG23	2.16	0.45
1:A:173:GLN:NE2	1:A:173:GLN:HA	2.28	0.45
1:C:173:GLN:NE2	1:C:453:GLN:HE22	2.09	0.45
1:A:44:SER:HB3	1:A:109:LEU:HD21	1.98	0.45
1:B:197:ASN:HD21	1:B:224:PHE:HA	1.80	0.45
1:B:368:PRO:O	1:B:407:ILE:HD11	2.17	0.45
1:C:20:ASP:HA	1:C:21:PRO:HD2	1.87	0.45
1:C:267:THR:HB	1:C:269:GLU:OE1	2.17	0.45
1:D:153:ILE:HG12	1:D:153:ILE:O	2.16	0.45
1:C:22:ILE:CD1	1:C:22:ILE:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:LEU:CD1	1:C:412:LEU:H	2.29	0.45
1:D:128:LYS:HE2	1:D:197:ASN:ND2	2.31	0.45
1:D:347:VAL:O	1:D:351:VAL:HG23	2.17	0.45
1:A:123:LEU:HD12	3:A:572:HOH:O	2.17	0.44
1:B:153:ILE:HA	1:B:172:SER:OG	2.17	0.44
1:B:431:ASN:HB3	1:B:434:ASN:ND2	2.32	0.44
1:A:80:VAL:O	1:A:81:PHE:CB	2.61	0.44
1:B:401:GLU:OE2	1:B:401:GLU:C	2.55	0.44
1:D:332:GLU:HG3	3:D:494:HOH:O	2.17	0.44
1:A:35:ARG:C	1:A:37:SER:H	2.21	0.44
1:B:366:LEU:HB3	1:B:432:PHE:CZ	2.53	0.44
1:C:407:ILE:HG13	1:C:430:PHE:HE2	1.81	0.44
1:C:78:LYS:C	1:C:80:VAL:N	2.71	0.44
1:D:189:LEU:HD13	1:D:247:PHE:CE2	2.52	0.44
1:C:374:ASP:O	1:C:377:LEU:HB2	2.17	0.44
1:D:117:ASP:CB	1:D:235:ILE:HD11	2.47	0.44
1:D:200:PRO:HA	1:D:228:SER:HG	1.79	0.44
1:A:38:GLU:O	1:A:42:GLN:HG3	2.18	0.44
1:D:183:THR:HG21	1:D:457:LEU:HD22	2.00	0.44
1:D:76:TRP:HE1	1:D:94:ASN:HD21	1.65	0.44
1:A:245:LEU:CD2	1:A:337:VAL:HG21	2.48	0.44
1:A:371:LEU:HD13	1:A:430:PHE:HA	1.99	0.44
1:A:52:GLU:HA	1:A:57:LEU:HB2	1.98	0.44
1:C:433:VAL:O	1:C:437:GLU:HG2	2.17	0.44
1:C:61:GLU:HG2	1:C:105:ILE:CD1	2.35	0.44
1:C:89:ASP:OD2	1:C:91:HIS:HB2	2.18	0.44
1:D:292:PRO:O	1:D:293:ASP:C	2.56	0.44
1:C:414:ASP:O	1:C:417:SER:OG	2.18	0.44
1:D:235:ILE:HG22	1:D:322:THR:HG22	2.00	0.44
1:D:275:LEU:HD11	1:D:295:LEU:HG	1.99	0.44
1:B:366:LEU:HD23	1:B:432:PHE:CG	2.53	0.44
1:B:384:VAL:CG1	1:B:388:GLN:HB2	2.47	0.44
1:B:311:SER:HB3	1:C:307:GLY:HA3	1.99	0.44
1:A:108:LYS:HE2	1:C:385:PRO:HG3	1.99	0.44
1:C:398:HIS:HA	1:C:401:GLU:HG2	1.99	0.44
1:C:406:THR:O	1:C:408:ASN:N	2.51	0.44
1:C:415:LEU:C	1:C:417:SER:H	2.21	0.44
1:A:355:LEU:C	1:A:355:LEU:HD12	2.37	0.44
1:C:100:GLU:HG3	1:C:100:GLU:O	2.17	0.43
1:C:98:LEU:O	1:C:98:LEU:HD13	2.18	0.43
1:D:28:SER:OG	1:D:30:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:CD	1:A:99:LYS:H	2.31	0.43
1:C:400:ALA:C	1:C:402:THR:H	2.22	0.43
1:D:400:ALA:HB2	1:D:410:LEU:CG	2.48	0.43
1:D:97:ARG:CZ	1:D:101:LEU:HD11	2.47	0.43
1:C:22:ILE:O	1:C:26:LEU:HG	2.18	0.43
1:B:296:GLU:HB3	1:C:325:LYS:HB3	2.00	0.43
1:B:412:LEU:HD11	1:B:422:PHE:O	2.18	0.43
1:C:260:GLU:O	1:C:264:ILE:HG12	2.18	0.43
1:C:422:PHE:HD1	1:C:426:VAL:HG21	1.81	0.43
1:B:110:ASN:ND2	1:B:113:ARG:HH21	2.16	0.43
1:B:20:ASP:CG	1:B:21:PRO:HD2	2.39	0.43
1:A:412:LEU:HG	1:A:416:LYS:HE2	2.01	0.43
1:B:141:LEU:O	1:B:141:LEU:HD23	2.19	0.43
1:B:419:SER:C	1:B:421:GLN:H	2.22	0.43
1:C:30:ILE:O	1:C:34:GLN:HG3	2.18	0.43
1:D:180:VAL:HG22	1:D:457:LEU:HD21	2.00	0.43
1:D:56:ILE:HG12	1:D:211:LEU:HD13	2.01	0.43
1:A:123:LEU:O	1:A:127:MET:HG3	2.19	0.43
1:A:128:LYS:HE3	1:A:197:ASN:ND2	2.34	0.43
1:A:265:TYR:HB3	1:A:272:PHE:HB2	2.00	0.43
1:C:364:LYS:HB2	1:C:364:LYS:HZ2	1.82	0.43
1:A:400:ALA:HB2	1:A:410:LEU:HD21	2.01	0.43
