



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 6PBZ / pdb_00006pbz
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

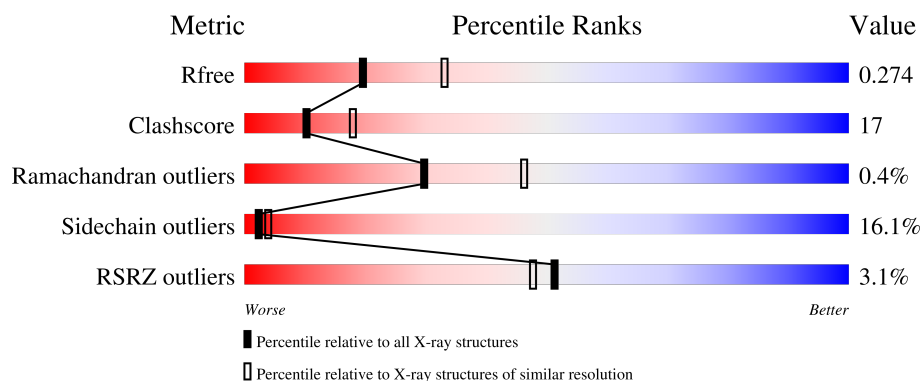
1 Overall quality at a glance

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_{free}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	494	70%25%..
1	B	494	% 55%36%6%.
1	C	494	4% 59%31%6%.
1	D	494	7% 57%28%7%8%

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	N	O	S	0	1	0
			3804	2394	689	703	18			
1	B	483	Total	C	N	O	S	0	0	0
			3787	2385	685	699	18			
1	C	477	Total	C	N	O	S	0	4	0
			3762	2369	684	690	19			
1	D	454	Total	C	N	O	S	0	1	0
			3550	2242	641	650	17			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

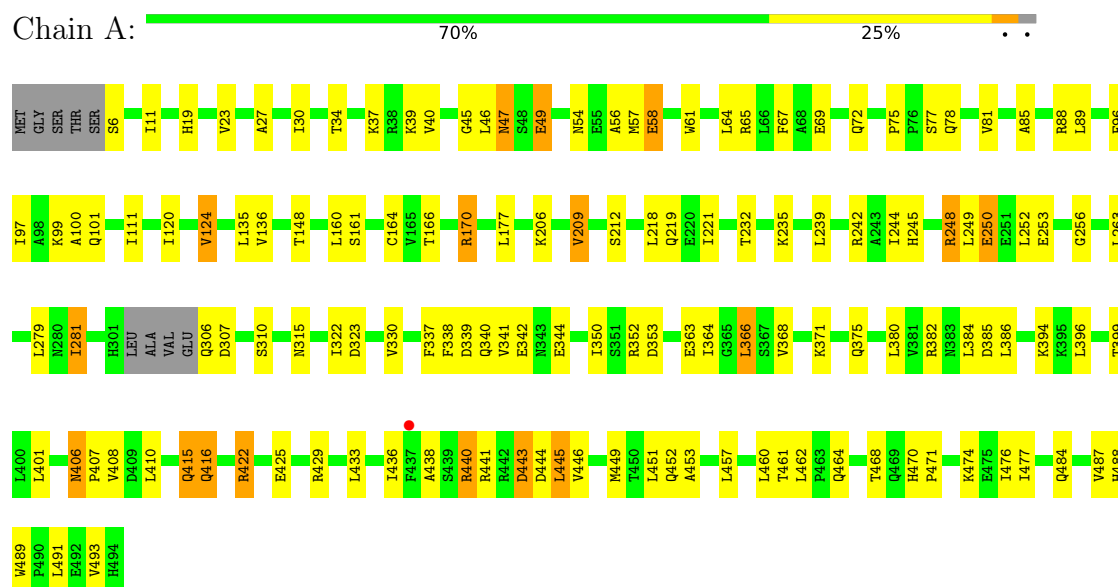
- Molecule 3 is water.

