



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM 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](mailto: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.

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

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

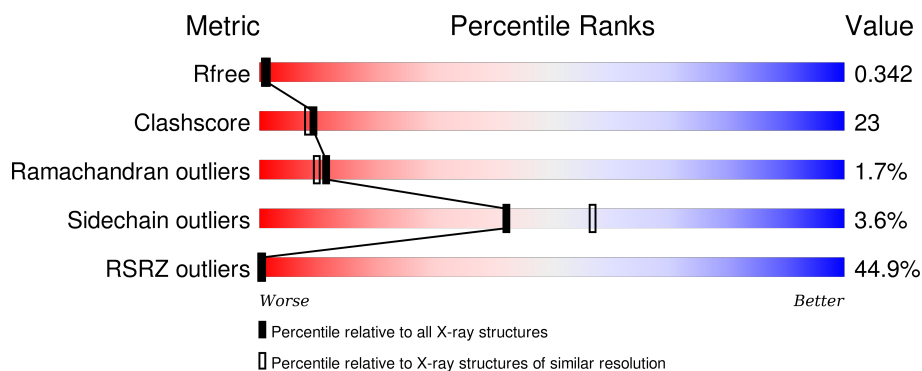
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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  $\geq 3$ , 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>50%</div> <div>57% 34% 5%</div> </div>
1	B	447	<div> <div>30%</div> <div>58% 34% 6%</div> </div>
1	C	447	<div> <div>63%</div> <div>52% 42% . .</div> </div>
1	D	447	<div> <div>29%</div> <div>60% 34% . .</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.

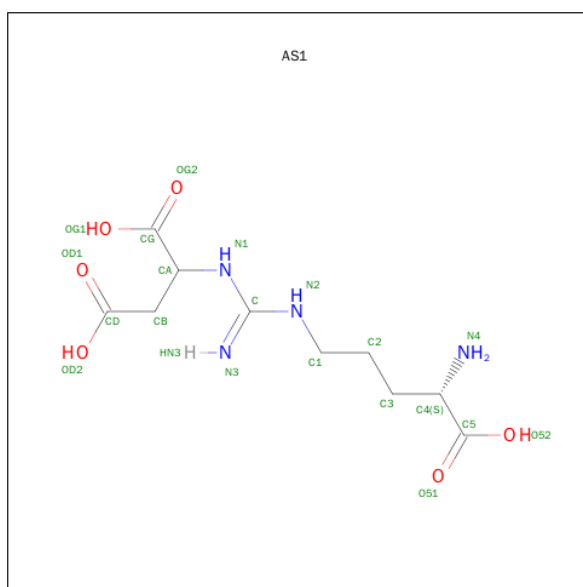
- Molecule 1 is a protein called DELTA 2 CRYSTALLIN.

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: C<sub>10</sub>H<sub>18</sub>N<sub>4</sub>O<sub>6</sub>).



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

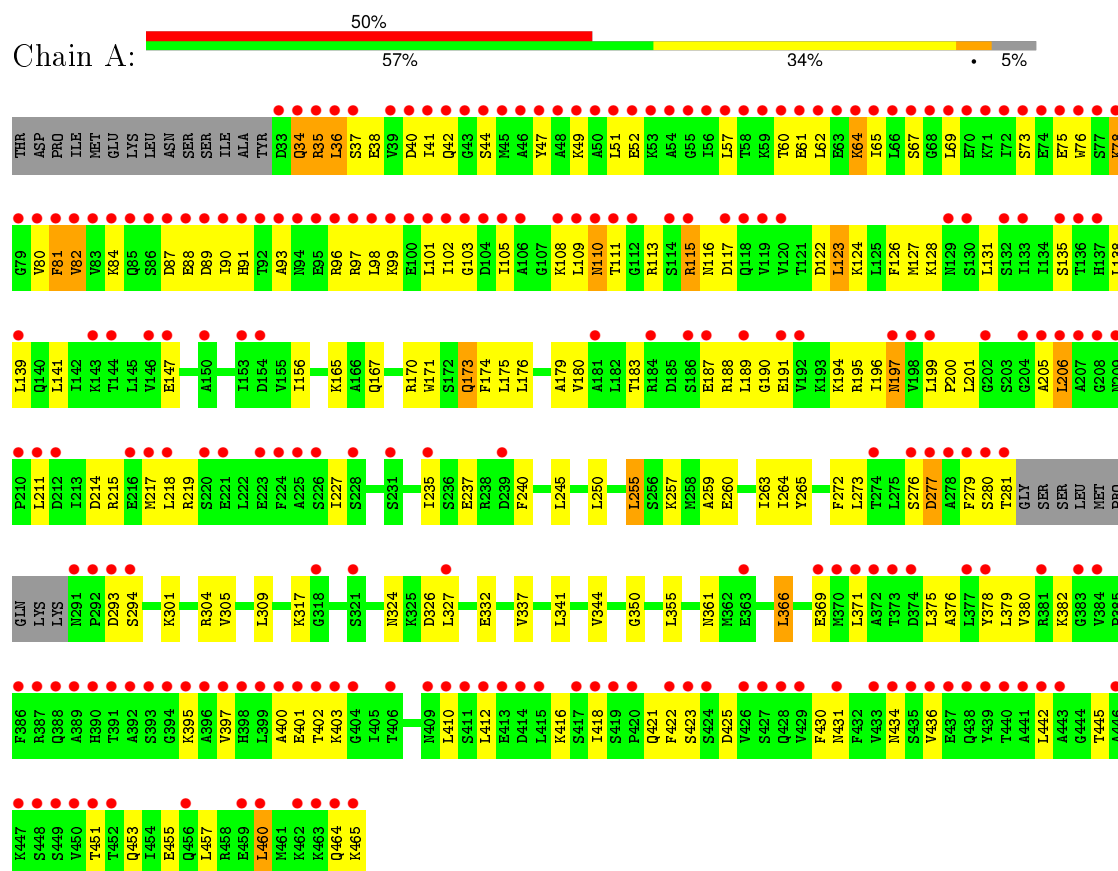
- Molecule 3 is water.

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

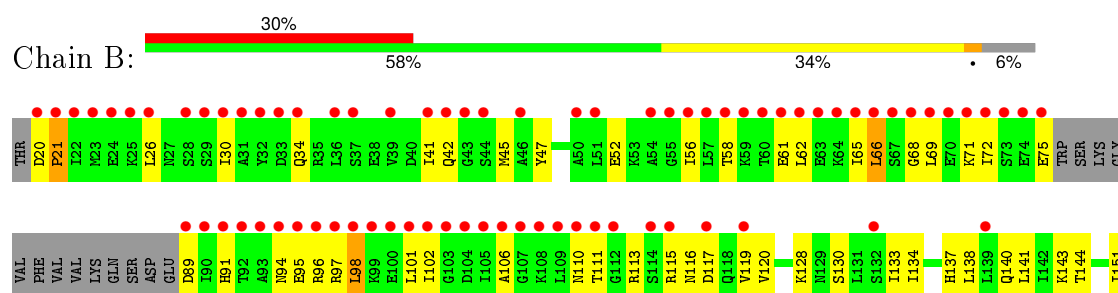
### 3 Residue-property plots

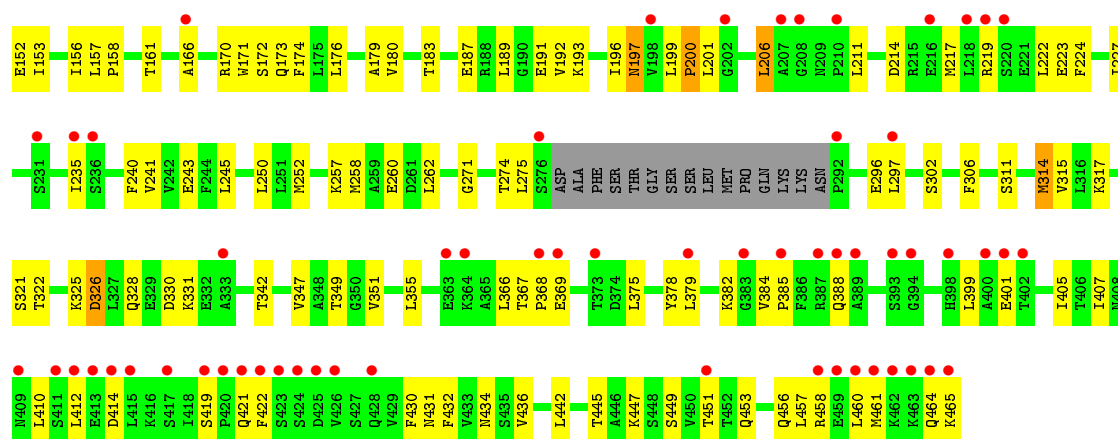
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: DELTA 2 CRYSTALLIN