1:A:464:GLN:O	1:A:465:LYS:HG2	2.19	0.43
1:A:75:GLU:O	1:A:78:LYS:HB2	2.18	0.43
1:C:104:ASP:C	1:C:106:ALA:H	2.20	0.43
1:D:405:ILE:HG13	1:D:406:THR:N	2.34	0.43
1:A:206:LEU:HD21	1:C:167:GLN:HG2	2.01	0.42
1:A:279:PHE:CZ	1:A:350:GLY:HA3	2.55	0.42
1:B:189:LEU:HD23	1:B:189:LEU:C	2.40	0.42
1:C:129:ASN:HB3	3:C:546:HOH:O	2.18	0.42
1:C:206:LEU:O	1:C:206:LEU:HD12	2.19	0.42
1:C:62:LEU:O	1:C:66:LEU:HD13	2.19	0.42
1:D:379:LEU:HD12	1:D:379:LEU:N	2.34	0.42
1:D:87:ASP:CG	1:D:96:ARG:HH21	2.22	0.42
1:A:281:THR:HB	1:A:293:ASP:OD1	2.19	0.42
1:A:255:LEU:HD23	1:A:344:VAL:HG11	2.00	0.42
1:B:115:ARG:NH2	1:B:115:ARG:HG3	2.34	0.42
1:A:206:LEU:HD21	1:C:167:GLN:CG	2.49	0.42
1:C:419:SER:HA	1:C:420:PRO:HD3	1.88	0.42
1:A:442:LEU:HB3	3:C:491:HOH:O	2.18	0.42
1:C:158:PRO:HG2	1:C:365:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ALA:O	1:C:380:VAL:HG23	2.18	0.42
1:D:137:HIS:HD2	3:D:475:HOH:O	2.02	0.42
1:A:35:ARG:HD2	1:A:126:PHE:CE1	2.54	0.42
1:B:449:SER:O	1:B:453:GLN:HG3	2.19	0.42
1:C:375:LEU:HD23	1:C:393:SER:HA	2.01	0.42
1:A:36:LEU:O	1:A:40:ASP:HB2	2.19	0.42
1:C:355:LEU:C	1:C:355:LEU:HD12	2.40	0.42
1:A:371:LEU:CD1	1:A:430:PHE:HA	2.49	0.42
1:A:41:ILE:HG21	1:A:73:SER:OG	2.19	0.42
1:B:407:ILE:HG13	1:B:430:PHE:HE2	1.85	0.42
1:B:68:GLY:O	1:B:72:ILE:HG13	2.19	0.42
1:C:325:LYS:HA	1:C:325:LYS:HE3	2.01	0.42
1:C:97:ARG:HD3	1:C:97:ARG:O	2.20	0.42
1:D:114:SER:O	1:D:118:GLN:HB2	2.20	0.42
1:A:115:ARG:HH11	1:A:116:ASN:ND2	2.18	0.42
1:B:96:ARG:NH1	1:B:96:ARG:HG2	2.34	0.42
1:D:203:SER:HB2	1:D:235:ILE:CD1	2.50	0.42
1:A:187:GLU:OE2	1:C:195:ARG:NH1	2.51	0.42
1:B:306:PHE:CE2	1:C:310:ALA:HB1	2.55	0.42
1:C:325:LYS:HE2	1:C:328:GLN:OE1	2.18	0.42
1:A:464:GLN:HA	1:A:464:GLN:NE2	2.34	0.42
1:B:317:LYS:HD3	1:B:317:LYS:C	2.40	0.42
1:B:42:GLN:HA	1:B:42:GLN:HE21	1.83	0.42
1:C:414:ASP:O	1:C:417:SER:CB	2.67	0.42
1:D:78:LYS:HB3	1:D:78:LYS:NZ	2.35	0.42
1:A:215:ARG:HA	1:A:218:LEU:HD12	2.02	0.42
1:A:326:ASP:HA	1:D:300:SER:HB3	2.01	0.42
1:C:113:ARG:HG2	1:C:114:SER:N	2.35	0.42
1:C:22:ILE:CD1	1:C:22:ILE:H	2.32	0.42
1:A:273:LEU:C	1:A:273:LEU:HD12	2.40	0.41
1:D:199:LEU:HD23	1:D:227:ILE:HG22	2.02	0.41
1:D:99:LYS:NZ	1:D:104:ASP:HA	2.35	0.41
1:A:301:LYS:O	1:A:305:VAL:HG23	2.20	0.41
1:D:317:LYS:C	1:D:317:LYS:HD3	2.41	0.41
1:A:431:ASN:CB	1:A:434:ASN:HD22	2.21	0.41
1:B:330:ASP:OD1	1:B:331:LYS:N	2.53	0.41
1:C:151:ILE:HG13	1:C:152:GLU:HG3	2.02	0.41
1:D:215:ARG:HH22	1:D:228:SER:CB	2.28	0.41
1:D:80:VAL:O	1:D:81:PHE:C	2.58	0.41
1:A:147:GLU:OE1	1:A:147:GLU:HA	2.20	0.41
1:B:347:VAL:O	1:B:351:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:GLU:HG2	1:D:270:PHE:CG	2.55	0.41
1:C:449:SER:O	1:C:453:GLN:HG3	2.21	0.41
1:D:407:ILE:HG13	1:D:430:PHE:CE2	2.53	0.41
1:D:460:LEU:HD22	1:D:460:LEU:HA	1.91	0.41
1:B:257:LYS:HB2	3:D:572:HOH:O	2.20	0.41
1:D:215:ARG:NH2	1:D:228:SER:HB2	2.27	0.41
1:D:292:PRO:O	1:D:295:LEU:N	2.50	0.41
1:D:98:LEU:HB3	1:D:106:ALA:CB	2.51	0.41
1:A:171:TRP:NE1	1:A:175:LEU:HD11	2.36	0.41
1:A:156:ILE:HG22	1:A:366:LEU:HD21	2.02	0.41
1:A:49:LYS:HB3	1:A:217:MET:CE	2.50	0.41
