



# Full wwPDB X-ray Structure Validation Report i

Aug 21, 2020 – 07:58 AM BST

PDB ID : 6PBZ  
Title : Crystal structure of Escherichia coli GppA  
Authors : Song, H.; Shaw, G.X.; Wang, C.; Ji, X.  
Deposited on : 2019-06-15  
Resolution : 2.48 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

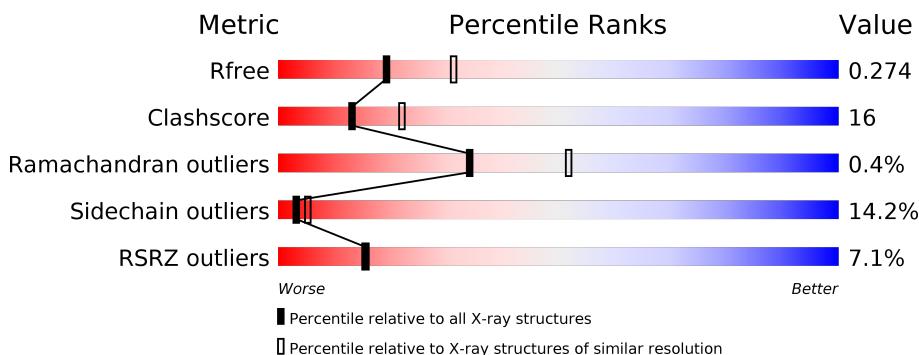
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

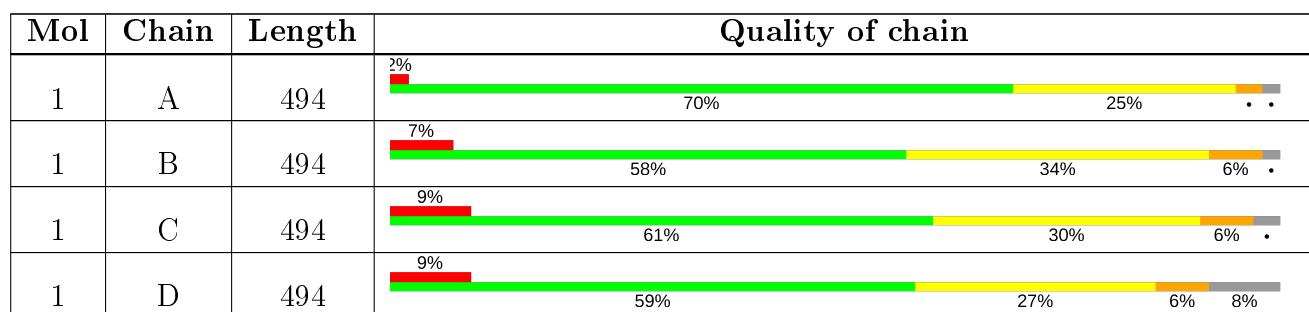
The reported resolution of this entry is 2.48 Å.

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 <sub>free</sub>	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15266 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 Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	485	Total	C 3804	N 2394	O 689	S 703	18	0	1	0
1	B	483	Total	C 3787	N 2385	O 685	S 699	18	0	0	0
1	C	477	Total	C 3762	N 2369	O 684	S 690	19	0	4	0
1	D	454	Total	C 3550	N 2242	O 641	S 650	17	0	1	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl 1	0	0
2	A	3	Total	Cl 3	0	0
2	D	2	Total	Cl 2	0	0
2	C	2	Total	Cl 2	0	0

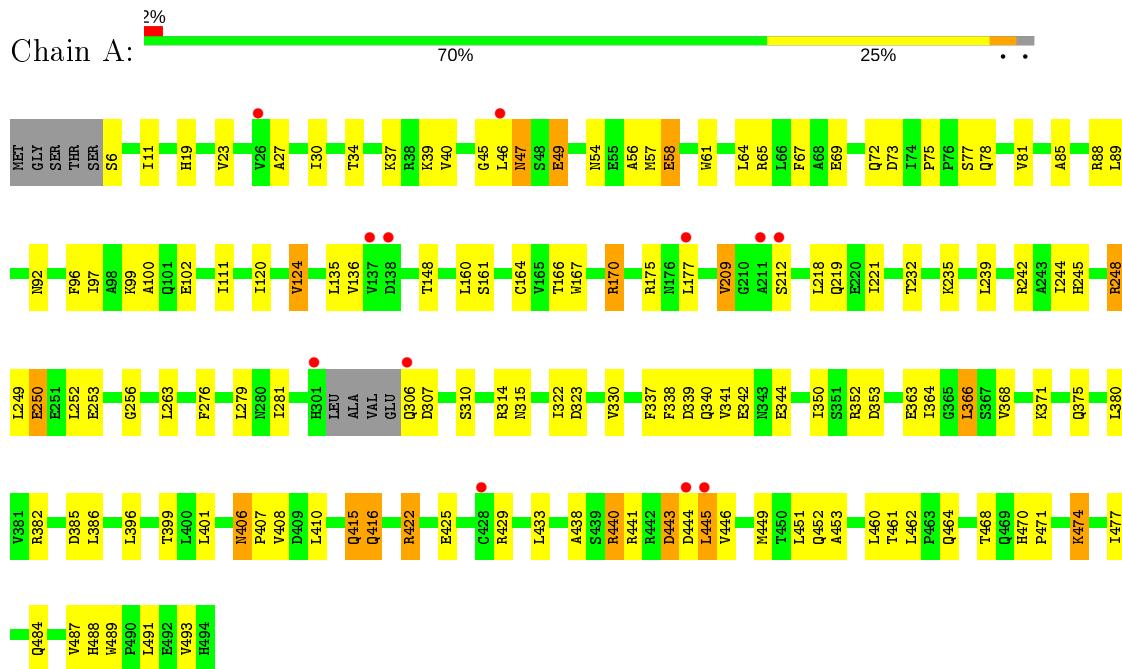
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O 113	0	0
3	B	45	Total	O 45	0	0
3	C	98	Total	O 98	0	0
3	D	99	Total	O 99	0	0