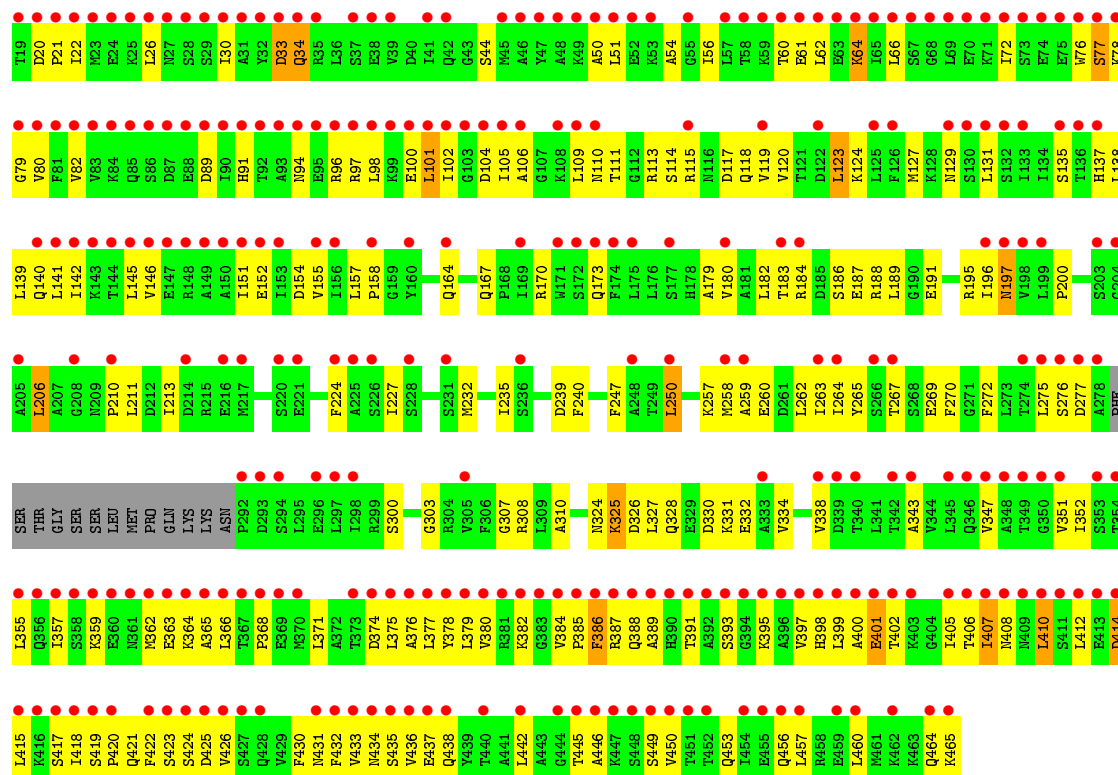


#### • Molecule 1: DELTA 2 CRYSTALLIN

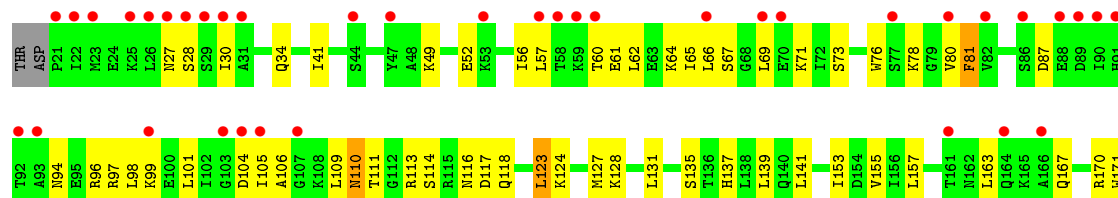


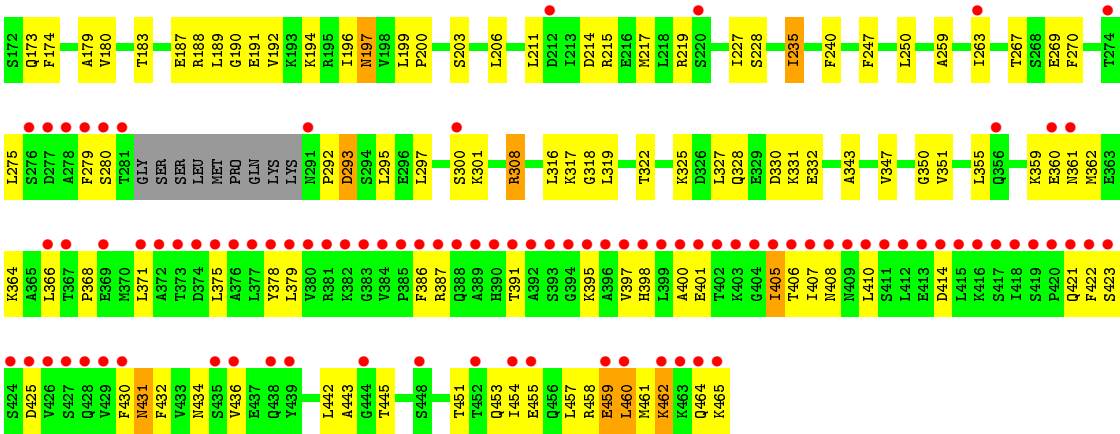


• Molecule 1: DELTA 2 CRYSTALLIN



• 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, $\alpha$ , $\beta$ , $\gamma$	94.58 Å 99.59 Å 107.14 Å 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.27 Å)	Xtriage
Refinement program	CNS 0.3C	Depositor
R, $R_{free}$	0.229 , 0.290 0.342 , 0.342	Depositor DCC
$R_{free}$ test set	6026 reflections (9.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 70.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 65834 reflections	Xtriage
$F_o, F_c$ correlation	0.78	EDS
Total number of atoms	13754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:C:123:LEU:HD12	3:C:514:HOH:O	1.80	0.81
1:B:140:GLN:O	1:B:144:THR:HG23	1.81	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:369:GLU:HG3	3:A:574:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:HG3	3:A:480:HOH:O	1.90	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:436:VAL:HG13	1:B:445:THR:HG23	1.75	0.69
1:B:111:THR:OG1	1:D:386:PHE:HB2	1.93	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:395:LYS:HD2	1:A:418:ILE:HG23	1.75	0.68
1:A:382:LYS:HE2	1:A:421:GLN:O	1.93	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:D:131:LEU:HD22	1:D:189:LEU:HD11	1.75	0.67
1:C:379:LEU:HB3	1:C:384:VAL:HB	1.76	0.67
1:A:87:ASP:HB3	1:A:96:ARG:HH21	1.59	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:378:TYR:HD2	1:A:379:LEU:HD12	1.61	0.66
1:A:190:GLY:O	1:A:194:LYS:HG2	1.96	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:D:400:ALA:HB2	1:D:410:LEU:HD21	1.78	0.65
1:C:22:ILE:N	1:C:22:ILE:HD12	2.11	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
2:D:0:AS1:CB	2:D:0:AS1:CG	2.72	0.64
1:C:435:SER:HA	1:C:438:GLN:HE21	1.61	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:90:ILE:HD12	1:A:93:ALA:HB3	1.79	0.64
1:A:173:GLN:HE22	1:A:453:GLN:HE22	1.46	0.64
1:D:461:MET:O	1:D:462:LYS:CB	2.46	0.63
1:C:431:ASN:HB3	1:C:434:ASN:HD22	1.61	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
2:D:0:AS1:H11	2:D:0:AS1:N2	1.99	0.62
1:C:386:PHE:HE2	1:C:387:ARG:NH2	1.96	0.62
1:B:442:LEU:HB3	3:D:498:HOH:O	1.98	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:C:374:ASP:CG	1:C:438:GLN:HE22	2.03	0.61
1:A:102:ILE:HG13	1:A:103:GLY:N	2.15	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:458:ARG:HA	1:B:461:MET:CE	2.30	0.60
1:B:214:ASP:OD2	1:B:217:MET:HB2	2.01	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:D:49:LYS:HZ3	1:D:66:LEU:HD21	1.65	0.60
1:A:170:ARG:HG3	1:A:436:VAL:HG11	1.82	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: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:D:459:GLU:OE1	1:D:462:LYS:HD3	2.02	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:A:176:LEU:O	1:A:180:VAL:HG23	2.01	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:C:456:GLN:O	1:C:460:LEU:HD23	2.02	0.59
1:B:258:MET:O	1:B:262:LEU:HD13	2.03	0.59
1:A:227:ILE:HD11	1:C:442:LEU:HD13	1.84	0.59
1:D:157:LEU:HA	1:D:366:LEU:HD11	1.84	0.59
1:C:401:GLU:O	1:C:401:GLU:OE1	2.21	0.59
1:C:366:LEU:HD23	1:C:432:PHE:CD2	2.37	0.59
1:C:60:THR:O	1:C:64:LYS:HD3	2.03	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:D:431:ASN:HB3	1:D:434:ASN:ND2	2.18	0.58
1:C:364:LYS:HB2	1:C:364:LYS:NZ	2.18	0.58
1:A:81:PHE:HZ	1:A:93:ALA:O	1.86	0.58
1:D:454:ILE:O	1:D:458:ARG:HB2	2.04	0.58
1:B:199:LEU:HD11	1:B:201:LEU:HB3	1.86	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:D:60:THR:CG2	1:D:64:LYS:HE2	2.34	0.58
1:C:387:ARG:O	1:C:391:THR:HG23	2.04	0.58
1:A:199:LEU:HD21	1:A:218:LEU:HB2	1.86	0.58
1:D:360:GLU:O	1:D:364:LYS:HG3	2.04	0.57
1:D:187:GLU:O	1:D:191:GLU:HG3	2.03	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:C:20:ASP:OD1	1:C:22:ILE:HD13	2.04	0.57
1:B:375:LEU:O	1:B:378:TYR:HB3	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:C:366:LEU:HB3	1:C:432:PHE:CE2	2.39	0.57
1:B:388:GLN:HA	1:B:388:GLN:HE21	1.70	0.57
1:B:385:PRO:HB2	1:B:388:GLN:HG2	1.85	0.57
1:B:196:ILE:HG12	1:B:240:PHE:HB2	1.87	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)
3:B:483:HOH:O	1:D:442:LEU:HB3	2.04	0.56
1:B:187:GLU:O	1:B:191:GLU:HG3	2.06	0.56
1:A:276:SER:O	1:A:277:ASP:CB	2.54	0.56
1:C:408:ASN:HB3	1:C:430:PHE:CD2	2.40	0.56
1:B:115:ARG:HH21	1:B:115:ARG:HG3	1.70	0.56
1:A:451:THR:O	1:A:455:GLU:HG3	2.05	0.56
1:C:412:LEU:HD12	1:C:412:LEU:N	2.20	0.56
1:A:89:ASP:OD2	1:A:91:HIS:HB2	2.05	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:C:399:LEU:O	1:C:402:THR:HB	2.06	0.56
1:C:20:ASP:OD2	1:C:22:ILE:HB	2.06	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: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:368:PRO:O	1:C:407:ILE:HD11	2.05	0.55
1:C:137:HIS:HE1	3:C:475:HOH:O	1.90	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:C:391:THR:O	1:C:395:LYS:HG3	2.07	0.55
1:A:99:LYS:HD2	1:A:99:LYS:H	1.71	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:N	1:A:101:LEU:HD22	2.21	0.54
1:C:164:GLN:HE22	1:D:267:THR:HA	1.73	0.54
1:B:128:LYS:NZ	1:B:197:ASN:ND2	2.55	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:81:PHE:HE2	1:A:93:ALA:HB1	1.72	0.54
1:C:412:LEU:H	1:C:412:LEU:HD12	1.72	0.54
1:A:34:GLN:HG3	1:A:35:ARG:N	2.22	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:C:119:VAL:HG22	3:C:528:HOH:O	2.07	0.54
1:A:259:ALA:O	1:A:263:ILE:HG13	2.07	0.54
1:A:171:TRP:O	1:A:174:PHE:HB3	2.08	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:C:324:ASN:O	1:C:327:LEU:HD23	2.09	0.53
1:B:325:LYS:HE2	1:B:328:GLN:OE1	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:D:292:PRO:HB3	1:D:295:LEU:HD12	1.89	0.53
1:B:41:ILE:HG23	1:B:69:LEU:HB3	1.90	0.53
1:B:378:TYR:HD2	1:B:379:LEU:HD12	1.72	0.53
1:B:117:ASP:HA	1:B:120:VAL:HG12	1.91	0.53
1:D:279:PHE:CZ	1:D:350:GLY:HA3	2.43	0.53
1:B:192:VAL:HG22	1:B:243:GLU:HB3	1.90	0.53
1:A:317:LYS:C	1:A:317:LYS:HD3	2.28	0.53
1:B:71:LYS:HD3	1:B:101:LEU:HD21	1.90	0.53
1:B:137:HIS:CE1	1:B:342:THR:HG23	2.44	0.53
1:C:124:LYS:HE2	1:C:240:PHE:CD2	2.44	0.53
1:C:431:ASN:CB	1:C:434:ASN:HD22	2.21	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: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:D:61:GLU:CG	1:D:105:ILE:HD11	2.39	0.52
1:A:442:LEU:HD13	1:C:227:ILE:HD11	1.91	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:403:LYS:CA	1:A:403:LYS:HE2	2.32	0.52
1:A:375:LEU:O	1:A:378:TYR:HB3	2.10	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:D:214:ASP:OD2	1:D:217:MET:HB2	2.10	0.52
1:B:65:ILE:O	1:B:65:ILE:HG22	2.10	0.52