1:A:87:ASP:CG	1:A:96:ARG:HH21	2.23	0.41
1:B:252:MET:HB3	1:B:302:SER:HA	2.03	0.41
1:B:321:SER:HB2	1:B:322:THR:HA	2.03	0.41
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.35	0.41
1:B:171:TRP:O	1:B:174:PHE:HB3	2.21	0.41
1:B:355:LEU:O	1:B:355:LEU:HD12	2.21	0.41
1:B:47:TYR:CE2	1:B:113:ARG:HB2	2.55	0.41
1:C:263:ILE:HG22	1:D:163:LEU:HD12	2.03	0.41
1:B:166:ALA:HB1	2:D:0:AS1:OD1	2.21	0.41
1:D:343:ALA:O	1:D:347:VAL:HG23	2.21	0.41
1:D:65:ILE:O	1:D:69:LEU:HG	2.21	0.41
1:B:241:VAL:O	1:B:245:LEU:HG	2.21	0.41
1:C:414:ASP:HB2	1:C:415:LEU:H	1.77	0.41
1:D:171:TRP:O	1:D:174:PHE:HB3	2.21	0.41
1:A:191:GLU:OE2	1:C:191:GLU:HB3	2.21	0.41
1:B:388:GLN:CA	1:B:388:GLN:HE21	2.32	0.41
1:B:94:ASN:C	1:B:96:ARG:H	2.24	0.41
1:A:442:LEU:CD1	1:C:227:ILE:HD11	2.51	0.40
1:D:308:ARG:HD2	3:D:467:HOH:O	2.21	0.40
1:D:400:ALA:CB	1:D:410:LEU:HD21	2.50	0.40
1:D:407:ILE:CG1	1:D:430:PHE:HE2	2.33	0.40
1:A:141:LEU:CD2	1:A:141:LEU:C	2.90	0.40
1:A:279:PHE:HB3	1:A:294:SER:CB	2.51	0.40
1:A:361:ASN:HD22	1:A:361:ASN:N	2.19	0.40
1:B:156:ILE:HG22	1:B:366:LEU:HD21	2.03	0.40
1:B:388:GLN:HA	1:B:388:GLN:NE2	2.36	0.40
1:B:421:GLN:HA	1:B:421:GLN:HE21	1.84	0.40
1:C:366:LEU:N	1:C:366:LEU:HD12	2.37	0.40
1:D:451:THR:O	1:D:455:GLU:HG3	2.22	0.40
1:B:141:LEU:C	1:B:141:LEU:HD23	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LEU:HD23	1:C:352:ILE:HG21	2.03	0.40
1:D:113:ARG:HG2	1:D:114:SER:N	2.37	0.40
1:B:130:SER:O	1:B:134:ILE:HG13	2.22	0.40
1:C:436:VAL:HG13	1:C:445:THR:HG23	2.03	0.40
1:A:379:LEU:HD11	1:A:422:PHE:CZ	2.56	0.40
1:B:157:LEU:HB2	1:B:158:PRO:CD	2.51	0.40
1:C:114:SER:O	1:C:118:GLN:HB2	2.22	0.40
1:C:123:LEU:O	1:C:127:MET:HG3	2.22	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	420/447 (94%)	379 (90%)	32 (8%)	9 (2%)	8	6
1	B	412/447 (92%)	382 (93%)	27 (7%)	3 (1%)	25	30
1	C	430/447 (96%)	389 (90%)	30 (7%)	11 (3%)	6	4
1	D	432/447 (97%)	397 (92%)	29 (7%)	6 (1%)	13	13
All	All	1694/1788 (95%)	1547 (91%)	118 (7%)	29 (2%)	11	9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PHE
1	A	82	VAL
1	A	84	LYS
1	A	88	GLU
1	A	206	LEU
1	C	276	SER
1	C	386	PHE

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Mol	Chain	Res	Type
1	D	206	LEU
1	D	462	LYS
1	A	36	LEU
1	A	277	ASP
1	B	66	LEU
1	B	206	LEU
1	C	407	ILE
1	C	410	LEU
1	D	293	ASP
1	A	34	GLN
1	C	79	GLY
1	C	206	LEU
1	D	443	ALA
1	B	21	PRO
1	C	277	ASP
1	D	81	PHE
1	A	35	ARG
1	C	34	GLN
1	C	77	SER
1	C	101	LEU
1	C	424	SER
1	D	405	ILE

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	369/392 (94%)	356 (96%)	13 (4%)	41	56
1	B	364/392 (93%)	355 (98%)	9 (2%)	53	70
1	C	377/392 (96%)	360 (96%)	17 (4%)	32	44
1	D	379/392 (97%)	365 (96%)	14 (4%)	39	53
All	All	1489/1568 (95%)	1436 (96%)	53 (4%)	40	55

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	78	LYS
1	A	110	ASN
1	A	115	ARG
1	A	123	LEU
1	A	138	LEU
1	A	173	GLN
1	A	197	ASN
1	A	200	PRO
1	A	237	GLU
1	A	255	LEU
1	A	366	LEU
1	A	460	LEU
1	B	75	GLU
1	B	95	GLU
1	B	98	LEU
1	B	138	LEU
1	B	197	ASN
1	B	200	PRO
1	B	250	LEU
1	B	314	MET
1	B	326	ASP
1	C	33	ASP
1	C	51	LEU
1	C	64	LYS
1	C	110	ASN
1	C	123	LEU
1	C	138	LEU