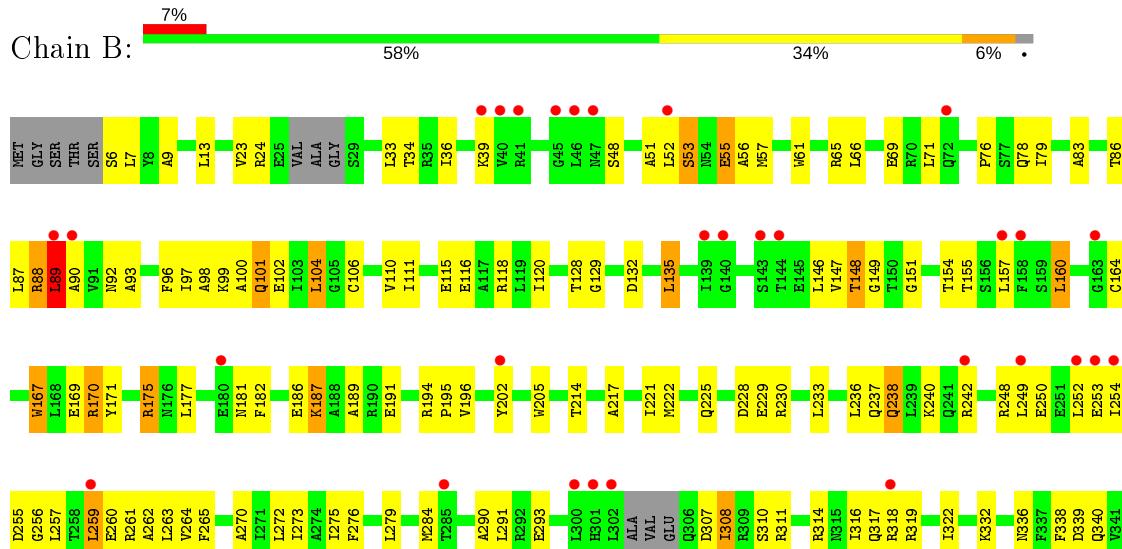
### 3 Residue-property plots

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

- Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase

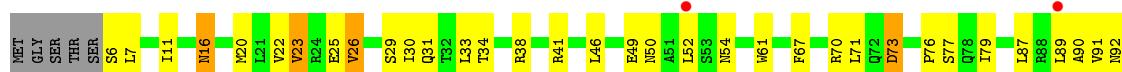


- Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase

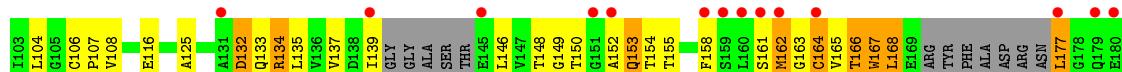


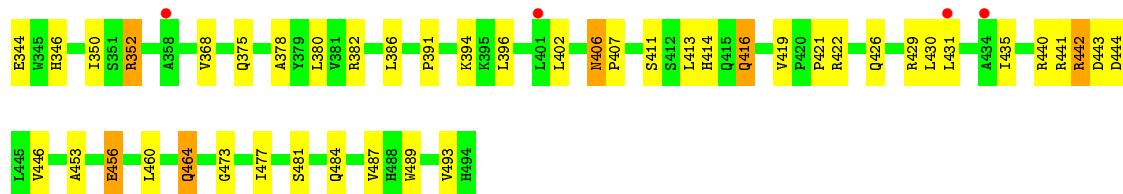


- Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase



- Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.83 Å    162.51 Å    165.67 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	29.46 – 2.48 29.46 – 2.47	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.46-2.48) 96.0 (29.46-2.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^{\text{1}}$	1.03 (at 2.48 Å)	Xtriage
Refinement program	PHENIX (dev_3352: ???)	Depositor
$R$ , $R_{free}$	0.225 , 0.274 0.227 , 0.274	Depositor DCC
$R_{free}$ test set	999 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, 0.333 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: CL

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	0.56	0/3865	0.69	0/5236
1	B	0.46	0/3847	0.66	0/5210
1	C	0.55	0/3822	0.69	0/5176
1	D	0.52	0/3605	0.71	0/4882
All	All	0.52	0/15139	0.69	0/20504