1:A:355:LEU:O	1:A:355:LEU:HD12	2.09	0.52
1:C:78:LYS:C	1:C:80:VAL:H	2.11	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:78:LYS:HB3	1:A:78:LYS:HZ2	1.75	0.51
1:A:219:ARG:HG2	1:A:219:ARG:NH1	2.25	0.51
1:A:167:GLN:HG2	3:A:568:HOH:O	2.10	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:A:337:VAL:O	1:A:341:LEU:HD13	2.10	0.51
1:D:110:ASN:ND2	1:D:113:ARG:HB3	2.24	0.51
1:B:197:ASN:ND2	1:B:224:PHE:HA	2.25	0.51
1:A:36:LEU:HD22	1:A:122:ASP:HB3	1.93	0.51
1:D:61:GLU:HG2	1:D:105:ILE:CD1	2.41	0.51
1:C:334:VAL:O	1:C:338:VAL:HG23	2.11	0.51
1:D:97:ARG:NE	1:D:101:LEU:HD11	2.26	0.51
1:C:265:TYR:HB3	1:C:272:PHE:HB2	1.93	0.51
1:D:459:GLU:OE1	1:D:459:GLU:HA	2.11	0.51
1:C:355:LEU:O	1:C:355:LEU:HD12	2.11	0.51
1:B:56:ILE:N	1:B:56:ILE:HD12	2.26	0.51
1:D:400:ALA:HB2	1:D:410:LEU:CD2	2.40	0.51
1:B:41:ILE:HD11	1:B:72:ILE:CG2	2.41	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: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:D:259:ALA:O	1:D:263:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:HIS:CD2	1:C:118:GLN:NE2	2.79	0.51
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.76	0.51
1:C:97:ARG:O	1:C:101:LEU:HB2	2.11	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:D:431:ASN:HB3	1:D:434:ASN:HD22	1.74	0.50
1:B:143:LYS:HZ2	1:B:143:LYS:HB2	1.74	0.50
1:A:436:VAL:HG13	1:A:445:THR:HG23	1.93	0.50
1:A:327:LEU:HD12	1:A:327:LEU:N	2.25	0.50
1:A:76:TRP:C	1:A:78:LYS:H	2.15	0.50
1:A:189:LEU:HD23	1:A:189:LEU:C	2.32	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:403:LYS:HA	1:A:403:LYS:CE	2.32	0.50
1:A:97:ARG:HG3	1:A:101:LEU:CD2	2.41	0.50
1:D:423:SER:HB3	1:D:425:ASP:OD2	2.12	0.50
1:C:111:THR:HG22	1:C:211:LEU:HD11	1.94	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:D:431:ASN:HD22	1:D:432:PHE:N	2.09	0.50
1:C:141:LEU:HD22	1:C:182:LEU:HD13	1.93	0.50
1:B:161:THR:HG21	2:D:0:AS1:HB1	1.93	0.49
1:A:81:PHE:CE2	1:A:93:ALA:HB1	2.47	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: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:408:ASN:HB3	1:D:430:PHE:CD2	2.47	0.49
1:C:141:LEU:HD23	1:C:141:LEU:C	2.33	0.49
1:D:375:LEU:O	1:D:378:TYR:HB3	2.12	0.49
1:A:431:ASN:HB3	1:A:434:ASN:ND2	2.19	0.49
1:C:379:LEU:H	1:C:379:LEU:CD1	2.26	0.49
1:A:257:LYS:HB2	3:C:500:HOH:O	2.13	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:D:436:VAL:HG13	1:D:445:THR:CG2	2.36	0.49
1:A:196:ILE:HG12	1:A:240:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:ASP:OD1	1:D:331:LYS:N	2.46	0.49
1:D:355:LEU:C	1:D:355:LEU:HD12	2.33	0.49
1:B:176:LEU:HD22	1:B:457:LEU:CD1	2.43	0.49
1:B:94:ASN:O	1:B:98:LEU:HB2	2.13	0.48
1:A:47:TYR:O	1:A:51:LEU:HB2	2.13	0.48
1:A:327:LEU:H	1:A:327:LEU:CD1	2.26	0.48
1:A:205:ALA:O	1:A:206:LEU:HB3	2.12	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:D:173:GLN:HA	1:D:173:GLN:NE2	2.27	0.48
1:A:135:SER:O	1:A:139:LEU:HD13	2.14	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:A:260:GLU:O	1:A:264:ILE:HG13	2.13	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:C:206:LEU:HD12	1:C:232:MET:HG2	1.96	0.48
1:B:66:LEU:O	1:B:66:LEU:HD23	2.13	0.48
1:C:50:ALA:CB	1:C:213:ILE:HD11	2.44	0.48
1:C:362:MET:O	1:C:366:LEU:CD1	2.61	0.48
1:A:35:ARG:O	1:A:37:SER:N	2.47	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:C:188:ARG:CZ	1:C:250:LEU:HD13	2.45	0.47
1:B:447:LYS:O	1:B:451:THR:HG23	2.14	0.47
1:A:117:ASP:HB3	1:A:235:ILE:HD11	1.97	0.47
1:C:398:HIS:CG	1:C:398:HIS:O	2.68	0.47
1:B:407:ILE:HG13	1:B:430:PHE:CE2	2.50	0.47
1:B:30:ILE:O	1:B:34:GLN:HG3	2.15	0.47
1:C:258:MET:O	1:C:262:LEU:HD13	2.15	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:30:ILE:O	1:D:34:GLN:HG3	2.15	0.47
1:D:61:GLU:CD	1:D:105:ILE:HD11	2.35	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: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: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:D:203:SER:HB2	1:D:235:ILE:HD13	1.98	0.46
1:C:419:SER:C	1:C:421:GLN:H	2.16	0.46
1:C:352:ILE:HG22	1:C:352:ILE:O	2.16	0.46
1:C:82:VAL:O	1:C:82:VAL:HG13	2.15	0.46
1:C:119:VAL:HG22	1:C:331:LYS:HZ2	1.81	0.46
1:B:189:LEU:O	1:B:189:LEU:HD23	2.14	0.46
1:D:366:LEU:HB3	1:D:432:PHE:CD2	2.50	0.46
1:D:131:LEU:HD22	1:D:189:LEU:CD1	2.43	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:B:89:ASP:OD1	1:B:91:HIS:HB2	2.16	0.46
1:B:431:ASN:HB3	1:B:434:ASN:HD22	1.81	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:C:384:VAL:HG12	1:C:389:ALA:HB2	1.97	0.46
1:D:52:GLU:HA	1:D:57:LEU:HB2	1.98	0.46
1:D:124:LYS:NZ	3:D:569:HOH:O	2.48	0.46
3:A:490:HOH:O	1:C:239:ASP:HB3	2.14	0.46
1:D:371:LEU:CD1	1:D:430:PHE:HA	2.46	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: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:N	1:C:379:LEU:CD1	2.79	0.46
1:D:368:PRO:O	1:D:407:ILE:HD11	2.16	0.46
1:C:380:VAL:HA	1:C:384:VAL:O	2.16	0.45
1:A:99:LYS:HD2	1:A:99:LYS:N	2.31	0.45
1:C:76:TRP:C	1:C:78:LYS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:SER:CB	1:D:235:ILE:HD13	2.46	0.45
1:D:123:LEU:HD22	1:D:127:MET:SD	2.56	0.45
1:C:423:SER:C	1:C:425:ASP:H	2.19	0.45
1:A:293:ASP:OD1	1:D:325:LYS:HE3	2.16	0.45
1:D:179:ALA:O	1:D:183:THR:HG23	2.16	0.45
1:A:110:ASN:O	1:A:110:ASN:ND2	2.50	0.45
1:D:173:GLN:HE22	1:D:453:GLN:NE2	2.08	0.45
1:A:176:LEU:HD22	1:A:457:LEU:HD12	1.97	0.45
1:A:47:TYR:CE2	1:A:113:ARG:HB2	2.51	0.45
1:A:61:GLU:CD	1:A:105:ILE:HD11	2.36	0.45
1:A:327:LEU:CD1	1:A:327:LEU:N	2.80	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:B:66:LEU:C	1:B:66:LEU:HD23	2.36	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:297:LEU:C	1:B:297:LEU:HD13	2.37	0.45
1:C:54:ALA:HB3	1:C:56:ILE:HD13	1.97	0.45
1:C:119:VAL:HG21	1:C:331:LYS:HZ1	1.82	0.45
1:B:58:THR:OG1	1:B:61:GLU:HG3	2.17	0.45
1:B:200:PRO:HB3	3:B:493:HOH:O	2.16	0.45
1:D:391:THR:O	1:D:395:LYS:HG3	2.16	0.45
1:D:170:ARG:HB3	3:D:540:HOH:O	2.17	0.45
1:C:91:HIS:CD2	1:C:115:ARG:HD2	2.51	0.45
1:B:275:LEU:HD11	1:B:351:VAL:HG13	1.99	0.45
1:C:140:GLN:HG2	3:C:544:HOH:O	2.15	0.45
1:C:206:LEU:CD1	1:C:232:MET:HG2	2.47	0.45
1:A:165:LYS:HE2	3:B:466:HOH:O	2.17	0.45
1:D:131:LEU:HD11	1:D:196:ILE:HD12	1.99	0.45
1:B:331:LYS:HE3	3:B:570:HOH:O	2.15	0.45
1:A:124:LYS:HE2	3:A:519:HOH:O	2.17	0.45
1:D:188:ARG:O	1:D:192:VAL:HG23	2.16	0.45
1:C:173:GLN:NE2	1:C:453:GLN:HE22	2.09	0.45
1:A:173:GLN:NE2	1:A:173:GLN:HA	2.28	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: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:A:44:SER:HB3	1:A:109:LEU:HD21	1.98	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:H	1:C:412:LEU:CD1	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:431:ASN:HB3	1:B:434:ASN:ND2	2.32	0.44
1:B:153:ILE:HA	1:B:172:SER:OG	2.17	0.44