1	C	197	ASN
1	C	200	PRO
1	C	210	PRO
1	C	247	PHE
1	C	250	LEU
1	C	308	ARG
1	C	325	LYS
1	C	326	ASP
1	C	388	GLN
1	C	401	GLU
1	C	414	ASP
1	D	27	ASN
1	D	109	LEU
1	D	110	ASN
1	D	123	LEU

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Mol	Chain	Res	Type
1	D	141	LEU
1	D	197	ASN
1	D	235	ILE
1	D	250	LEU
1	D	308	ARG
1	D	327	LEU
1	D	414	ASP
1	D	431	ASN
1	D	459	GLU
1	D	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	94	ASN
1	A	110	ASN
1	A	116	ASN
1	A	129	ASN
1	A	137	HIS
1	A	167	GLN
1	A	173	GLN
1	A	197	ASN
1	A	291	ASN
1	A	361	ASN
1	A	409	ASN
1	A	421	GLN
1	A	434	ASN
1	A	464	GLN
1	B	34	GLN
1	B	42	GLN
1	B	110	ASN
1	B	118	GLN
1	B	129	ASN
1	B	137	HIS
1	B	173	GLN
1	B	197	ASN
1	B	324	ASN
1	B	388	GLN
1	B	409	ASN
1	B	421	GLN
1	B	434	ASN

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Mol	Chain	Res	Type
1	C	42	GLN
1	C	91	HIS
1	C	94	ASN
1	C	116	ASN
1	C	118	GLN
1	C	129	ASN
1	C	137	HIS
1	C	164	GLN
1	C	173	GLN
1	C	197	ASN
1	C	324	ASN
1	C	361	ASN
1	C	409	ASN
1	C	434	ASN
1	C	438	GLN
1	D	27	ASN
1	D	94	ASN
1	D	110	ASN
1	D	116	ASN
1	D	118	GLN
1	D	129	ASN
1	D	137	HIS
1	D	173	GLN
1	D	197	ASN
1	D	291	ASN
1	D	328	GLN
1	D	356	GLN
1	D	421	GLN
1	D	431	ASN
1	D	434	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AS1	D	0	-	7,19,19	8.70	5 (71%)	8,24,24	11.75	8 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AS1	D	0	-	2/2/6/8	0/13/23/23	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	0	AS1	CA-N1	-6.06	1.38	1.46
2	D	0	AS1	C-N1	2.11	1.39	1.34
2	D	0	AS1	C-N3	4.38	1.42	1.29
2	D	0	AS1	C1-N2	10.21	1.69	1.46
2	D	0	AS1	CB-CA	19.06	1.79	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	N2-C-N3	-5.95	109.01	120.18
2	D	0	AS1	CA-N1-C	4.54	130.96	122.06
2	D	0	AS1	CB-CA-N1	4.58	118.08	108.94
2	D	0	AS1	CD-CB-CA	6.31	127.78	114.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	N2-C-N1	8.44	136.45	116.88
2	D	0	AS1	C1-N2-C	13.67	149.61	123.69
2	D	0	AS1	C3-C2-C1	17.65	164.84	112.11
2	D	0	AS1	C2-C1-N2	20.45	170.98	112.18

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	0	AS1	C4
2	D	0	AS1	CA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	0	AS1	9	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	424/447 (94%)	2.26	215 (50%) 0 0	17, 37, 85, 95	0
1	B	418/447 (93%)	1.54	131 (31%) 0 0	14, 35, 76, 98	0
1	C	434/447 (97%)	2.86	267 (61%) 0 0	18, 42, 95, 100	0
1	D	436/447 (97%)	1.54	124 (28%) 1 1	17, 36, 87, 99	0
All	All	1712/1788 (95%)	2.06	737 (43%) 0 0	14, 38, 87, 100	0

All (737) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	278	ALA	14.3
1	D	404	GLY	13.0
1	A	82	VAL	11.8
1	C	398	HIS	11.7
1	C	80	VAL	10.5
1	A	383	GLY	9.6
1	C	19	THR	9.4
1	C	413	GLU	8.8
1	C	394	GLY	8.8
1	C	400	ALA	8.6
1	A	402	THR	8.6
1	B	21	PRO	8.4
1	B	292	PRO	8.3
1	D	402	THR	8.2
1	C	415	LEU	8.1
1	C	387	ARG	7.8
1	C	77	SER	7.8
1	D	418	ILE	7.7
1	A	386	PHE	7.7
1	A	83	VAL	7.6
1	C	67	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	424	SER	7.5
1	C	393	SER	7.4
1	C	414	ASP	7.3
1	D	29	SER	7.3
1	A	34	GLN	7.2
1	C	25	LYS	7.2
1	A	85	GLN	7.1
1	C	60	THR	7.0
1	D	414	ASP	7.0
1	D	396	ALA	6.7