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	3804	0	3851	86	0
1	B	3787	0	3837	142	0
1	C	3762	0	3814	152	0
1	D	3550	0	3606	129	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	1	0
2	D	2	0	0	0	0
3	A	113	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	0	3	0
3	C	98	0	0	4	0
3	D	99	0	0	4	0
All	All	15266	0	15108	489	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 16.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:MET:SD	1:D:391:PRO:HB2	1.55	1.46
1:D:162:MET:HB3	1:D:167:TRP:CZ3	1.77	1.19
1:D:7:LEU:HG	1:D:74:ILE:CD1	1.75	1.16
1:D:222:MET:CE	1:D:235:LYS:HD3	1.86	1.05
1:D:223:MET:SD	1:D:391:PRO:CB	2.46	1.03
1:D:464[A]:GLN:HA	1:D:464[A]:GLN:HE21	1.24	1.02
1:C:170:ARG:HG2	1:C:170:ARG:HH11	1.26	1.00
1:D:7:LEU:CG	1:D:74:ILE:HD13	1.91	1.00
1:C:180:GLU:O	1:C:183:ASP:HB3	1.66	0.96
1:B:83:ALA:HB1	1:B:87:LEU:HD12	1.46	0.94
1:D:75:PRO:HG2	1:D:78:GLN:HG3	1.47	0.93
1:D:7:LEU:HG	1:D:74:ILE:HD13	0.94	0.93
1:C:26:VAL:HG12	1:D:321:MET:HE3	1.52	0.91
1:D:222:MET:HE3	1:D:235:LYS:HD3	1.52	0.90
1:C:166:THR:O	1:C:170:ARG:HD3	1.72	0.88
1:B:146:LEU:HD13	1:B:160:LEU:CD2	2.05	0.87
1:A:406:ASN:HB3	1:A:407:PRO:CD	2.04	0.86
1:A:57:MET:HG3	1:A:96:PHE:HD1	1.40	0.85
1:D:396:LEU:HB2	1:D:416:GLN:HG3	1.58	0.85
1:D:223:MET:CE	1:D:391:PRO:HB2	2.09	0.83
1:B:310:SER:HB3	1:B:314:ARG:HH12	1.43	0.83
1:B:146:LEU:CD1	1:B:160:LEU:CD2	2.57	0.83
1:B:175:ARG:CZ	1:B:175:ARG:HB2	2.08	0.82
1:C:179:GLN:H	1:C:244:ILE:HD12	1.45	0.82
1:D:162:MET:CB	1:D:167:TRP:CZ3	2.62	0.82
1:C:166:THR:O	1:C:170:ARG:HB2	1.80	0.81
1:D:464[A]:GLN:HA	1:D:464[A]:GLN:NE2	1.95	0.81
1:D:168:LEU:HD12	1:D:168:LEU:O	1.81	0.80
1:C:170:ARG:HG2	1:C:170:ARG:NH1	1.95	0.80
1:D:177:LEU:HD21	1:D:247:GLY:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TRP:HH2	1:D:192:VAL:HG21	1.47	0.79
1:D:84:THR:HG22	1:D:85:ALA:H	1.48	0.79
1:C:214:THR:HG21	1:C:268:GLY:HA3	1.64	0.77
1:D:210:GLY:HA3	1:D:215:VAL:HG21	1.66	0.77
1:B:83:ALA:CB	1:B:87:LEU:HD12	2.14	0.77
1:C:26:VAL:HG12	1:D:321:MET:CE	2.14	0.77
1:D:222:MET:HE1	1:D:235:LYS:HD3	1.66	0.77
1:C:242:ARG:NH2	1:C:246:CYS:SG	2.57	0.76
1:D:183:ASP:HA	1:D:186:GLU:HB2	1.67	0.75
1:C:167:TRP:HD1	1:C:185:ALA:HB1	1.52	0.75
1:D:7:LEU:HD23	1:D:7:LEU:H	1.52	0.75
1:C:182:PHE:CD2	1:C:240:LYS:HG3	2.22	0.75
1:D:406:ASN:HB3	1:D:407:PRO:HD2	1.67	0.75
1:D:132:ASP:HB3	1:D:150:THR:HG23	1.68	0.73
1:B:167:TRP:HE1	1:B:189:ALA:HB2	1.53	0.73
1:D:7:LEU:H	1:D:7:LEU:CD2	2.03	0.72
1:B:456:GLU:O	1:B:490:PRO:HG2	1.89	0.72
1:D:406:ASN:HB3	1:D:407:PRO:CD	2.19	0.72
1:B:242:ARG:HD2	1:B:254:ILE:HG22	1.72	0.71
1:A:45:GLY:HA3	1:A:56:ALA:HB2	1.72	0.71
1:D:162:MET:HB3	1:D:167:TRP:CE3	2.24	0.71
1:C:167:TRP:CD1	1:C:185:ALA:HB1	2.25	0.71
1:B:240:LYS:HD2	1:B:273:ILE:HD12	1.73	0.70
1:B:236:LEU:HD13	1:B:273:ILE:HG22	1.74	0.70
1:B:484:GLN:HB3	1:B:489:TRP:HB2	1.73	0.69
1:C:182:PHE:C	1:C:186:GLU:HG3	2.13	0.69
1:B:317:GLN:HA	1:B:322:ILE:HD12	1.74	0.69
1:C:390:THR:HG23	1:C:393:GLN:H	1.56	0.69
1:D:168:LEU:HD12	1:D:168:LEU:C	2.13	0.69
1:B:167:TRP:NE1	1:B:189:ALA:HB2	2.07	0.69
1:C:117:ALA:HB2	1:C:145:GLU:HG2	1.74	0.69
1:A:406:ASN:HB3	1:A:407:PRO:HD2	1.73	0.68
1:B:24:ARG:HB2	1:B:33:LEU:HD11	1.75	0.68
1:C:182:PHE:HB3	1:C:186:GLU:OE2	1.93	0.68
1:D:414:HIS:CD2	1:D:421:PRO:HB3	2.29	0.68
1:C:182:PHE:HZ	1:C:243:ALA:HB1	1.58	0.67
1:A:57:MET:HG3	1:A:96:PHE:CD1	2.28	0.67
1:C:182:PHE:HD2	1:C:240:LYS:HG3	1.60	0.67
1:B:146:LEU:HD11	1:B:160:LEU:HD23	1.76	0.67
1:C:406:ASN:HB3	1:C:407:PRO:CD	2.25	0.67
1:C:442:ARG:HB2	1:C:445:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:HB	1:A:487:VAL:HG21	1.76	0.67
1:C:157:LEU:O	1:C:157:LEU:HD23	1.95	0.67
1:B:416:GLN:HG2	1:B:418:ALA:H	1.60	0.66
1:C:186:GLU:O	1:C:190:ARG:HG3	1.96	0.66
1:C:233:LEU:H	1:C:233:LEU:HD13	1.60	0.66
1:B:444:ASP:OD1	1:B:445:LEU:HD23	1.96	0.65
1:C:20:MET:HE1	1:C:70:ARG:HD2	1.79	0.65
1:B:175:ARG:O	1:B:248:ARG:HA	1.96	0.65
1:A:396:LEU:HD13	1:A:416:GLN:HG3	1.79	0.65
1:C:97:ILE:O	1:C:101:GLN:HG3	1.97	0.64
1:D:301:HIS:H	1:D:301:HIS:CD2	2.12	0.64
1:B:250:GLU:OE1	1:C:263:LEU:HG	1.96	0.64
1:A:248:ARG:CZ	1:A:250:GLU:HG3	2.28	0.64
1:B:146:LEU:CD1	1:B:160:LEU:HD23	2.28	0.64
1:B:39:LYS:HD3	1:C:245:HIS:CD2	2.33	0.64
1:D:7:LEU:CG	1:D:74:ILE:CD1	2.65	0.64
1:A:27:ALA:HB3	1:A:315:ASN:ND2	2.13	0.63
1:C:162:MET:CE	1:C:189:ALA:HB1	2.29	0.63
1:D:149:GLY:HA2	1:D:155:THR:HG23	1.81	0.63
1:D:167:TRP:CH2	1:D:192:VAL:HG21	2.31	0.63
1:D:236:LEU:HD13	1:D:273:ILE:HG22	1.81	0.63
1:D:186:GLU:OE2	1:D:273:ILE:HD11	1.98	0.63
1:A:440:ARG:HB3	1:A:445:LEU:HD23	1.81	0.62
1:D:220:GLU:O	1:D:224:ALA:HB2	2.00	0.62
1:A:307:ASP:OD2	1:A:310:SER:CB	2.47	0.62
1:B:175:ARG:HB3	1:B:249:LEU:H	1.64	0.62
1:D:162:MET:HA	1:D:167:TRP:HZ3	1.64	0.62
1:C:182:PHE:O	1:C:186:GLU:CG	2.47	0.62
1:D:263:LEU:HG	1:D:264:VAL:HG13	1.82	0.62
1:D:133:GLN:HG3	1:D:206:LYS:H	1.64	0.62
1:C:477:ILE:HG21	1:C:493:VAL:HG21	1.82	0.61
1:D:223:MET:HE1	1:D:391:PRO:CB	2.30	0.61
1:D:344:GLU:HG2	1:D:453:ALA:O	2.00	0.61
1:A:406:ASN:HB3	1:A:407:PRO:HD3	1.83	0.61
1:C:30:ILE:HG12	1:C:300:LEU:HD21	1.82	0.61
1:C:170:ARG:HB3	1:C:171:TYR:CD1	2.35	0.61
1:D:223:MET:CE	1:D:391:PRO:CB	2.77	0.61
1:B:34:THR:HB	1:B:36:ILE:HD11	1.82	0.61
1:A:350:ILE:HD12	1:A:350:ILE:H	1.65	0.61
1:C:406:ASN:HB3	1:C:407:PRO:HD2	1.83	0.61
1:B:310:SER:HB3	1:B:314:ARG:NH1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:GLN:NE2	2:C:501:CL:CL	2.68	0.61
1:D:464[A]:GLN:CA	1:D:464[A]:GLN:HE21	2.07	0.61
1:C:76:PRO:HA	1:C:79:ILE:HD12	1.84	0.60
1:C:26:VAL:HG21	1:C:31:GLN:HE21	1.66	0.60