1:A:80:VAL:O	1:A:81:PHE:CB	2.61	0.44
1:D:332:GLU:HG3	3:D:494:HOH:O	2.17	0.44
1:B:401:GLU:OE2	1:B:401:GLU:C	2.55	0.44
1:D:189:LEU:HD13	1:D:247:PHE:CE2	2.52	0.44
1:C:407:ILE:HG13	1:C:430:PHE:HE2	1.81	0.44
1:A:35:ARG:C	1:A:37:SER:H	2.21	0.44
1:C:78:LYS:C	1:C:80:VAL:N	2.71	0.44
1:B:366:LEU:HB3	1:B:432:PHE:CZ	2.53	0.44
1:D:200:PRO:HA	1:D:228:SER:HG	1.79	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:183:THR:HG21	1:D:457:LEU:HD22	2.00	0.44
1:A:38:GLU:O	1:A:42:GLN:HG3	2.18	0.44
1:D:76:TRP:HE1	1:D:94:ASN:HD21	1.65	0.44
1:C:61:GLU:HG2	1:C:105:ILE:CD1	2.35	0.44
1:D:292:PRO:O	1:D:293:ASP:C	2.56	0.44
1:A:52:GLU:HA	1:A:57:LEU:HB2	1.98	0.44
1:A:245:LEU:CD2	1:A:337:VAL:HG21	2.48	0.44
1:C:89:ASP:OD2	1:C:91:HIS:HB2	2.18	0.44
1:C:433:VAL:O	1:C:437:GLU:HG2	2.17	0.44
1:A:371:LEU:HD13	1:A:430:PHE:HA	1.99	0.44
1:D:275:LEU:HD11	1:D:295:LEU:HG	1.99	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:C:415:LEU:C	1:C:417:SER:H	2.21	0.44
1:C:398:HIS:HA	1:C:401:GLU:HG2	1.99	0.44
1:B:311:SER:HB3	1:C:307:GLY:HA3	1.99	0.44
1:B:384:VAL:CG1	1:B:388:GLN:HB2	2.47	0.44
1:C:406:THR:O	1:C:408:ASN:N	2.51	0.44
1:B:366:LEU:HD23	1:B:432:PHE:CG	2.53	0.44
1:A:108:LYS:HE2	1:C:385:PRO:HG3	1.99	0.44
1:A:355:LEU:C	1:A:355:LEU:HD12	2.37	0.44
1:C:98:LEU:O	1:C:98:LEU:HD13	2.18	0.43
1:C:100:GLU:HG3	1:C:100:GLU:O	2.17	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: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:A:99:LYS:CD	1:A:99:LYS:H	2.31	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:412:LEU:HD11	1:B:422:PHE:O	2.18	0.43
1:C:422:PHE:HD1	1:C:426:VAL:HG21	1.81	0.43
1:B:296:GLU:HB3	1:C:325:LYS:HB3	2.00	0.43
1:C:260:GLU:O	1:C:264:ILE:HG12	2.18	0.43
1:B:20:ASP:CG	1:B:21:PRO:HD2	2.39	0.43
1:B:110:ASN:ND2	1:B:113:ARG:HH21	2.16	0.43
1:D:56:ILE:HG12	1:D:211:LEU:HD13	2.01	0.43
1:B:419:SER:C	1:B:421:GLN:H	2.22	0.43
1:D:180:VAL:HG22	1:D:457:LEU:HD21	2.00	0.43
1:C:30:ILE:O	1:C:34:GLN:HG3	2.18	0.43
1:B:141:LEU:O	1:B:141:LEU:HD23	2.19	0.43
1:A:412:LEU:HG	1:A:416:LYS:HE2	2.01	0.43
1:A:123:LEU:O	1:A:127:MET:HG3	2.19	0.43
1:C:364:LYS:HB2	1:C:364:LYS:HZ2	1.82	0.43
1:A:265:TYR:HB3	1:A:272:PHE:HB2	2.00	0.43
1:A:128:LYS:HE3	1:A:197:ASN:ND2	2.34	0.43
1:A:75:GLU:O	1:A:78:LYS:HB2	2.18	0.43
1:A:464:GLN:O	1:A:465:LYS:HG2	2.19	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:400:ALA:HB2	1:A:410:LEU:HD21	2.01	0.43
1:D:87:ASP:CG	1:D:96:ARG:HH21	2.22	0.42
1:D:379:LEU:HD12	1:D:379:LEU:N	2.34	0.42
1:A:206:LEU:HD21	1:C:167:GLN:HG2	2.01	0.42
1:C:206:LEU:O	1:C:206:LEU:HD12	2.19	0.42
1:B:189:LEU:HD23	1:B:189:LEU:C	2.40	0.42
1:A:279:PHE:CZ	1:A:350:GLY:HA3	2.55	0.42
1:C:62:LEU:O	1:C:66:LEU:HD13	2.19	0.42
1:C:129:ASN:HB3	3:C:546:HOH:O	2.18	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: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:C:376:ALA:O	1:C:380:VAL:HG23	2.18	0.42
1:A:442:LEU:HB3	3:C:491:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:HIS:HD2	3:D:475:HOH:O	2.02	0.42
1:C:158:PRO:HG2	1:C:365:ALA:HB1	2.01	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:35:ARG:HD2	1:A:126:PHE:CE1	2.54	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:B:68:GLY:O	1:B:72:ILE:HG13	2.19	0.42
1:D:114:SER:O	1:D:118:GLN:HB2	2.20	0.42
1:C:97:ARG:HD3	1:C:97:ARG:O	2.20	0.42
1:B:407:ILE:HG13	1:B:430:PHE:HE2	1.85	0.42
1:A:371:LEU:CD1	1:A:430:PHE:HA	2.49	0.42
1:C:325:LYS:HA	1:C:325:LYS:HE3	2.01	0.42
1:A:41:ILE:HG21	1:A:73:SER:OG	2.19	0.42
1:B:96:ARG:NH1	1:B:96:ARG:HG2	2.34	0.42
1:A:115:ARG:HH11	1:A:116:ASN:ND2	2.18	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:C:325:LYS:HE2	1:C:328:GLN:OE1	2.18	0.42
1:B:306:PHE:CE2	1:C:310:ALA:HB1	2.55	0.42
1:C:414:ASP:O	1:C:417:SER:CB	2.67	0.42
1:A:464:GLN:HA	1:A:464:GLN:NE2	2.34	0.42
1:B:42:GLN:HA	1:B:42:GLN:HE21	1.83	0.42
1:B:317:LYS:HD3	1:B:317:LYS:C	2.40	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:C:22:ILE:H	1:C:22:ILE:CD1	2.32	0.42
1:C:113:ARG:HG2	1:C:114:SER:N	2.35	0.42
1:A:326:ASP:HA	1:D:300:SER:HB3	2.01	0.42
1:D:199:LEU:HD23	1:D:227:ILE:HG22	2.02	0.41
1:A:273:LEU:C	1:A:273:LEU:HD12	2.40	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: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:C:151:ILE:HG13	1:C:152:GLU:HG3	2.02	0.41
1:C:449:SER:O	1:C:453:GLN:HG3	2.21	0.41
1:C:269:GLU:HG2	1:D:270:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ILE:HG13	1:D:430:PHE:CE2	2.53	0.41
1:B:347:VAL:O	1:B:351:VAL:HG23	2.21	0.41
1:D:460:LEU:HD22	1:D:460:LEU:HA	1.91	0.41
1:A:147:GLU:OE1	1:A:147:GLU:HA	2.20	0.41
1:D:292:PRO:O	1:D:295:LEU:N	2.50	0.41
1:D:215:ARG:NH2	1:D:228:SER:HB2	2.27	0.41
1:D:98:LEU:HB3	1:D:106:ALA:CB	2.51	0.41
1:B:257:LYS:HB2	3:D:572:HOH:O	2.20	0.41
1:A:87:ASP:CG	1:A:96:ARG:HH21	2.23	0.41
1:A:49:LYS:HB3	1:A:217:MET:CE	2.50	0.41
1:A:171:TRP:NE1	1:A:175:LEU:HD11	2.36	0.41
1:B:252:MET:HB3	1:B:302:SER:HA	2.03	0.41
1:A:156:ILE:HG22	1:A:366:LEU:HD21	2.02	0.41
1:B:321:SER:HB2	1:B:322:THR:HA	2.03	0.41
1:B:166:ALA:HB1	2:D:0:AS1:OD1	2.21	0.41
1:C:414:ASP:HB2	1:C:415:LEU:H	1.77	0.41
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.35	0.41
1:C:263:ILE:HG22	1:D:163:LEU:HD12	2.03	0.41
1:D:343:ALA:O	1:D:347:VAL:HG23	2.21	0.41
1:B:47:TYR:CE2	1:B:113:ARG:HB2	2.55	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: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:D:171:TRP:O	1:D:174:PHE:HB3	2.21	0.41
1:B:94:ASN:C	1:B:96:ARG:H	2.24	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: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: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:C:366:LEU:N	1:C:366:LEU:HD12	2.37	0.40
1:B:388:GLN:HA	1:B:388:GLN:NE2	2.36	0.40
1:A:141:LEU:C	1:A:141:LEU:CD2	2.90	0.40
1:B:421:GLN:HA	1:B:421:GLN:HE21	1.84	0.40
1:B:156:ILE:HG22	1:B:366:LEU:HD21	2.03	0.40
1:A:279:PHE:HB3	1:A:294:SER:CB	2.51	0.40
1:D:451:THR:O	1:D:455:GLU:HG3	2.22	0.40
1:A:361:ASN:N	1:A:361:ASN:HD22	2.19	0.40
1:D:113:ARG:HG2	1:D:114:SER:N	2.37	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:B:141:LEU:C	1:B:141:LEU:HD23	2.42	0.40
1:C:436:VAL:HG13	1:C:445:THR:HG23	2.03	0.40
1:B:130:SER:O	1:B:134:ILE:HG13	2.22	0.40
1:C:123:LEU:O	1:C:127:MET:HG3	2.22	0.40
1:A:379:LEU:HD11	1:A:422:PHE:CZ	2.56	0.40
1:C:114:SER:O	1:C:118:GLN:HB2	2.22	0.40
1:B:157:LEU:HB2	1:B:158:PRO:CD	2.51	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%)	9	7
1	B	412/447 (92%)	382 (93%)	27 (7%)	3 (1%)	26	31
1	C	430/447 (96%)	389 (90%)	30 (7%)	11 (3%)	7	4
1	D	432/447 (97%)	397 (92%)	29 (7%)	6 (1%)	14	13
All	All	1694/1788 (95%)	1547 (91%)	118 (7%)	29 (2%)	11	10