1	B	29	SER	6.7
1	A	400	ALA	6.6
1	C	93	ALA	6.6
1	C	151	ILE	6.5
1	C	434	ASN	6.5
1	C	220	SER	6.4
1	C	83	VAL	6.4
1	C	412	LEU	6.4
1	B	402	THR	6.3
1	C	73	SER	6.3
1	A	465	LYS	6.3
1	C	391	THR	6.3
1	A	84	LYS	6.2
1	C	401	GLU	6.2
1	D	392	ALA	6.2
1	D	281	THR	6.2
1	C	464	GLN	6.1
1	C	399	LEU	6.1
1	C	427	SER	6.1
1	D	411	SER	6.1
1	C	402	THR	6.0
1	D	391	THR	6.0
1	C	31	ALA	6.0
1	C	396	ALA	6.0
1	C	423	SER	6.0
1	A	96	ARG	6.0
1	C	101	LEU	6.0
1	C	65	ILE	6.0
1	D	397	VAL	6.0
1	D	389	ALA	5.9
1	A	391	THR	5.9
1	A	110	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	411	SER	5.9
1	D	417	SER	5.8
1	C	102	ILE	5.8
1	C	422	PHE	5.8
1	C	99	LYS	5.8
1	D	419	SER	5.8
1	D	401	GLU	5.7
1	B	24	GLU	5.6
1	C	57	LEU	5.6
1	C	64	LYS	5.6
1	C	425	ASP	5.6
1	C	389	ALA	5.5
1	A	460	LEU	5.5
1	D	409	ASN	5.5
1	A	100	GLU	5.4
1	C	448	SER	5.4
1	C	109	LEU	5.4
1	C	90	ILE	5.4
1	D	405	ILE	5.4
1	C	68	GLY	5.4
1	D	380	VAL	5.4
1	A	406	THR	5.4
1	A	98	LEU	5.4
1	A	35	ARG	5.4
1	B	411	SER	5.3
1	A	398	HIS	5.3
1	D	388	GLN	5.3
1	C	376	ALA	5.3
1	A	401	GLU	5.3
1	C	133	ILE	5.3
1	C	408	ASN	5.3
1	B	401	GLU	5.2
1	C	410	LEU	5.2
1	A	449	SER	5.2
1	A	86	SER	5.2
1	D	403	LYS	5.1
1	D	277	ASP	5.1
1	C	78	LYS	5.1
1	C	26	LEU	5.1
1	A	37	SER	5.1
1	C	105	ILE	5.1
1	D	420	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	5.0
1	C	46	ALA	5.0
1	D	398	HIS	5.0
1	C	292	PRO	4.9
1	C	76	TRP	4.9
1	D	421	GLN	4.9
1	A	57	LEU	4.9
1	B	25	LYS	4.9
1	C	71	LYS	4.9
1	A	415	LEU	4.9
1	C	377	LEU	4.9
1	A	373	THR	4.9
1	B	58	THR	4.9
1	B	400	ALA	4.8
1	B	26	LEU	4.8
1	A	464	GLN	4.8
1	A	69	LEU	4.8
1	C	358	SER	4.8
1	D	26	LEU	4.8
1	B	71	LYS	4.8
1	C	418	ILE	4.7
1	C	452	THR	4.7
1	A	112	GLY	4.7
1	C	386	PHE	4.7
1	C	368	PRO	4.7
1	A	66	LEU	4.7
1	C	52	GLU	4.7
1	C	342	THR	4.7
1	D	378	TYR	4.7
1	C	74	GLU	4.7
1	C	98	LEU	4.7
1	C	274	THR	4.7
1	C	451	THR	4.7
1	A	41	ILE	4.7
1	C	426	VAL	4.6
1	B	92	THR	4.6
1	C	21	PRO	4.6
1	D	408	ASN	4.6
1	B	23	MET	4.6
1	D	390	HIS	4.6
1	A	411	SER	4.6
1	D	413	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	58	THR	4.6
1	C	72	ILE	4.6
1	B	103	GLY	4.6
1	D	25	LYS	4.6
1	A	389	ALA	4.5
1	B	93	ALA	4.5
1	B	68	GLY	4.5
1	A	60	THR	4.5
1	A	436	VAL	4.5
1	A	81	PHE	4.5
1	C	132	SER	4.5
1	B	104	ASP	4.5
1	C	366	LEU	4.5
1	C	82	VAL	4.5
1	A	56	ILE	4.5
1	D	427	SER	4.4
1	C	30	ILE	4.4
1	A	74	GLU	4.4
1	D	278	ALA	4.4
1	C	357	ILE	4.4
1	D	394	GLY	4.4
1	D	406	THR	4.4
1	A	33	ASP	4.4
1	A	277	ASP	4.4
1	A	374	ASP	4.4
1	B	464	GLN	4.4
1	C	388	GLN	4.4
1	D	425	ASP	4.4
1	A	80	VAL	4.4
1	C	41	ILE	4.4
1	A	63	GLU	4.4
1	C	62	LEU	4.4
1	C	86	SER	4.4
1	A	150	ALA	4.4
1	C	276	SER	4.4
1	D	439	TYR	4.3
1	B	101	LEU	4.3
1	C	390	HIS	4.3
1	D	379	LEU	4.3
1	A	397	VAL	4.3
1	C	88	GLU	4.3
1	C	409	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	105	ILE	4.3
1	B	75	GLU	4.3
1	C	89	ASP	4.3
1	D	426	VAL	4.3
1	C	338	VAL	4.3
1	D	430	PHE	4.2
1	C	293	ASP	4.2
1	C	361	ASN	4.2
1	C	369	GLU	4.2
1	A	220	SER	4.2
1	D	399	LEU	4.2
1	A	92	THR	4.2
1	D	428	GLN	4.2
1	C	433	VAL	4.2
1	B	105	ILE	4.2
1	C	395	LYS	4.2
1	C	373	THR	4.1
1	B	51	LEU	4.1
1	A	97	ARG	4.1
1	B	28	SER	4.1
1	C	449	SER	4.1
1	D	386	PHE	4.1