1:D:139:ILE:HG22	1:D:139:ILE:O	2.00	0.60
1:C:162:MET:HE1	1:C:189:ALA:HB1	1.82	0.60
1:B:146:LEU:CD1	1:B:160:LEU:HD22	2.31	0.60
1:A:307:ASP:OD2	1:A:310:SER:HB2	2.01	0.59
1:A:88:ARG:NH1	1:A:111:ILE:O	2.34	0.59
1:A:75:PRO:HG2	1:A:78:GLN:HG3	1.84	0.59
1:D:47:ASN:HD21	1:D:51:ALA:HB3	1.68	0.59
1:A:242:ARG:HH21	1:A:253:GLU:HG3	1.67	0.58
1:C:210:GLY:HA3	1:C:215:VAL:HG11	1.84	0.58
1:C:258:THR:HG22	1:C:261:ARG:H	1.69	0.58
1:D:164:CYS:SG	1:D:264:VAL:HG11	2.44	0.58
1:D:456:GLU:H	1:D:456:GLU:CD	2.06	0.58
1:B:440:ARG:NH2	3:B:603:HOH:O	2.36	0.58
1:C:29:SER:HB3	1:C:315[A]:ASN:CG	2.24	0.58
1:C:25:GLU:HA	1:C:30:ILE:HD12	1.86	0.58
1:B:217:ALA:HB2	1:B:261:ARG:HD2	1.87	0.57
1:C:168:LEU:HB2	1:C:267:SER:OG	2.04	0.57
1:B:115:GLU:OE1	1:B:118:ARG:NH1	2.37	0.57
1:B:52:LEU:O	1:B:92:ASN:ND2	2.38	0.57
1:D:162:MET:HA	1:D:167:TRP:CZ3	2.39	0.57
1:B:405:THR:O	1:B:406:ASN:HB2	2.05	0.57
1:D:106:CYS:HB2	1:D:107:PRO:HD2	1.84	0.57
1:B:132:ASP:O	1:B:151:GLY:N	2.32	0.57
1:A:323:ASP:OD2	1:A:441:ARG:NH1	2.37	0.57
1:A:221:ILE:HA	1:A:256:GLY:HA3	1.86	0.56
1:C:449:MET:HG2	1:C:462:LEU:HD23	1.86	0.56
1:B:149:GLY:HA2	1:B:155:THR:HG23	1.87	0.56
1:B:52:LEU:H	1:B:92:ASN:HB3	1.71	0.56
1:D:350:ILE:HD12	1:D:350:ILE:H	1.69	0.56
1:C:50:ASN:ND2	1:C:89:LEU:O	2.38	0.56
1:C:182:PHE:O	1:C:186:GLU:HG2	2.06	0.56
1:D:422:ARG:O	1:D:426:GLN:HG3	2.05	0.56
1:C:26:VAL:CG2	1:C:31:GLN:HG2	2.35	0.56
1:C:378:ALA:O	1:C:382[B]:ARG:HG3	2.07	0.56
1:B:233:LEU:HA	1:B:236:LEU:HB2	1.87	0.55
1:C:182:PHE:O	1:C:186:GLU:HG3	2.06	0.55
1:C:263:LEU:H	1:C:263:LEU:HD23	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:THR:HG22	1:C:393:GLN:CG	2.37	0.55
1:B:6:SER:HB3	1:B:78:GLN:HE22	1.70	0.55
1:C:239:LEU:O	1:C:243:ALA:N	2.39	0.55
1:C:440:ARG:HG3	1:C:445:LEU:HD13	1.89	0.55
1:A:177:LEU:O	1:A:244:ILE:HA	2.06	0.55
1:B:55:GLU:HG2	1:B:56:ALA:N	2.20	0.55
1:C:29:SER:HB3	1:C:315[A]:ASN:ND2	2.21	0.55
1:D:440:ARG:HB2	3:D:652:HOH:O	2.06	0.55
1:C:157:LEU:C	1:C:157:LEU:HD23	2.27	0.54
1:D:484:GLN:HB3	1:D:489:TRP:HB2	1.89	0.54
1:B:7:LEU:O	1:B:78:GLN:NE2	2.40	0.54
1:C:261:ARG:HG3	1:C:261:ARG:HH11	1.72	0.54
1:D:338:PHE:CD1	1:D:352:ARG:HG3	2.41	0.54
1:A:19:HIS:CE1	1:A:37:LYS:HD3	2.43	0.54
1:C:170:ARG:CG	1:C:170:ARG:HH11	2.08	0.54
1:C:182:PHE:HZ	1:C:243:ALA:CB	2.19	0.54
1:A:371:LYS:HB2	3:A:612:HOH:O	2.07	0.54
1:D:162:MET:CA	1:D:167:TRP:HZ3	2.20	0.54
1:B:451:LEU:HD11	1:B:458:LEU:HD22	1.90	0.54
1:A:6:SER:N	3:A:607:HOH:O	2.40	0.54
1:C:90:ALA:HB3	1:C:93:ALA:HB2	1.90	0.54
1:D:442:ARG:NH2	1:D:444:ASP:OD1	2.40	0.54
1:B:51:ALA:HB1	1:B:92:ASN:HB2	1.90	0.54
1:C:319:ARG:NH2	3:C:603:HOH:O	2.41	0.54
1:B:449:MET:HG2	1:B:462:LEU:HD23	1.90	0.54
1:C:182:PHE:CE2	1:C:240:LYS:HG3	2.42	0.53
1:D:319:ARG:HD2	3:D:618:HOH:O	2.07	0.53
1:B:149:GLY:HA2	1:B:155:THR:H	1.73	0.53
1:B:250:GLU:CD	1:C:263:LEU:CD1	2.77	0.53
1:C:165:VAL:O	1:C:168:LEU:HB3	2.08	0.53
1:C:171:TYR:O	1:C:181:ASN:OD1	2.26	0.53
1:C:7:LEU:HD21	1:D:441:ARG:HD2	1.90	0.53
1:C:167:TRP:NE1	1:C:189:ALA:HB2	2.23	0.53
1:C:209:VAL:CG1	1:C:287:ALA:HB2	2.38	0.53
1:C:23:VAL:HG13	1:C:30:ILE:HG13	1.91	0.53
1:D:97:ILE:HG23	1:D:108:VAL:HB	1.89	0.53
1:D:164:CYS:SG	1:D:264:VAL:HB	2.48	0.52
1:D:406:ASN:CB	1:D:407:PRO:CD	2.88	0.52
1:B:237:GLN:HA	1:B:240:LYS:HB2	1.91	0.52
1:D:177:LEU:HD21	1:D:247:GLY:N	2.19	0.52
1:D:162:MET:CA	1:D:167:TRP:CZ3	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:ARG:CZ	1:D:489:TRP:HB3	2.40	0.52
1:B:338:PHE:CZ	1:B:347:LEU:HB3	2.45	0.52
1:A:337:PHE:O	1:A:341:VAL:HG22	2.10	0.52
1:B:250:GLU:OE1	1:C:263:LEU:CG	2.58	0.52
1:B:444:ASP:OD1	1:B:445:LEU:CD2	2.58	0.52
1:C:263:LEU:CD2	1:C:263:LEU:N	2.73	0.52
1:D:97:ILE:O	1:D:101:GLN:HG3	2.09	0.52
1:B:57:MET:SD	1:B:96:PHE:HB2	2.50	0.51
1:B:225:GLN:HG2	1:B:255:ASP:HB3	1.91	0.51
1:D:27:ALA:HA	1:D:318:ARG:HH21	1.74	0.51
1:A:375[A]:GLN:NE2	3:A:609:HOH:O	2.42	0.51
1:A:61:TRP:O	1:A:65:ARG:HG3	2.10	0.51
1:D:222:MET:HE3	1:D:235:LYS:CD	2.33	0.51
1:C:50:ASN:O	1:C:91:VAL:HG22	2.11	0.51
1:D:38:ARG:NH1	1:D:70:ARG:HH12	2.09	0.51
1:A:338:PHE:CD1	1:A:352:ARG:HG3	2.45	0.51
1:B:146:LEU:N	1:B:146:LEU:HD12	2.26	0.51
1:C:305:GLU:HG3	1:C:311:ARG:HD3	1.93	0.51
1:C:186:GLU:OE2	1:C:273:ILE:HD11	2.11	0.51
1:D:193:LEU:HD11	1:D:278:GLU:HB3	1.92	0.51
1:C:344:GLU:HG2	1:C:453:ALA:O	2.11	0.50
1:D:7:LEU:N	1:D:7:LEU:CD2	2.71	0.50
1:A:452:GLN:OE1	3:A:601:HOH:O	2.20	0.50
1:D:125:ALA:HA	1:D:134:ARG:NH1	2.26	0.50
1:D:275:ILE:O	1:D:279:LEU:HB2	2.12	0.50
1:D:315:ASN:O	1:D:319:ARG:HG3	2.12	0.50
1:B:147:VAL:HG22	1:B:157:LEU:HA	1.93	0.50
1:B:175:ARG:HG2	1:B:249:LEU:HB3	1.93	0.50
1:B:9:ALA:HB3	1:B:79:ILE:HG12	1.94	0.50
1:A:57:MET:HG2	1:A:61:TRP:CH2	2.47	0.50
1:B:164:CYS:HB3	1:B:264:VAL:HB	1.93	0.50
1:D:473:GLY:O	1:D:477:ILE:HG13	2.12	0.50
1:A:64:LEU:HD12	1:A:100:ALA:HB1	1.94	0.50
1:C:263:LEU:HD23	1:C:263:LEU:N	2.26	0.50
1:B:221:ILE:HA	1:B:256:GLY:HA3	1.93	0.50
1:D:386:LEU:HD12	1:D:394:LYS:HG3	1.94	0.50
1:C:156:SER:HB2	1:C:158:PHE:CE2	2.47	0.50
1:C:46:LEU:HD13	1:C:52:LEU:HD12	1.94	0.49
1:D:163:GLY:C	1:D:166:THR:HG23	2.32	0.49
1:B:414:HIS:CD2	1:B:421:PRO:HB3	2.48	0.49
1:B:187:LYS:O	1:B:191:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:N	1:C:247:GLY:O	2.44	0.49
1:A:339:ASP:O	1:A:342:GLU:HG2	2.13	0.49
1:B:147:VAL:HG22	1:B:157:LEU:HG	1.94	0.49
1:C:440:ARG:HD2	1:D:69:GLU:O	2.13	0.49
1:D:27:ALA:HA	1:D:318:ARG:NH2	2.28	0.49
1:D:235:LYS:O	1:D:239:LEU:HB2	2.12	0.49
1:A:443:ASP:O	1:A:446:VAL:HG22	2.13	0.49
1:A:425:GLU:HG2	1:A:489:TRP:HZ2	1.77	0.49
1:B:449:MET:HB3	1:B:460:LEU:HD11	1.94	0.49
1:C:183:ASP:N	1:C:186:GLU:HG3	2.28	0.49