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%)	43	58
1	B	364/392 (93%)	355 (98%)	9 (2%)	55	73
1	C	377/392 (96%)	360 (96%)	17 (4%)	34	46
1	D	379/392 (97%)	365 (96%)	14 (4%)	41	55
All	All	1489/1568 (95%)	1436 (96%)	53 (4%)	42	57

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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	-	10,19,19	7.16	5 (50%)	9,24,24	10.70	8 (88%)

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	-5.95	1.38	1.46
2	D	0	AS1	C-N1	2.02	1.39	1.34
2	D	0	AS1	C-N3	5.23	1.42	1.29
2	D	0	AS1	C1-N2	10.12	1.69	1.46
2	D	0	AS1	CB-CA	18.41	1.79	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	N1-C-N3	-3.50	114.55	120.46
2	D	0	AS1	C3-C4-N4	2.71	118.21	110.52
2	D	0	AS1	CB-CA-N1	3.32	118.08	108.23
2	D	0	AS1	CA-N1-C	4.54	130.96	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	0	AS1	N2-C-N1	8.56	136.45	117.02
2	D	0	AS1	C1-N2-C	14.41	149.61	123.43
2	D	0	AS1	C3-C2-C1	17.10	164.84	112.13
2	D	0	AS1	C2-C1-N2	20.07	170.98	112.19