1	B	100	GLU	4.1
1	A	65	ILE	4.1
1	C	84	LYS	4.1
1	D	30	ILE	4.1
1	C	104	ASP	4.1
1	A	387	ARG	4.1
1	A	462	LYS	4.1
1	A	73	SER	4.1
1	A	448	SER	4.1
1	C	363	GLU	4.1
1	C	96	ARG	4.1
1	C	37	SER	4.1
1	B	54	ALA	4.0
1	C	45	MET	4.0
1	C	362	MET	4.0
1	A	417	SER	4.0
1	A	414	ASP	4.0
1	C	462	LYS	4.0
1	D	465	LYS	4.0
1	A	89	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	67	SER	4.0
1	D	372	ALA	4.0
1	C	103	GLY	4.0
1	C	59	LYS	4.0
1	D	279	PHE	4.0
1	B	89	ASP	4.0
1	B	70	GLU	4.0
1	C	95	GLU	4.0
1	C	378	TYR	3.9
1	A	392	ALA	3.9
1	D	416	LYS	3.9
1	B	102	ILE	3.9
1	A	54	ALA	3.9
1	D	373	THR	3.9
1	A	39	VAL	3.9
1	B	419	SER	3.9
1	D	104	ASP	3.9
1	A	72	ILE	3.9
1	A	103	GLY	3.9
1	B	74	GLU	3.9
1	A	217	MET	3.9
1	A	58	THR	3.9
1	C	403	LYS	3.8
1	C	97	ARG	3.8
1	A	292	PRO	3.8
1	C	364	LYS	3.8
1	A	95	GLU	3.8
1	A	369	GLU	3.8
1	B	91	HIS	3.8
1	B	22	ILE	3.8
1	B	65	ILE	3.8
1	C	48	ALA	3.8
1	A	62	LEU	3.8
1	C	354	THR	3.8
1	C	66	LEU	3.8
1	D	375	LEU	3.8
1	A	423	SER	3.8
1	A	434	ASN	3.8
1	A	280	SER	3.8
1	A	111	THR	3.7
1	C	75	GLU	3.7
1	C	28	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	3.7
1	A	136	THR	3.7
1	A	281	THR	3.7
1	B	111	THR	3.7
1	C	22	ILE	3.7
1	C	454	ILE	3.7
1	A	186	SER	3.7
1	A	378	TYR	3.7
1	C	225	ALA	3.7
1	C	450	VAL	3.7
1	C	431	ASN	3.7
1	C	455	GLU	3.7
1	A	226	SER	3.7
1	B	276	SER	3.7
1	B	56	ILE	3.7
1	B	63	GLU	3.7
1	A	212	ASP	3.7
1	A	91	HIS	3.7
1	B	90	ILE	3.7
1	C	153	ILE	3.7
1	C	217	MET	3.7
1	B	20	ASP	3.6
1	A	102	ILE	3.6
1	D	369	GLU	3.6
1	A	77	SER	3.6
1	A	68	GLY	3.6
1	A	404	GLY	3.6
1	B	110	ASN	3.6
1	A	276	SER	3.6
1	D	424	SER	3.6
1	B	46	ALA	3.6
1	A	90	ILE	3.6
1	D	384	VAL	3.6
1	D	387	ARG	3.6
1	C	465	LYS	3.6
1	A	278	ALA	3.5
1	A	93	ALA	3.5
1	C	296	GLU	3.5
1	A	429	VAL	3.5
1	D	455	GLU	3.5
1	A	46	ALA	3.5
1	C	392	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	353	SER	3.5
1	D	393	SER	3.5
1	C	457	LEU	3.5
1	C	384	VAL	3.5
1	B	60	THR	3.5
1	C	150	ALA	3.5
1	A	211	LEU	3.4
1	B	72	ILE	3.4
1	D	460	LEU	3.4
1	A	413	GLU	3.4
1	C	459	GLU	3.4
1	A	210	PRO	3.4
1	B	412	LEU	3.4
1	A	132	SER	3.4
1	C	397	VAL	3.4
1	A	71	LYS	3.4
1	B	465	LYS	3.4
1	A	224	PHE	3.4
1	B	30	ILE	3.4
1	B	62	LEU	3.4
1	C	50	ALA	3.4
1	D	400	ALA	3.4
1	B	115	ARG	3.4
1	D	21	PRO	3.4
1	C	92	THR	3.4
1	A	388	GLN	3.4
1	A	403	LYS	3.4
1	A	50	ALA	3.4
1	D	412	LEU	3.4
1	C	416	LYS	3.4
1	C	380	VAL	3.3
1	A	394	GLY	3.3
1	B	394	GLY	3.3
1	C	266	SER	3.3
1	C	183	THR	3.3
1	D	395	LYS	3.3
1	C	277	ASP	3.3
1	C	136	THR	3.3
1	D	291	ASN	3.3
1	B	95	GLU	3.3
1	D	69	LEU	3.3
1	C	420	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	381	ARG	3.3
1	C	140	GLN	3.3
1	C	360	GLU	3.3
1	A	225	ALA	3.3
1	A	36	LEU	3.3
1	D	107	GLY	3.3
1	B	398	HIS	3.3
1	C	456	GLN	3.3
1	B	106	ALA	3.3
1	B	235	ILE	3.3
1	D	464	GLN	3.3
1	B	216	GLU	3.3
1	B	69	LEU	3.3
1	C	175	LEU	3.3
1	C	379	LEU	3.3
1	A	216	GLU	3.3
1	B	94	ASN	3.2
1	A	442	LEU	3.2
1	C	20	ASP	3.2
1	A	452	THR	3.2
1	B	99	LYS	3.2
1	B	31	ALA	3.2
1	A	67	SER	3.2
1	D	410	LEU	3.2
1	D	103	GLY	3.2
1	B	369	GLU	3.2
1	C	130	SER	3.2
1	B	421	GLN	3.2
1	B	61	GLU	3.2
1	C	155	VAL	3.2
1	A	115	ARG	3.2
1	A	443	ALA	3.2
1	D	220	SER	3.2
1	A	88	GLU	3.2