1:C:300:LEU:HB3	1:C:302:LEU:HG	1.94	0.49
1:A:19:HIS:HE1	1:A:37:LYS:HD3	1.78	0.49
1:B:250:GLU:OE1	1:C:263:LEU:CD1	2.60	0.49
1:B:175:ARG:CZ	1:B:175:ARG:CB	2.86	0.48
1:C:11:ILE:HG12	1:C:20:MET:HG3	1.95	0.48
1:C:386:LEU:HD12	1:C:394:LYS:HG2	1.94	0.48
1:D:396:LEU:HB2	1:D:416:GLN:CG	2.39	0.48
1:B:316:ILE:HD12	1:B:384:LEU:HD13	1.95	0.48
1:A:433:LEU:HD21	1:A:491:LEU:HD21	1.95	0.48
1:B:146:LEU:HD13	1:B:160:LEU:HD21	1.91	0.48
1:D:49:GLU:HG2	1:D:49:GLU:O	2.12	0.48
1:A:443:ASP:OD1	1:A:443:ASP:N	2.35	0.48
1:C:182:PHE:C	1:C:186:GLU:CG	2.80	0.48
1:A:11:ILE:HB	1:A:81:VAL:HG13	1.96	0.48
1:B:88:ARG:NH1	1:B:111:ILE:O	2.47	0.48
1:B:386:LEU:HD12	1:B:394:LYS:HG3	1.96	0.48
1:A:120:ILE:O	1:A:124:VAL:HG13	2.14	0.48
1:A:45:GLY:HA3	1:A:56:ALA:CB	2.43	0.48
1:D:133:GLN:HA	1:D:149:GLY:O	2.13	0.48
1:A:54:ASN:O	1:A:58:GLU:HB2	2.13	0.47
1:A:410:LEU:HD11	1:A:487:VAL:HG13	1.96	0.47
1:C:271:ILE:O	1:C:275:ILE:HG13	2.14	0.47
1:B:175:ARG:HH12	1:B:248:ARG:HG2	1.78	0.47
1:C:61:TRP:CD2	1:C:99:LYS:HD3	2.48	0.47
1:B:170:ARG:HG3	1:B:171:TYR:CD2	2.49	0.47
1:B:53:SER:OG	1:B:55:GLU:OE1	2.20	0.47
1:C:16:ASN:HD21	1:C:41:ARG:HG3	1.79	0.47
1:C:431:LEU:O	1:C:435:ILE:HG13	2.14	0.47
1:D:125:ALA:HA	1:D:134:ARG:HH12	1.79	0.47
1:D:233:LEU:O	1:D:237:GLN:HG2	2.15	0.47
1:D:271:ILE:O	1:D:275:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:HB3	1:A:474:LYS:HE2	1.58	0.47
1:B:262:ALA:HA	1:B:265:PHE:HB2	1.96	0.47
1:B:236:LEU:HD21	1:B:272:LEU:HD23	1.97	0.47
1:B:473:GLY:O	1:B:477:ILE:HG13	2.15	0.47
1:B:98:ALA:O	1:B:102:GLU:HG2	2.14	0.47
1:C:182:PHE:CZ	1:C:243:ALA:CB	2.97	0.47
1:D:199:GLU:OE2	1:D:203:HIS:HE1	1.98	0.47
1:A:471:PRO:HG2	1:B:66:LEU:HD23	1.96	0.47
1:C:406:ASN:CB	1:C:407:PRO:CD	2.93	0.47
1:C:197:ALA:HB2	1:C:278:GLU:OE2	2.14	0.47
1:C:164:CYS:HB2	1:C:264:VAL:HG22	1.97	0.47
1:B:13:LEU:HB2	1:B:83:ALA:HA	1.97	0.47
1:D:46:LEU:HA	1:D:46:LEU:HD12	1.71	0.47
1:A:338:PHE:O	1:A:342:GLU:N	2.48	0.47
1:B:61:TRP:O	1:B:65:ARG:HG2	2.14	0.47
1:C:179:GLN:N	1:C:244:ILE:HD12	2.23	0.47
1:A:368:VAL:O	1:B:384:LEU:HD23	2.16	0.46
1:C:390:THR:HG22	1:C:393:GLN:CD	2.36	0.46
1:D:378:ALA:HB2	1:D:402:LEU:HB2	1.97	0.46
1:C:187:LYS:HA	1:C:190:ARG:HB2	1.96	0.46
1:A:279:LEU:HB2	1:A:281:ILE:HD12	1.96	0.46
1:C:131:ALA:HB3	1:C:207:VAL:HG23	1.97	0.46
1:B:146:LEU:HD13	1:B:160:LEU:HD22	1.92	0.46
1:D:431:LEU:O	1:D:435:ILE:HG13	2.16	0.46
1:B:336:ASN:O	1:B:340:GLN:HG3	2.15	0.46
1:B:484:GLN:O	1:B:487:VAL:HG12	2.15	0.46
1:A:488:HIS:CE1	1:C:420:PRO:HG3	2.50	0.46
1:B:408:VAL:HG22	1:B:432:ARG:NH1	2.30	0.46
1:B:466:TRP:CE2	1:B:470:HIS:ND1	2.84	0.46
1:B:429:ARG:HG2	1:B:489:TRP:CE3	2.50	0.46
1:C:22:VAL:HG12	1:C:23:VAL:H	1.81	0.46
1:C:450:THR:HG22	1:C:452:GLN:NE2	2.30	0.46
1:B:414:HIS:NE2	1:B:425:GLU:OE2	2.40	0.46
1:C:115:GLU:HG3	3:C:697:HOH:O	2.16	0.46
1:C:261:ARG:HG3	1:C:261:ARG:NH1	2.31	0.46
1:C:317:GLN:HB3	1:C:324:ILE:HD11	1.97	0.46
1:C:329:ARG:NH1	1:C:441:ARG:HA	2.31	0.46
1:D:201:ARG:HB2	1:D:201:ARG:HH11	1.81	0.46
1:B:76:PRO:HB3	1:B:106:CYS:HB3	1.97	0.46
1:B:275:ILE:O	1:B:279:LEU:HB2	2.16	0.46
1:B:52:LEU:H	1:B:92:ASN:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:HE1	1:C:70:ARG:HH11	1.81	0.46
1:C:315[B]:ASN:HA	1:C:318:ARG:HG3	1.97	0.46
1:C:390:THR:CG2	1:C:393:GLN:H	2.26	0.46
1:B:101:GLN:HE21	1:B:101:GLN:HB2	1.45	0.46
1:C:452:GLN:HG2	1:C:459:THR:O	2.16	0.46
1:C:73:ASP:OD2	1:D:442:ARG:HD3	2.16	0.46
1:D:341:VAL:HG12	1:D:453:ALA:HB2	1.98	0.46
1:D:24:ARG:HG2	1:D:26:VAL:HG13	1.96	0.46
1:B:406:ASN:O	1:B:407:PRO:C	2.55	0.45
1:B:248:ARG:NH1	1:C:41:ARG:HG2	2.30	0.45
1:D:164:CYS:SG	1:D:264:VAL:CG1	3.04	0.45
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.74	0.45
1:B:480:GLU:O	1:B:484:GLN:HG3	2.16	0.45
1:A:363:GLU:OE1	1:A:441:ARG:NH2	2.48	0.45
1:A:322:ILE:HD11	1:A:364:ILE:HB	1.98	0.45
1:B:170:ARG:HG3	1:B:171:TYR:CE2	2.51	0.45
1:C:26:VAL:HG21	1:C:31:GLN:HG2	1.98	0.45
1:A:340:GLN:OE1	1:A:451:LEU:N	2.31	0.45
1:B:396:LEU:HB2	1:B:416:GLN:HG3	1.98	0.45
1:C:61:TRP:CE2	1:C:99:LYS:HD3	2.51	0.45
1:D:269:LEU:O	1:D:273:ILE:HG23	2.16	0.45
1:A:27:ALA:HB3	1:A:315:ASN:HD21	1.80	0.45
1:A:85:ALA:HA	1:A:88:ARG:HG2	1.97	0.45
1:B:450:THR:O	1:B:460:LEU:HD12	2.16	0.45
1:C:237:GLN:NE2	1:C:240:LYS:HD3	2.31	0.45
1:B:250:GLU:OE1	1:C:263:LEU:HD11	2.17	0.45
1:B:456:GLU:O	1:B:490:PRO:CG	2.63	0.45
1:C:163:GLY:O	1:C:167:TRP:HB2	2.16	0.45
1:C:437:PHE:CE1	1:C:462:LEU:HD21	2.52	0.45
1:D:429:ARG:HG2	1:D:489:TRP:CE3	2.51	0.45
1:C:183:ASP:CA	1:C:186:GLU:HG3	2.47	0.45
1:C:238:GLN:O	1:C:242:ARG:HB2	2.17	0.45
1:A:460:LEU:O	1:A:493:VAL:HA	2.17	0.45
1:A:484:GLN:HB3	1:A:489:TRP:HB2	1.99	0.45
1:B:89:LEU:O	1:B:90:ALA:C	2.55	0.45
1:D:190:ARG:O	1:D:194:ARG:HB2	2.17	0.45
1:C:314:ARG:O	1:C:318:ARG:HG2	2.16	0.45
1:C:336:ASN:O	1:C:340:GLN:HG3	2.16	0.45
1:B:128:THR:HG22	1:B:129:GLY:O	2.17	0.44
1:C:206:LYS:HD3	1:C:206:LYS:HA	1.82	0.44
1:B:106:CYS:HB2	3:B:610:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TRP:CZ2	1:B:99:LYS:HB3	2.52	0.44
1:A:344:GLU:HG2	1:A:453:ALA:O	2.18	0.44
1:D:164:CYS:SG	1:D:264:VAL:CB	3.06	0.44
1:B:186:GLU:HG2	1:B:270:ALA:HB1	2.00	0.44
1:D:219:GLN:NE2	1:D:391:PRO:HG2	2.33	0.44
1:D:242:ARG:HD2	1:D:242:ARG:HA	1.34	0.44
1:A:382:ARG:HD3	3:A:630:HOH:O	2.18	0.44
1:C:222:MET:HG2	1:C:227:MET:HE2	2.00	0.44
1:D:152:ALA:N	3:D:604:HOH:O	2.35	0.44
1:B:250:GLU:OE2	1:C:263:LEU:HD12	2.17	0.44
1:B:395:LYS:NZ	1:B:415:GLN:HG3	2.32	0.44
1:B:429:ARG:O	1:B:433:LEU:HG	2.18	0.44
1:A:235:LYS:O	1:A:239:LEU:HG	2.17	0.44
1:C:222:MET:HE3	1:C:235:LYS:HD3	1.99	0.44
1:D:177:LEU:HD23	1:D:244:ILE:HA	1.98	0.44