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	424/447 (94%)	2.37	222 (52%) 0 0	17, 37, 85, 95	0
1	B	418/447 (93%)	1.63	135 (32%) 1 1	14, 35, 76, 98	0
1	C	434/447 (97%)	2.99	280 (64%) 0 0	18, 42, 95, 100	0
1	D	436/447 (97%)	1.63	131 (30%) 1 1	17, 36, 87, 99	0
All	All	1712/1788 (95%)	2.16	768 (44%) 0 0	14, 38, 87, 100	0

All (768) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	278	ALA	14.8
1	D	404	GLY	13.4
1	A	82	VAL	12.2
1	C	398	HIS	12.0
1	C	80	VAL	10.9
1	A	383	GLY	9.9
1	C	19	THR	9.8
1	C	394	GLY	9.1
1	C	413	GLU	9.0
1	A	402	THR	8.9
1	C	400	ALA	8.9
1	B	21	PRO	8.6
1	B	292	PRO	8.6
1	D	402	THR	8.5
1	C	415	LEU	8.3
1	D	418	ILE	8.0
1	C	77	SER	8.0
1	A	386	PHE	8.0
1	C	387	ARG	8.0
1	A	83	VAL	7.9
1	C	67	SER	7.8

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Mol	Chain	Res	Type	RSRZ
1	C	424	SER	7.8
1	C	393	SER	7.7
1	C	414	ASP	7.5
1	D	29	SER	7.5
1	A	34	GLN	7.4
1	C	25	LYS	7.3
1	C	60	THR	7.3
1	A	85	GLN	7.3
1	D	414	ASP	7.2
1	D	396	ALA	6.9
1	B	29	SER	6.9
1	A	400	ALA	6.9
1	C	93	ALA	6.8
1	C	151	ILE	6.8
1	C	434	ASN	6.7
1	C	83	VAL	6.6
1	C	220	SER	6.6
1	C	412	LEU	6.6
1	B	402	THR	6.6
1	C	73	SER	6.5
1	C	391	THR	6.5
1	A	465	LYS	6.4
1	D	392	ALA	6.4
1	D	281	THR	6.4
1	A	84	LYS	6.4
1	C	401	GLU	6.4
1	C	402	THR	6.3
1	D	391	THR	6.3
1	C	399	LEU	6.3
1	C	31	ALA	6.3
1	C	396	ALA	6.3
1	C	427	SER	6.3
1	D	411	SER	6.3
1	C	423	SER	6.2
1	C	464	GLN	6.2
1	D	397	VAL	6.2
1	C	65	ILE	6.2
1	C	101	LEU	6.2
1	D	389	ALA	6.2
1	A	391	THR	6.1
1	A	96	ARG	6.1
1	A	110	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	411	SER	6.0
1	C	102	ILE	6.0
1	D	417	SER	6.0
1	C	422	PHE	6.0
1	D	419	SER	5.9
1	C	99	LYS	5.9
1	D	401	GLU	5.9
1	B	24	GLU	5.8
1	C	57	LEU	5.8
1	C	389	ALA	5.8
1	C	425	ASP	5.7
1	C	64	LYS	5.7
1	A	460	LEU	5.6
1	D	409	ASN	5.6
1	D	380	VAL	5.6
1	C	109	LEU	5.6
1	C	448	SER	5.6
1	C	90	ILE	5.6
1	D	405	ILE	5.6
1	A	406	THR	5.6
1	A	100	GLU	5.6
1	C	68	GLY	5.6
1	A	98	LEU	5.6
1	B	411	SER	5.5
1	A	398	HIS	5.5
1	C	376	ALA	5.5
1	C	133	ILE	5.5
1	A	35	ARG	5.5
1	D	388	GLN	5.5
1	C	408	ASN	5.4
1	A	401	GLU	5.4
1	C	410	LEU	5.4
1	A	449	SER	5.4
1	A	86	SER	5.3
1	B	401	GLU	5.3
1	D	277	ASP	5.3
1	C	26	LEU	5.3
1	C	105	ILE	5.3
1	D	420	PRO	5.3
1	A	37	SER	5.3
1	C	46	ALA	5.2
1	B	98	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	403	LYS	5.2
1	C	78	LYS	5.2
1	D	398	HIS	5.1
1	C	292	PRO	5.1
1	C	76	TRP	5.1
1	A	57	LEU	5.1
1	A	415	LEU	5.1
1	D	421	GLN	5.1
1	A	373	THR	5.0
1	B	58	THR	5.0
1	C	377	LEU	5.0
1	B	400	ALA	5.0
1	B	25	LYS	5.0
1	B	26	LEU	5.0
1	C	71	LYS	5.0
1	A	69	LEU	5.0
1	D	26	LEU	5.0
1	C	358	SER	4.9
1	A	464	GLN	4.9
1	C	418	ILE	4.9
1	C	452	THR	4.9
1	A	112	GLY	4.9
1	C	368	PRO	4.9
1	C	386	PHE	4.9
1	C	342	THR	4.9
1	A	66	LEU	4.9
1	C	274	THR	4.9
1	C	451	THR	4.9
1	C	426	VAL	4.9
1	B	71	LYS	4.9
1	C	98	LEU	4.9
1	A	41	ILE	4.9
1	B	92	THR	4.8
1	C	52	GLU	4.8
1	D	378	TYR	4.8
1	C	21	PRO	4.8
1	C	74	GLU	4.8
1	D	408	ASN	4.8
1	D	390	HIS	4.8
1	B	23	MET	4.8
1	C	58	THR	4.8
1	C	72	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	411	SER	4.8
1	B	103	GLY	4.7
1	A	389	ALA	4.7
1	B	93	ALA	4.7
1	A	436	VAL	4.7
1	D	413	GLU	4.7
1	A	60	THR	4.7
1	B	68	GLY	4.7
1	C	82	VAL	4.7
1	A	81	PHE	4.7
1	C	366	LEU	4.7
1	C	132	SER	4.7
1	A	56	ILE	4.7
1	B	104	ASP	4.7
1	D	25	LYS	4.7
1	C	30	ILE	4.6
1	D	427	SER	4.6
1	D	278	ALA	4.6
1	C	357	ILE	4.6
1	D	406	THR	4.6
1	A	80	VAL	4.6
1	D	394	GLY	4.6
1	A	33	ASP	4.6
1	A	277	ASP	4.6
1	A	374	ASP	4.6
1	C	41	ILE	4.6
1	A	74	GLU	4.6
1	D	425	ASP	4.6
1	C	62	LEU	4.5
1	C	388	GLN	4.5
1	A	150	ALA	4.5
1	A	397	VAL	4.5
1	B	464	GLN	4.5
1	C	86	SER	4.5
1	C	276	SER	4.5
1	A	63	GLU	4.5
1	C	390	HIS	4.5
1	B	101	LEU	4.5
1	D	379	LEU	4.5
1	D	426	VAL	4.5
1	D	439	TYR	4.5
1	A	105	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	338	VAL	4.5
1	C	409	ASN	4.5
1	C	88	GLU	4.4
1	C	89	ASP	4.4
1	B	75	GLU	4.4
1	D	430	PHE	4.4
1	C	293	ASP	4.4
1	C	361	ASN	4.4
1	C	433	VAL	4.4
1	D	399	LEU	4.3
1	A	92	THR	4.3
1	A	220	SER	4.3
1	B	105	ILE	4.3
1	C	373	THR	4.3
1	C	369	GLU	4.3
1	B	51	LEU	4.3
1	B	28	SER	4.3
1	C	449	SER	4.3
1	D	386	PHE	4.3
1	D	428	GLN	4.3
1	A	65	ILE	4.3
1	D	30	ILE	4.3
1	C	395	LYS	4.2
1	A	97	ARG	4.2
1	C	104	ASP	4.2
1	B	100	GLU	4.2
1	A	73	SER	4.2
1	A	448	SER	4.2
1	B	54	ALA	4.2
1	C	37	SER	4.2
1	C	84	LYS	4.2
1	C	363	GLU	4.2
1	C	45	MET	4.2
1	C	362	MET	4.2
1	A	387	ARG	4.2
1	A	417	SER	4.2
1	A	414	ASP	4.2
1	A	462	LYS	4.2
1	D	372	ALA	4.2
1	C	96	ARG	4.2
1	B	67	SER	4.2
1	C	103	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	ASP	4.2
1	D	279	PHE	4.1
1	B	89	ASP	4.1
1	C	462	LYS	4.1
1	D	465	LYS	4.1
1	A	392	ALA	4.1
1	A	39	VAL	4.1
1	B	102	ILE	4.1
1	A	54	ALA	4.1
1	D	373	THR	4.1
1	C	59	LYS	4.1