1	D	91	HIS	3.2
1	D	436	VAL	3.2
1	B	109	LEU	3.2
1	C	110	ASN	3.2
1	C	87	ASP	3.2
1	A	451	THR	3.2
1	C	137	HIS	3.2
1	D	463	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	372	ALA	3.2
1	C	460	LEU	3.2
1	C	405	ILE	3.1
1	D	462	LYS	3.1
1	C	70	GLU	3.1
1	A	371	LEU	3.1
1	B	44	SER	3.1
1	C	359	LYS	3.1
1	C	106	ALA	3.1
1	B	96	ARG	3.1
1	A	450	VAL	3.1
1	B	32	TYR	3.1
1	C	69	LEU	3.1
1	C	355	LEU	3.1
1	A	221	GLU	3.1
1	C	144	THR	3.1
1	C	85	GLN	3.1
1	C	351	VAL	3.1
1	C	436	VAL	3.1
1	A	410	LEU	3.1
1	A	427	SER	3.1
1	C	94	ASN	3.1
1	C	348	ALA	3.1
1	B	413	GLU	3.1
1	B	424	SER	3.1
1	B	57	LEU	3.1
1	C	367	THR	3.1
1	C	91	HIS	3.0
1	B	37	SER	3.0
1	C	23	MET	3.0
1	A	279	PHE	3.0
1	A	363	GLU	3.0
1	C	435	SER	3.0
1	B	385	PRO	3.0
1	A	94	ASN	3.0
1	B	462	LYS	3.0
1	A	446	ALA	3.0
1	D	407	ILE	3.0
1	B	236	SER	3.0
1	B	423	SER	3.0
1	A	106	ALA	3.0
1	B	220	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	448	SER	3.0
1	A	59	LYS	3.0
1	C	81	PHE	3.0
1	B	107	GLY	3.0
1	B	425	ASP	3.0
1	C	428	GLN	3.0
1	C	438	GLN	3.0
1	B	373	THR	3.0
1	A	53	LYS	3.0
1	A	139	LEU	2.9
1	C	42	GLN	2.9
1	C	214	ASP	2.9
1	A	133	ILE	2.9
1	C	119	VAL	2.9
1	C	381	ARG	2.9
1	C	29	SER	2.9
1	D	89	ASP	2.9
1	B	41	ILE	2.9
1	B	426	VAL	2.9
1	D	429	VAL	2.9
1	A	64	LYS	2.9
1	D	86	SER	2.9
1	C	184	ARG	2.9
1	C	27	ASN	2.9
1	C	263	ILE	2.9
1	A	130	SER	2.9
1	C	177	SER	2.9
1	A	318	GLY	2.9
1	B	34	GLN	2.9
1	B	389	ALA	2.9
1	D	382	LYS	2.9
1	A	137	HIS	2.9
1	C	226	SER	2.9
1	A	192	VAL	2.9
1	C	250	LEU	2.9
1	C	259	ALA	2.9
1	A	235	ILE	2.8
1	A	419	SER	2.8
1	C	340	THR	2.8
1	D	59	LYS	2.8
1	D	367	THR	2.8
1	C	258	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	90	ILE	2.8
1	D	92	THR	2.8
1	C	53	LYS	2.8
1	C	149	ALA	2.8
1	D	356	GLN	2.8
1	A	129	ASN	2.8
1	C	349	THR	2.8
1	D	376	ALA	2.8
1	C	204	GLY	2.8
1	D	276	SER	2.8
1	A	181	ALA	2.8
1	A	396	ALA	2.8
1	B	108	LYS	2.8
1	D	212	ASP	2.8
1	D	280	SER	2.8
1	D	366	LEU	2.8
1	A	99	LYS	2.8
1	A	205	ALA	2.7
1	A	381	ARG	2.8
1	C	343	ALA	2.7
1	A	208	GLY	2.7
1	B	210	PRO	2.7
1	D	415	LEU	2.7
1	B	451	THR	2.7
1	A	55	GLY	2.7
1	C	24	GLU	2.7
1	B	415	LEU	2.7
1	C	275	LEU	2.7
1	A	231	SER	2.7
1	B	420	PRO	2.7
1	C	365	ALA	2.7
1	A	109	LEU	2.7
1	A	447	LYS	2.7
1	C	297	LEU	2.7
1	D	60	THR	2.7
1	B	64	LYS	2.7
1	D	28	SER	2.7
1	A	420	PRO	2.6
1	C	231	SER	2.6
1	A	78	LYS	2.6
1	A	147	GLU	2.6
1	A	293	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	441	ALA	2.6
1	B	387	ARG	2.6
1	A	412	LEU	2.6
1	C	339	ASP	2.6
1	D	423	SER	2.6
1	A	209	ASN	2.6
1	A	418	ILE	2.6
1	C	196	ILE	2.6
1	B	463	LYS	2.6
1	D	161	THR	2.6
1	D	377	LEU	2.6
1	A	104	ASP	2.6
1	D	438	GLN	2.6
1	A	228	SER	2.6
1	A	433	VAL	2.6
1	D	80	VAL	2.6
1	C	148	ARG	2.6
1	C	447	LYS	2.6
1	A	87	ASP	2.6
1	B	42	GLN	2.6
1	B	383	GLY	2.6
1	C	346	GLN	2.6
1	C	129	ASN	2.6
1	B	393	SER	2.6
1	C	135	SER	2.6
1	C	385	PRO	2.6
1	D	53	LYS	2.6
1	A	44	SER	2.5
1	A	184	ARG	2.5
1	C	445	THR	2.5
1	D	58	THR	2.5
1	A	101	LEU	2.5
1	D	164	GLN	2.5
1	C	147	GLU	2.5
1	C	382	LYS	2.5
1	A	117	ASP	2.5
1	A	189	LEU	2.5
1	A	399	LEU	2.5
1	B	460	LEU	2.5
1	A	79	GLY	2.5
1	A	424	SER	2.5
1	A	61	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	34	GLN	2.5