1:A:69:GLU:O	1:A:72:GLN:HG2	2.17	0.43
1:B:290:ALA:H	1:B:293:GLU:HB2	1.83	0.43
1:B:339:ASP:OD1	1:B:352:ARG:NH1	2.51	0.43
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.71	0.43
1:D:182:PHE:CE2	1:D:244:ILE:HG12	2.52	0.43
1:A:250:GLU:HB2	1:D:263:LEU:HD13	2.01	0.43
1:C:265:PHE:CE2	1:C:269:LEU:HD22	2.53	0.43
1:C:484:GLN:HB3	1:C:489:TRP:HB2	1.99	0.43
1:D:193:LEU:HG	1:D:278:GLU:HG2	2.00	0.43
1:A:422:ARG:HD3	1:A:422:ARG:HA	1.64	0.43
1:C:162:MET:HE3	1:C:189:ALA:HB1	2.00	0.43
1:C:20:MET:CE	1:C:70:ARG:HD2	2.48	0.43
1:D:338:PHE:CE1	1:D:352:ARG:HG3	2.53	0.43
1:A:396:LEU:O	1:A:399:THR:HG22	2.18	0.43
1:B:338:PHE:CZ	1:B:352:ARG:HB2	2.53	0.43
1:C:162:MET:HG2	1:C:167:TRP:CH2	2.53	0.43
1:D:64:LEU:HD22	1:D:104:LEU:HD21	2.00	0.43
1:A:61:TRP:CE2	1:A:99:LYS:HD3	2.54	0.43
1:B:229:GLU:OE1	1:B:390:THR:HB	2.19	0.43
1:B:270:ALA:HA	1:B:273:ILE:HD11	1.99	0.43
1:B:342:GLU:HG3	1:B:343:ASN:N	2.32	0.43
1:B:250:GLU:OE2	1:C:263:LEU:CD1	2.67	0.43
1:A:136:VAL:HA	1:A:209:VAL:O	2.19	0.43
1:B:262:ALA:HA	1:B:265:PHE:CB	2.49	0.43
1:C:194:ARG:HA	1:C:194:ARG:HD2	1.79	0.43
1:B:100:ALA:O	1:B:104:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HG	1:B:260:GLU:N	2.33	0.43
1:B:460:LEU:O	1:B:493:VAL:HA	2.19	0.43
1:D:223:MET:HE1	1:D:391:PRO:HB3	2.01	0.43
1:A:440:ARG:HD3	1:A:440:ARG:HA	1.73	0.43
1:C:46:LEU:HD21	1:C:89:LEU:HD11	2.01	0.43
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.86	0.43
1:A:415:GLN:HB3	1:A:415:GLN:HE21	1.55	0.42
1:C:229:GLU:OE1	1:C:390:THR:OG1	2.37	0.42
1:D:84:THR:HG23	1:D:116:GLU:OE1	2.19	0.42
1:B:270:ALA:O	1:B:273:ILE:HG12	2.18	0.42
1:B:454:ASN:HD22	1:B:454:ASN:HA	1.52	0.42
1:D:426:GLN:O	1:D:430:LEU:HG	2.18	0.42
1:B:457:LEU:HA	1:B:490:PRO:HG2	2.01	0.42
1:D:201:ARG:NH1	1:D:201:ARG:HB2	2.34	0.42
1:A:449:MET:HG2	1:A:462:LEU:HD23	2.00	0.42
1:A:61:TRP:CZ2	1:A:99:LYS:HD3	2.54	0.42
1:B:97:ILE:HG22	1:B:101:GLN:HE22	1.84	0.42
1:C:193:LEU:HD21	1:C:275:ILE:HG12	2.01	0.42
1:A:242:ARG:NH2	1:A:253:GLU:HG3	2.34	0.42
1:A:477:ILE:CG2	1:A:493:VAL:HG11	2.49	0.42
1:C:305:GLU:CD	1:C:314:ARG:HH22	2.23	0.42
1:D:36:ILE:HD13	1:D:36:ILE:HA	1.83	0.42
1:A:46:LEU:HA	1:A:46:LEU:HD12	1.93	0.42
1:B:238:GLN:OE1	1:B:242:ARG:NH2	2.52	0.42
1:B:404:GLN:HB2	1:B:435:ILE:CD1	2.49	0.42
1:B:308:ILE:O	1:B:311:ARG:N	2.52	0.42
1:B:61:TRP:CE3	1:B:99:LYS:HD3	2.55	0.42
1:C:384:LEU:HD23	1:D:368:VAL:O	2.19	0.42
1:D:137:VAL:HG22	1:D:146:LEU:HD23	2.01	0.42
1:D:199:GLU:OE2	1:D:203:HIS:CE1	2.72	0.42
1:B:146:LEU:HD11	1:B:160:LEU:CD2	2.36	0.42
1:B:194:ARG:N	1:B:195:PRO:HD2	2.34	0.42
1:B:230:ARG:NH1	1:B:230:ARG:HB2	2.35	0.42
1:C:121:TYR:HE1	1:C:152:ALA:HA	1.84	0.42
1:D:153:GLN:HA	1:D:153:GLN:HE21	1.85	0.42
1:D:332:LYS:HG3	1:D:333:VAL:N	2.34	0.42
1:D:416:GLN:OE1	1:D:419:VAL:N	2.42	0.42
1:B:135:LEU:HB2	1:B:205:TRP:CG	2.55	0.42
1:B:429:ARG:CZ	1:B:489:TRP:HB3	2.50	0.42
1:C:134:ARG:NH2	3:C:605:HOH:O	2.40	0.42
1:C:219:GLN:HA	1:C:219:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG22	1:A:438:ALA:HB3	2.02	0.42
1:C:395:LYS:HE2	3:C:601:HOH:O	2.19	0.42
1:A:166:THR:O	1:A:170:ARG:HG2	2.20	0.41
1:A:429:ARG:HG2	1:A:489:TRP:CE3	2.55	0.41
1:A:406:ASN:CB	1:A:407:PRO:CD	2.81	0.41
1:B:364:ILE:HG12	1:B:380:LEU:HD13	2.01	0.41
1:A:232:THR:OG1	1:A:235:LYS:HG3	2.20	0.41
1:B:148:THR:HB	1:B:155:THR:OG1	2.19	0.41
1:C:30:ILE:CG1	1:C:300:LEU:HD21	2.48	0.41
1:B:421:PRO:O	1:B:425:GLU:HG3	2.20	0.41
1:D:214:THR:O	1:D:217:ALA:N	2.52	0.41
1:A:30:ILE:HG21	1:A:30:ILE:HD13	1.68	0.41
1:A:11:ILE:HD12	1:A:67:PHE:CD2	2.55	0.41
1:A:338:PHE:CE1	1:A:352:ARG:HG3	2.56	0.41
1:D:272:LEU:O	1:D:276:PHE:N	2.52	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.86	0.41
1:A:47:ASN:HD21	1:A:49:GLU:HB2	1.85	0.41
1:B:89:LEU:HA	1:B:89:LEU:HD12	1.72	0.41
1:C:190:ARG:HA	1:C:193:LEU:HB2	2.02	0.41
1:C:326:GLN:HG2	1:C:441:ARG:NH1	2.35	0.41
1:C:369:ASP:OD2	1:C:371:LYS:NZ	2.48	0.41
1:C:38:ARG:HD2	1:C:67:PHE:CE1	2.55	0.41
1:D:11:ILE:HD11	1:D:71:LEU:HD21	2.03	0.41
1:D:163:GLY:CA	1:D:166:THR:HG23	2.51	0.41
1:A:385:ASP:O	1:A:386:LEU:HD23	2.21	0.41
1:A:39:LYS:HB3	1:A:39:LYS:HE2	1.91	0.41
1:A:470:HIS:HB3	1:B:69:GLU:OE2	2.21	0.41
1:C:451:LEU:HA	1:C:451:LEU:HD12	1.86	0.41
1:D:222:MET:CE	1:D:235:LYS:CD	2.77	0.41
1:B:221:ILE:HD11	1:B:257:LEU:HD13	2.03	0.41
1:B:413:LEU:HD12	1:B:413:LEU:HA	1.84	0.41
1:C:185:ALA:HA	1:C:188:ALA:HB3	2.03	0.41
1:B:442:ARG:HD2	3:B:634:HOH:O	2.21	0.41
1:C:315[A]:ASN:HA	1:C:318:ARG:HG3	2.02	0.41
1:D:163:GLY:HA3	1:D:166:THR:CG2	2.51	0.41
1:A:245:HIS:HE1	3:D:677:HOH:O	2.04	0.40
1:B:160:LEU:HD11	1:B:196:VAL:HG11	2.02	0.40
1:B:13:LEU:HD12	1:B:83:ALA:HB2	2.02	0.40
1:C:187:LYS:O	1:C:191:GLU:HG3	2.21	0.40
1:C:38:ARG:HD2	1:C:67:PHE:HE1	1.86	0.40
1:D:443:ASP:O	1:D:446:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:O	1:B:120:ILE:HG13	2.22	0.40
1:D:378:ALA:O	1:D:382:ARG:HG3	2.21	0.40
1:A:364:ILE:HG12	1:A:380:LEU:HD13	2.04	0.40
1:B:90:ALA:HB3	1:B:93:ALA:HB2	2.03	0.40
1:C:190:ARG:O	1:C:194:ARG:N	2.55	0.40
1:C:30:ILE:HD13	1:C:300:LEU:HD11	2.03	0.40
1:B:332:LYS:HB2	1:B:332:LYS:HE2	1.74	0.40
1:B:61:TRP:CZ3	1:B:99:LYS:HD3	2.57	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	482/494 (98%)	463 (96%)	18 (4%)	1 (0%)	47 66
1	B	477/494 (97%)	448 (94%)	26 (6%)	3 (1%)	25 40
1	C	475/494 (96%)	449 (94%)	25 (5%)	1 (0%)	47 66
1	D	443/494 (90%)	419 (95%)	22 (5%)	2 (0%)	29 46
All	All	1877/1976 (95%)	1779 (95%)	91 (5%)	7 (0%)	34 52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	LEU
1	B	407	PRO
1	D	164	CYS
1	A	406	ASN
1	B	406	ASN
1	C	406	ASN
1	D	406	ASN