1	B	70	GLU	4.1
1	C	95	GLU	4.1
1	C	378	TYR	4.1
1	A	72	ILE	4.1
1	B	419	SER	4.1
1	D	104	ASP	4.0
1	A	103	GLY	4.0
1	A	58	THR	4.0
1	D	416	LYS	4.0
1	A	217	MET	4.0
1	A	292	PRO	4.0
1	B	74	GLU	4.0
1	B	22	ILE	4.0
1	B	65	ILE	4.0
1	C	48	ALA	4.0
1	C	354	THR	4.0
1	B	91	HIS	4.0
1	A	62	LEU	4.0
1	C	66	LEU	4.0
1	D	375	LEU	4.0
1	C	97	ARG	3.9
1	C	403	LYS	3.9
1	A	95	GLU	3.9
1	A	369	GLU	3.9
1	A	423	SER	3.9
1	C	364	LYS	3.9
1	A	434	ASN	3.9
1	A	111	THR	3.9
1	A	280	SER	3.9
1	C	28	SER	3.9
1	B	66	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	136	THR	3.9
1	A	281	THR	3.9
1	B	111	THR	3.9
1	C	22	ILE	3.9
1	C	454	ILE	3.9
1	C	450	VAL	3.9
1	C	75	GLU	3.9
1	C	225	ALA	3.9
1	A	186	SER	3.8
1	B	56	ILE	3.8
1	C	431	ASN	3.8
1	A	226	SER	3.8
1	B	90	ILE	3.8
1	B	276	SER	3.8
1	C	153	ILE	3.8
1	A	378	TYR	3.8
1	A	91	HIS	3.8
1	A	212	ASP	3.8
1	C	455	GLU	3.8
1	C	217	MET	3.8
1	A	102	ILE	3.8
1	B	63	GLU	3.8
1	A	68	GLY	3.8
1	A	404	GLY	3.8
1	B	20	ASP	3.8
1	A	77	SER	3.7
1	B	110	ASN	3.7
1	D	384	VAL	3.7
1	A	276	SER	3.7
1	B	46	ALA	3.7
1	A	90	ILE	3.7
1	D	369	GLU	3.7
1	D	424	SER	3.7
1	A	278	ALA	3.7
1	A	429	VAL	3.7
1	A	93	ALA	3.7
1	A	46	ALA	3.7
1	C	392	ALA	3.7
1	C	384	VAL	3.7
1	D	387	ARG	3.7
1	C	296	GLU	3.6
1	C	465	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	353	SER	3.6
1	C	457	LEU	3.6
1	D	393	SER	3.6
1	D	455	GLU	3.6
1	B	60	THR	3.6
1	C	150	ALA	3.6
1	B	72	ILE	3.6
1	C	397	VAL	3.6
1	A	211	LEU	3.6
1	D	460	LEU	3.6
1	A	210	PRO	3.6
1	B	412	LEU	3.6
1	A	132	SER	3.6
1	A	224	PHE	3.6
1	B	30	ILE	3.5
1	A	413	GLU	3.5
1	C	459	GLU	3.5
1	C	50	ALA	3.5
1	D	400	ALA	3.5
1	B	62	LEU	3.5
1	C	92	THR	3.5
1	D	21	PRO	3.5
1	C	380	VAL	3.5
1	A	50	ALA	3.5
1	A	71	LYS	3.5
1	B	465	LYS	3.5
1	D	412	LEU	3.5
1	C	183	THR	3.5
1	A	394	GLY	3.5
1	B	394	GLY	3.5
1	C	266	SER	3.5
1	B	115	ARG	3.5
1	C	136	THR	3.5
1	A	388	GLN	3.5
1	C	277	ASP	3.5
1	D	69	LEU	3.5
1	C	420	PRO	3.5
1	D	291	ASN	3.5
1	A	225	ALA	3.5
1	A	403	LYS	3.4
1	A	36	LEU	3.4
1	D	107	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	398	HIS	3.4
1	C	416	LYS	3.4
1	B	106	ALA	3.4
1	B	235	ILE	3.4
1	B	95	GLU	3.4
1	D	395	LYS	3.4
1	C	140	GLN	3.4
1	C	360	GLU	3.4
1	B	69	LEU	3.4
1	C	175	LEU	3.4
1	C	379	LEU	3.4
1	D	381	ARG	3.4
1	C	456	GLN	3.4
1	A	442	LEU	3.4
1	A	452	THR	3.4
1	D	464	GLN	3.4
1	B	31	ALA	3.4
1	B	94	ASN	3.4
1	C	20	ASP	3.4
1	B	216	GLU	3.4
1	C	155	VAL	3.4
1	D	410	LEU	3.4
1	A	67	SER	3.4
1	D	103	GLY	3.4
1	A	216	GLU	3.4
1	D	436	VAL	3.3
1	A	443	ALA	3.3
1	C	130	SER	3.3
1	D	220	SER	3.3
1	D	91	HIS	3.3
1	B	369	GLU	3.3
1	B	99	LYS	3.3
1	A	451	THR	3.3
1	B	109	LEU	3.3
1	B	421	GLN	3.3
1	A	372	ALA	3.3
1	B	61	GLU	3.3
1	C	137	HIS	3.3
1	C	405	ILE	3.3
1	C	87	ASP	3.3
1	C	110	ASN	3.3
1	A	88	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	460	LEU	3.3
1	A	115	ARG	3.3
1	A	371	LEU	3.3
1	A	450	VAL	3.3
1	C	106	ALA	3.3
1	B	44	SER	3.3
1	C	351	VAL	3.3
1	C	436	VAL	3.3
1	D	463	LYS	3.2
1	C	144	THR	3.2
1	C	70	GLU	3.2
1	C	69	LEU	3.2
1	C	355	LEU	3.2
1	D	462	LYS	3.2
1	B	32	TYR	3.2
1	A	410	LEU	3.2
1	C	348	ALA	3.2
1	A	427	SER	3.2
1	C	359	LYS	3.2
1	C	367	THR	3.2
1	C	94	ASN	3.2
1	B	96	ARG	3.2
1	A	221	GLU	3.2
1	B	57	LEU	3.2
1	C	85	GLN	3.2
1	B	424	SER	3.2
1	C	91	HIS	3.2
1	B	37	SER	3.2
1	A	279	PHE	3.2
1	B	413	GLU	3.2
1	B	385	PRO	3.2
1	C	23	MET	3.2
1	C	435	SER	3.2
1	D	407	ILE	3.1
1	A	446	ALA	3.1
1	A	94	ASN	3.1
1	A	363	GLU	3.1
1	A	106	ALA	3.1
1	B	236	SER	3.1
1	B	423	SER	3.1
1	B	107	GLY	3.1
1	C	81	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	220	SER	3.1
1	D	448	SER	3.1
1	B	425	ASP	3.1
1	C	119	VAL	3.1
1	B	373	THR	3.1
1	A	133	ILE	3.1
1	A	139	LEU	3.1
1	B	462	LYS	3.1
1	B	426	VAL	3.1
1	C	428	GLN	3.1
1	B	41	ILE	3.1
1	C	214	ASP	3.1
1	C	438	GLN	3.1
1	D	429	VAL	3.1
1	A	59	LYS	3.1
1	C	29	SER	3.1
1	D	89	ASP	3.1
1	C	42	GLN	3.0
1	A	53	LYS	3.0
1	C	263	ILE	3.0
1	C	381	ARG	3.0
1	A	192	VAL	3.0
1	D	86	SER	3.0
1	B	389	ALA	3.0
1	C	27	ASN	3.0
1	A	318	GLY	3.0
1	A	130	SER	3.0
1	C	177	SER	3.0
1	A	137	HIS	3.0
1	C	259	ALA	3.0
1	A	235	ILE	3.0
1	C	250	LEU	3.0
1	C	226	SER	3.0
1	C	184	ARG	3.0
1	A	64	LYS	3.0
1	B	34	GLN	3.0
1	A	419	SER	3.0
1	C	340	THR	3.0
1	D	367	THR	3.0
1	D	90	ILE	3.0
1	D	92	THR	3.0
1	D	382	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	149	ALA	2.9
1	C	349	THR	2.9
1	C	258	MET	2.9
1	D	376	ALA	2.9
1	A	129	ASN	2.9
1	C	204	GLY	2.9
1	D	59	LYS	2.9
1	A	181	ALA	2.9
1	A	396	ALA	2.9
1	D	276	SER	2.9
1	D	356	GLN	2.9
1	D	366	LEU	2.9
1	A	205	ALA	2.9
1	C	343	ALA	2.9
1	D	280	SER	2.9
1	D	212	ASP	2.9
1	C	53	LYS	2.9
1	A	208	GLY	2.9
1	B	210	PRO	2.9
1	B	451	THR	2.9
1	D	415	LEU	2.9
1	A	55	GLY	2.8
1	B	108	LYS	2.8
1	B	415	LEU	2.8
1	C	275	LEU	2.8
1	A	381	ARG	2.8
1	C	365	ALA	2.8
1	A	99	LYS	2.8