1	A	108	LYS	2.5
1	A	422	PHE	2.5
1	D	166	ALA	2.5
1	A	52	GLU	2.5
1	A	223	GLU	2.5
1	C	142	ILE	2.5
1	A	206	LEU	2.5
1	A	70	GLU	2.5
1	D	82	VAL	2.5
1	A	135	SER	2.5
1	B	97	ARG	2.5
1	C	145	LEU	2.5
1	A	45	MET	2.5
1	B	39	VAL	2.5
1	C	432	PHE	2.5
1	D	383	GLY	2.5
1	B	417	SER	2.4
1	D	77	SER	2.4
1	A	426	VAL	2.4
1	C	146	VAL	2.4
1	C	180	VAL	2.4
1	A	437	GLU	2.4
1	C	197	ASN	2.4
1	A	390	HIS	2.4
1	D	459	GLU	2.4
1	A	47	TYR	2.4
1	B	33	ASP	2.4
1	C	33	ASP	2.4
1	A	459	GLU	2.4
1	C	100	GLU	2.4
1	D	93	ALA	2.4
1	B	55	GLY	2.4
1	C	38	GLU	2.4
1	A	153	ILE	2.4
1	B	218	LEU	2.4
1	D	23	MET	2.4
1	C	39	VAL	2.4
1	C	198	VAL	2.4
1	C	374	ASP	2.4
1	A	114	SER	2.4
1	C	172	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	57	LEU	2.4
1	A	40	ASP	2.4
1	A	154	ASP	2.4
1	B	414	ASP	2.4
1	C	370	MET	2.4
1	D	385	PRO	2.4
1	A	291	ASN	2.4
1	A	51	LEU	2.4
1	A	327	LEU	2.4
1	C	125	LEU	2.4
1	A	428	GLN	2.4
1	B	363	GLU	2.4
1	D	88	GLU	2.4
1	A	409	ASN	2.4
1	B	409	ASN	2.4
1	D	300	SER	2.4
1	A	48	ALA	2.3
1	A	377	LEU	2.3
1	B	50	ALA	2.3
1	D	360	GLU	2.3
1	A	118	GLN	2.3
1	B	73	SER	2.3
1	A	187	GLU	2.3
1	A	143	LYS	2.3
1	A	431	ASN	2.3
1	C	294	SER	2.3
1	C	419	SER	2.3
1	B	112	GLY	2.3
1	B	139	LEU	2.3
1	C	141	LEU	2.3
1	A	144	THR	2.3
1	C	63	GLU	2.3
1	A	119	VAL	2.3
1	C	347	VAL	2.3
1	D	22	ILE	2.3
1	C	383	GLY	2.3
1	B	459	GLU	2.3
1	C	210	PRO	2.3
1	C	108	LYS	2.3
1	D	105	ILE	2.3
1	C	440	THR	2.3
1	C	442	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	GLY	2.3
1	C	208	GLY	2.3
1	A	198	VAL	2.3
1	C	171	TRP	2.3
1	B	368	PRO	2.3
1	D	99	LYS	2.3
1	B	231	SER	2.3
1	C	264	ILE	2.3
1	C	375	LEU	2.2
1	C	437	GLU	2.2
1	B	59	LYS	2.2
1	C	122	ASP	2.2
1	B	166	ALA	2.2
1	D	274	THR	2.2
1	A	456	GLN	2.2
1	A	191	GLU	2.2
1	B	198	VAL	2.2
1	B	428	GLN	2.2
1	A	76	TRP	2.2
1	C	115	ARG	2.2
1	C	236	SER	2.2
1	B	208	GLY	2.2
1	C	248	ALA	2.2
1	D	27	ASN	2.2
1	A	439	TYR	2.2
1	C	160	TYR	2.2
1	C	156	ILE	2.2
1	D	361	ASN	2.2
1	B	297	LEU	2.2
1	C	345	LEU	2.2
1	D	371	LEU	2.2
1	A	120	VAL	2.2
1	A	204	GLY	2.2
1	C	267	THR	2.2
1	C	406	THR	2.2
1	C	169	ILE	2.2
1	C	216	GLU	2.2
1	B	422	PHE	2.2
1	D	422	PHE	2.2
1	C	203	SER	2.2
1	D	374	ASP	2.2
1	A	42	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	49	LYS	2.1
1	A	294	SER	2.1
1	D	435	SER	2.1
1	A	43	GLY	2.1
1	B	219	ARG	2.1
1	C	305	VAL	2.1
1	A	440	THR	2.1
1	A	393	SER	2.1
1	B	132	SER	2.1
1	C	417	SER	2.1
1	B	461	MET	2.1
1	C	32	TYR	2.1
1	C	49	LYS	2.1
1	A	239	ASP	2.1
1	A	438	GLN	2.1
1	B	379	LEU	2.1
1	B	117	ASP	2.1
1	C	174	PHE	2.1
1	C	407	ILE	2.1
1	A	218	LEU	2.1
1	C	173	GLN	2.1
1	D	452	THR	2.1
1	A	197	ASN	2.1
1	A	395	LYS	2.1
1	C	350	GLY	2.1
1	C	164	GLN	2.1
1	C	221	GLU	2.1
1	C	205	ALA	2.1
1	A	202	GLY	2.1
1	C	224	PHE	2.1
1	D	47	TYR	2.1
1	B	388	GLN	2.0
1	C	61	GLU	2.0
1	B	364	LYS	2.0
1	A	75	GLU	2.0
1	B	119	VAL	2.0
1	B	458	ARG	2.0
1	B	202	GLY	2.0
1	A	435	SER	2.0
1	C	356	GLN	2.0
1	C	143	LYS	2.0
1	C	47	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	MET	2.0
1	C	444	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	AS1	D	0	20/20	0.65	0.39	1.62	30,60,82,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.