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	404/410 (98%)	358 (89%)	46 (11%)	5   10
1	B	403/410 (98%)	344 (85%)	59 (15%)	3   5
1	C	399/410 (97%)	342 (86%)	57 (14%)	3   5
1	D	378/410 (92%)	315 (83%)	63 (17%)	2   3
All	All	1584/1640 (97%)	1359 (86%)	225 (14%)	3   5

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	34	THR
1	A	40	VAL
1	A	47	ASN
1	A	49	GLU
1	A	58	GLU
1	A	73	ASP
1	A	77	SER
1	A	89	LEU
1	A	92	ASN
1	A	97	ILE
1	A	102	GLU
1	A	124	VAL
1	A	135	LEU
1	A	148	THR
1	A	160	LEU
1	A	161	SER
1	A	164	CYS
1	A	167	TRP
1	A	170	ARG
1	A	175	ARG
1	A	209	VAL
1	A	212	SER
1	A	219	GLN

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Mol	Chain	Res	Type
1	A	248	ARG
1	A	249	LEU
1	A	250	GLU
1	A	252	LEU
1	A	263	LEU
1	A	276	PHE
1	A	306	GLN
1	A	314	ARG
1	A	353	ASP
1	A	366	LEU
1	A	401	LEU
1	A	415	GLN
1	A	416	GLN
1	A	422	ARG
1	A	440	ARG
1	A	443	ASP
1	A	444	ASP
1	A	445	LEU
1	A	461	THR
1	A	464	GLN
1	A	468	THR
1	A	474	LYS
1	B	23	VAL
1	B	48	SER
1	B	53	SER
1	B	55	GLU
1	B	71	LEU
1	B	86	THR
1	B	88	ARG
1	B	89	LEU
1	B	101	GLN
1	B	104	LEU
1	B	110	VAL
1	B	135	LEU
1	B	148	THR
1	B	154	THR
1	B	160	LEU
1	B	167	TRP
1	B	169	GLU
1	B	170	ARG
1	B	175	ARG
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	181	ASN
1	B	182	PHE
1	B	187	LYS
1	B	202	TYR
1	B	214	THR
1	B	222	MET
1	B	228	ASP
1	B	238	GLN
1	B	252	LEU
1	B	253	GLU
1	B	259	LEU
1	B	263	LEU
1	B	276	PHE
1	B	284	MET
1	B	291	LEU
1	B	307	ASP
1	B	308	ILE
1	B	318	ARG
1	B	319	ARG
1	B	342	GLU
1	B	345	TRP
1	B	356	ILE
1	B	385	ASP
1	B	390	THR
1	B	396	LEU
1	B	413	LEU
1	B	415	GLN
1	B	416	GLN
1	B	417	ASN
1	B	422	ARG
1	B	423	VAL
1	B	440	ARG
1	B	444	ASP
1	B	454	ASN
1	B	464	GLN
1	B	487	VAL
1	B	491	LEU
1	B	493	VAL
1	B	494	HIS
1	C	6	SER
1	C	16	ASN
1	C	23	VAL