1	B	420	PRO	2.8
1	A	109	LEU	2.8
1	A	231	SER	2.8
1	D	60	THR	2.8
1	C	24	GLU	2.8
1	C	297	LEU	2.8
1	D	28	SER	2.8
1	A	420	PRO	2.8
1	C	231	SER	2.8
1	A	447	LYS	2.8
1	A	441	ALA	2.8
1	A	293	ASP	2.7
1	B	64	LYS	2.7
1	A	412	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	418	ILE	2.7
1	C	196	ILE	2.7
1	D	161	THR	2.7
1	D	423	SER	2.7
1	C	339	ASP	2.7
1	A	209	ASN	2.7
1	A	433	VAL	2.7
1	D	80	VAL	2.7
1	A	147	GLU	2.7
1	D	377	LEU	2.7
1	A	78	LYS	2.7
1	B	387	ARG	2.7
1	A	104	ASP	2.7
1	A	228	SER	2.7
1	B	383	GLY	2.7
1	C	385	PRO	2.7
1	A	87	ASP	2.7
1	B	393	SER	2.7
1	C	135	SER	2.7
1	C	129	ASN	2.7
1	C	445	THR	2.7
1	D	58	THR	2.7
1	B	463	LYS	2.7
1	D	438	GLN	2.7
1	A	101	LEU	2.7
1	A	44	SER	2.7
1	B	42	GLN	2.7
1	C	346	GLN	2.7
1	C	148	ARG	2.7
1	C	447	LYS	2.7
1	A	189	LEU	2.6
1	A	399	LEU	2.6
1	B	460	LEU	2.6
1	A	79	GLY	2.6
1	A	117	ASP	2.6
1	A	424	SER	2.6
1	D	82	VAL	2.6
1	D	164	GLN	2.6
1	A	184	ARG	2.6
1	C	147	GLU	2.6
1	C	142	ILE	2.6
1	D	166	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	422	PHE	2.6
1	D	53	LYS	2.6
1	B	39	VAL	2.6
1	A	206	LEU	2.6
1	C	382	LYS	2.6
1	A	61	GLU	2.6
1	C	34	GLN	2.6
1	A	135	SER	2.6
1	A	426	VAL	2.6
1	C	145	LEU	2.6
1	C	146	VAL	2.6
1	C	180	VAL	2.6
1	A	52	GLU	2.6
1	A	223	GLU	2.6
1	C	432	PHE	2.6
1	A	108	LYS	2.6
1	D	383	GLY	2.6
1	A	70	GLU	2.6
1	A	45	MET	2.6
1	B	417	SER	2.6
1	D	77	SER	2.6
1	A	390	HIS	2.6
1	B	97	ARG	2.6
1	C	197	ASN	2.6
1	D	93	ALA	2.5
1	A	437	GLU	2.5
1	C	39	VAL	2.5
1	C	198	VAL	2.5
1	A	153	ILE	2.5
1	B	33	ASP	2.5
1	C	33	ASP	2.5
1	B	55	GLY	2.5
1	A	47	TYR	2.5
1	D	459	GLU	2.5
1	B	218	LEU	2.5
1	A	459	GLU	2.5
1	C	100	GLU	2.5
1	C	374	ASP	2.5
1	D	23	MET	2.5
1	D	57	LEU	2.5
1	A	114	SER	2.5
1	C	172	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	38	GLU	2.5
1	D	385	PRO	2.5
1	A	40	ASP	2.5
1	A	154	ASP	2.5
1	B	414	ASP	2.5
1	A	51	LEU	2.5
1	A	327	LEU	2.5
1	C	125	LEU	2.5
1	C	370	MET	2.5
1	A	291	ASN	2.5
1	A	48	ALA	2.5
1	B	50	ALA	2.5
1	D	300	SER	2.5
1	A	377	LEU	2.5
1	A	409	ASN	2.5
1	B	409	ASN	2.5
1	B	73	SER	2.4
1	A	428	GLN	2.4
1	B	363	GLU	2.4
1	D	88	GLU	2.4
1	A	119	VAL	2.4
1	C	347	VAL	2.4
1	B	112	GLY	2.4
1	C	294	SER	2.4
1	C	419	SER	2.4
1	A	144	THR	2.4
1	A	431	ASN	2.4
1	D	360	GLU	2.4
1	A	118	GLN	2.4
1	B	139	LEU	2.4
1	C	141	LEU	2.4
1	D	22	ILE	2.4
1	A	187	GLU	2.4
1	A	198	VAL	2.4
1	D	105	ILE	2.4
1	C	383	GLY	2.4
1	A	143	LYS	2.4
1	C	440	THR	2.4
1	C	210	PRO	2.4
1	C	63	GLU	2.4
1	C	442	LEU	2.4
1	B	43	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	208	GLY	2.4
1	C	264	ILE	2.4
1	C	171	TRP	2.4
1	B	368	PRO	2.4
1	C	375	LEU	2.4
1	B	198	VAL	2.4
1	B	231	SER	2.4
1	B	459	GLU	2.4
1	B	166	ALA	2.4
1	D	274	THR	2.4
1	C	122	ASP	2.3
1	C	108	LYS	2.3
1	C	248	ALA	2.3
1	A	76	TRP	2.3
1	C	437	GLU	2.3
1	B	208	GLY	2.3
1	C	236	SER	2.3
1	D	99	LYS	2.3
1	A	120	VAL	2.3
1	C	156	ILE	2.3
1	D	27	ASN	2.3
1	B	59	LYS	2.3
1	B	297	LEU	2.3
1	C	345	LEU	2.3
1	D	371	LEU	2.3
1	A	456	GLN	2.3
1	B	428	GLN	2.3
1	A	191	GLU	2.3
1	A	439	TYR	2.3
1	C	160	TYR	2.3
1	C	169	ILE	2.3
1	C	267	THR	2.3
1	C	406	THR	2.3
1	D	361	ASN	2.3
1	A	204	GLY	2.3
1	C	115	ARG	2.3
1	B	422	PHE	2.3
1	D	422	PHE	2.3
1	C	305	VAL	2.3
1	C	203	SER	2.3
1	D	374	ASP	2.3
1	C	216	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	2.2
1	A	440	THR	2.2
1	A	294	SER	2.2
1	D	435	SER	2.2
1	A	42	GLN	2.2
1	A	393	SER	2.2
1	B	132	SER	2.2
1	C	417	SER	2.2
1	B	379	LEU	2.2
1	B	461	MET	2.2
1	A	239	ASP	2.2
1	B	219	ARG	2.2
1	C	407	ILE	2.2
1	A	49	LYS	2.2
1	C	32	TYR	2.2
1	C	174	PHE	2.2
1	A	218	LEU	2.2
1	B	117	ASP	2.2
1	D	452	THR	2.2
1	A	438	GLN	2.2
1	C	350	GLY	2.2
1	C	49	LYS	2.2
1	A	197	ASN	2.2
1	C	205	ALA	2.2
1	B	119	VAL	2.2
1	A	202	GLY	2.2
1	C	224	PHE	2.2
1	C	173	GLN	2.2
1	C	164	GLN	2.1
1	C	221	GLU	2.1
1	D	47	TYR	2.1
1	A	395	LYS	2.1
1	B	202	GLY	2.1
1	B	388	GLN	2.1
1	C	61	GLU	2.1
1	A	384	VAL	2.1
1	A	435	SER	2.1
1	A	75	GLU	2.1
1	C	444	GLY	2.1
1	D	454	ILE	2.1
1	B	364	LYS	2.1
1	C	158	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	458	ARG	2.1
1	C	47	TYR	2.1
1	A	370	MET	2.1
1	C	51	LEU	2.1
1	C	356	GLN	2.1
1	D	31	ALA	2.1
1	C	298	ILE	2.1
1	A	199	LEU	2.1
1	C	55	GLY	2.1
1	C	143	LYS	2.1
1	C	228	SER	2.1
1	D	263	ILE	2.1
1	A	274	THR	2.1
1	C	126	PHE	2.1
1	C	333	ALA	2.1
1	C	35	ARG	2.0
1	C	131	LEU	2.0
1	C	199	LEU	2.0
1	D	66	LEU	2.0
1	C	446	ALA	2.0
1	A	321	SER	2.0
1	D	44	SER	2.0
1	C	152	GLU	2.0
1	D	70	GLU	2.0
1	B	207	ALA	2.0
1	C	79	GLY	2.0
1	D	444	GLY	2.0
1	A	463	LYS	2.0
1	A	146	VAL	2.0
1	A	207	ALA	2.0
1	B	36	LEU	2.0
1	B	333	ALA	2.0
1	B	114	SER	2.0

## 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 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	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.