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Mol	Chain	Res	Type
1	C	26	VAL
1	C	33	LEU
1	C	34	THR
1	C	49	GLU
1	C	54	ASN
1	C	71	LEU
1	C	73	ASP
1	C	77	SER
1	C	87	LEU
1	C	92	ASN
1	C	115	GLU
1	C	134	ARG
1	C	135	LEU
1	C	156	SER
1	C	161	SER
1	C	166	THR
1	C	167	TRP
1	C	170	ARG
1	C	187	LYS
1	C	192	VAL
1	C	194	ARG
1	C	196	VAL
1	C	201	ARG
1	C	202	TYR
1	C	209	VAL
1	C	214	THR
1	C	221	ILE
1	C	225	GLN
1	C	229	GLU
1	C	233	LEU
1	C	238	GLN
1	C	242	ARG
1	C	258	THR
1	C	259	LEU
1	C	263	LEU
1	C	264	VAL
1	C	267	SER
1	C	296	VAL
1	C	300	LEU
1	C	304	VAL
1	C	310	SER
1	C	314	ARG

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Mol	Chain	Res	Type
1	C	318	ARG
1	C	325	ASP
1	C	372	GLN
1	C	415	GLN
1	C	422	ARG
1	C	440	ARG
1	C	442	ARG
1	C	452	GLN
1	C	456	GLU
1	C	464	GLN
1	C	468	THR
1	C	487	VAL
1	D	6	SER
1	D	7	LEU
1	D	16	ASN
1	D	17	SER
1	D	23	VAL
1	D	31	GLN
1	D	33	LEU
1	D	37	LYS
1	D	46	LEU
1	D	53	SER
1	D	54	ASN
1	D	71	LEU
1	D	89	LEU
1	D	91	VAL
1	D	92	ASN
1	D	102	GLU
1	D	132	ASP
1	D	134	ARG
1	D	135	LEU
1	D	148	THR
1	D	153	GLN
1	D	154	THR
1	D	158	PHE
1	D	161	SER
1	D	162	MET
1	D	165	VAL
1	D	166	THR
1	D	167	TRP
1	D	168	LEU
1	D	177	LEU

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Mol	Chain	Res	Type
1	D	182	PHE
1	D	183	ASP
1	D	193	LEU
1	D	201	ARG
1	D	207	VAL
1	D	212	SER
1	D	214	THR
1	D	222	MET
1	D	234	GLU
1	D	239	LEU
1	D	241	GLN
1	D	242	ARG
1	D	273	ILE
1	D	276	PHE
1	D	281	ILE
1	D	282	GLN
1	D	301	HIS
1	D	328	GLN
1	D	332	LYS
1	D	346	HIS
1	D	352	ARG
1	D	375	GLN
1	D	411	SER
1	D	413	LEU
1	D	416	GLN
1	D	442	ARG
1	D	456	GLU
1	D	460	LEU
1	D	464[A]	GLN
1	D	464[B]	GLN
1	D	481	SER
1	D	487	VAL
1	D	493	VAL

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

Mol	Chain	Res	Type
1	A	19	HIS
1	A	50	ASN
1	A	203	HIS
1	A	219	GLN
1	A	238	GLN

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Mol	Chain	Res	Type
1	A	315	ASN
1	A	415	GLN
1	A	464	GLN
1	A	488	HIS
1	B	78	GLN
1	B	153	GLN
1	B	343	ASN
1	B	415	GLN
1	B	426	GLN
1	B	454	ASN
1	C	16	ASN
1	C	31	GLN
1	C	50	ASN
1	C	181	ASN
1	C	219	GLN
1	C	225	GLN
1	C	237	GLN
1	C	241	GLN
1	C	245	HIS
1	C	336	ASN
1	C	452	GLN
1	C	470	HIS
1	C	479	GLN
1	C	482	GLN
1	D	16	ASN
1	D	19	HIS
1	D	126	HIS
1	D	153	GLN
1	D	179	GLN
1	D	203	HIS
1	D	237	GLN
1	D	241	GLN
1	D	301	HIS
1	D	375	GLN
1	D	414	HIS
1	D	415	GLN
1	D	479	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 i

### 6.1 Protein, DNA and RNA chains i

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	485/494 (98%)	-0.14	12 (2%) 57 59	46, 70, 94, 115	0
1	B	483/494 (97%)	0.39	35 (7%) 15 15	30, 94, 142, 165	0
1	C	477/494 (96%)	0.19	42 (8%) 10 9	39, 76, 148, 176	0
1	D	454/494 (91%)	0.31	45 (9%) 7 6	46, 73, 165, 188	0
All	All	1899/1976 (96%)	0.18	134 (7%) 16 15	30, 77, 148, 188	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	LEU	7.4
1	C	243	ALA	7.3
1	D	223	MET	6.7
1	D	160	LEU	6.1
1	D	158	PHE	5.5
1	B	252	LEU	5.5
1	B	46	LEU	5.4
1	D	245	HIS	5.1
1	D	159	SER	5.0
1	D	242	ARG	5.0
1	C	139	ILE	4.8
1	B	259	LEU	4.6
1	C	204	GLY	4.5
1	D	182	PHE	4.4
1	D	226	GLY	4.3
1	D	301	HIS	4.3
1	C	177	LEU	4.2
1	D	193	LEU	4.2
1	C	142	ALA	4.2
1	C	157	LEU	4.2
1	C	52	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	182	PHE	4.0
1	D	162	MET	4.0
1	D	161	SER	4.0
1	C	244	ILE	4.0
1	D	219	GLN	3.9
1	A	301	HIS	3.9
1	D	218	LEU	3.9
1	B	254	ILE	3.8
1	C	248	ARG	3.7
1	D	180	GLU	3.7
1	C	240	LYS	3.7
1	D	246	CYS	3.7
1	D	220	GLU	3.6
1	C	171	TYR	3.6
1	C	141	GLY	3.6
1	C	263	LEU	3.6
1	D	164	CYS	3.5
1	D	202	TYR	3.4
1	C	194	ARG	3.4
1	B	249	LEU	3.3
1	B	301	HIS	3.3
1	A	212	SER	3.3
1	B	444	ASP	3.2
1	B	253	GLU	3.2
1	C	180	GLU	3.2
1	C	163	GLY	3.2
1	B	41	ARG	3.1
1	A	445	LEU	3.1
1	D	196	VAL	3.1
1	D	224	ALA	3.1
1	A	137	VAL	3.1
1	C	246	CYS	3.1
1	D	179	GLN	3.1
1	C	89	LEU	3.0
1	B	45	GLY	3.0
1	B	140	GLY	3.0
1	D	139	ILE	3.0
1	D	247	GLY	3.0
1	D	184	ALA	2.9
1	C	196	VAL	2.9
1	C	267	SER	2.9
1	B	180	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	2.9
1	C	202	TYR	2.8
1	C	442	ARG	2.8
1	B	431	LEU	2.8
1	D	197	ALA	2.8
1	C	214	THR	2.7
1	C	140	GLY	2.7
1	C	241	GLN	2.7
1	D	201	ARG	2.7
1	D	151	GLY	2.6
1	C	282	GLN	2.6
1	B	39	LYS	2.6
1	B	435	ILE	2.6
1	A	306	GLN	2.6
1	B	488	HIS	2.6
1	B	52	LEU	2.5
1	D	200	LEU	2.5
1	C	201	ARG	2.5
1	A	26	VAL	2.5
1	A	444	ASP	2.5
1	B	300	LEU	2.5
1	B	285	THR	2.5
1	D	431	LEU	2.4
1	B	40	VAL	2.4
1	D	262	ALA	2.4
1	B	139	ILE	2.4
1	D	434	ALA	2.4
1	B	72	GLN	2.4
1	C	247	GLY	2.4
1	D	195	PRO	2.3
1	D	221	ILE	2.3
1	D	234	GLU	2.3
1	B	163	GLY	2.3
1	C	191	GLU	2.3
1	D	181	ASN	2.3
1	B	144	THR	2.3
1	B	318	ARG	2.2
1	B	242	ARG	2.2
1	D	145	GLU	2.2
1	D	401	LEU	2.2
1	A	211	ALA	2.2
1	A	46	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	200	LEU	2.2
1	C	304	VAL	2.2
1	C	148	THR	2.2
1	B	455	HIS	2.2
1	C	192	VAL	2.2
1	C	159	SER	2.2
1	C	206	LYS	2.1
1	B	202	TYR	2.1
1	C	264	VAL	2.1
1	A	138	ASP	2.1
1	B	47	ASN	2.1
1	A	177	LEU	2.1
1	B	90	ALA	2.1
1	D	358	ALA	2.1
1	D	273	ILE	2.1
1	B	157	LEU	2.1
1	D	235	LYS	2.1
1	D	131	ALA	2.1
1	C	195	PRO	2.1
1	A	428	CYS	2.1
1	C	164	CYS	2.1
1	B	143	SER	2.1
1	C	268	GLY	2.1
1	D	191	GLU	2.1
1	C	137	VAL	2.0
1	B	89	LEU	2.0
1	B	158	PHE	2.0
1	D	152	ALA	2.0
1	C	269	LEU	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	D	502	1/1	0.75	0.07	109,109,109,109	0
2	CL	B	501	1/1	0.77	0.23	115,115,115,115	0
2	CL	A	501	1/1	0.90	0.13	95,95,95,95	0
2	CL	C	501	1/1	0.91	0.25	92,92,92,92	0
2	CL	D	501	1/1	0.91	0.10	77,77,77,77	0
2	CL	C	502	1/1	0.95	0.10	90,90,90,90	0
2	CL	A	502	1/1	0.95	0.12	81,81,81,81	0
2	CL	A	503	1/1	0.96	0.06	81,81,81,81	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.