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

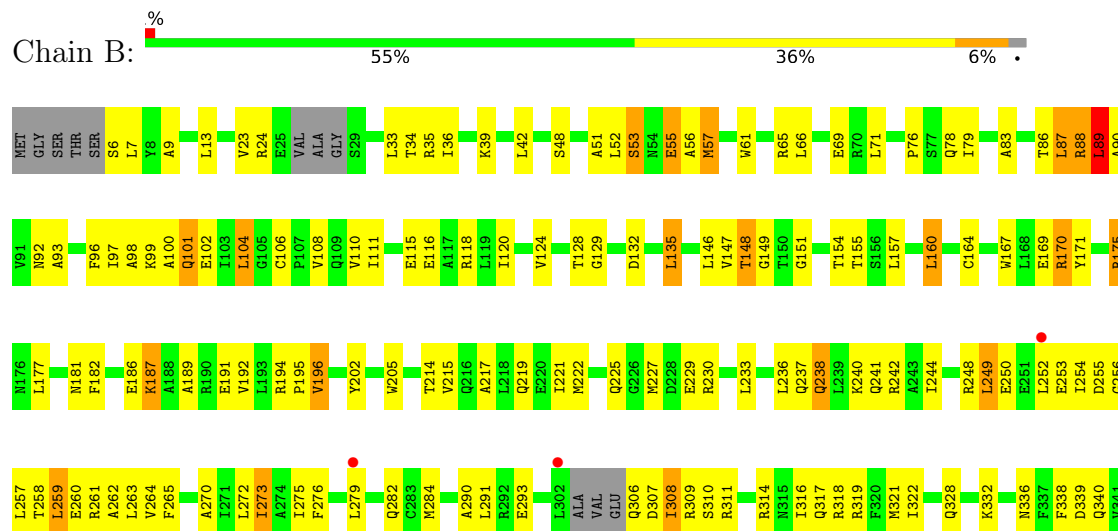
3 Residue-property plots

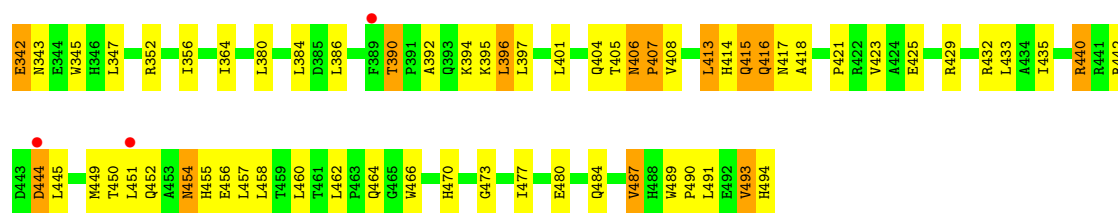
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

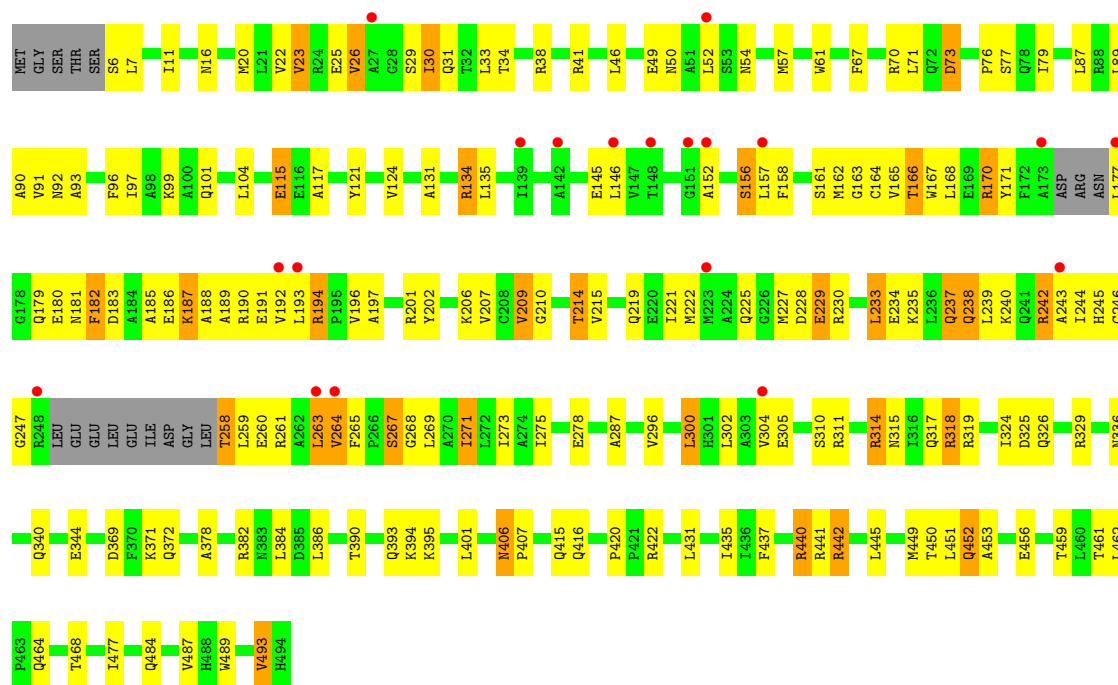


- Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase

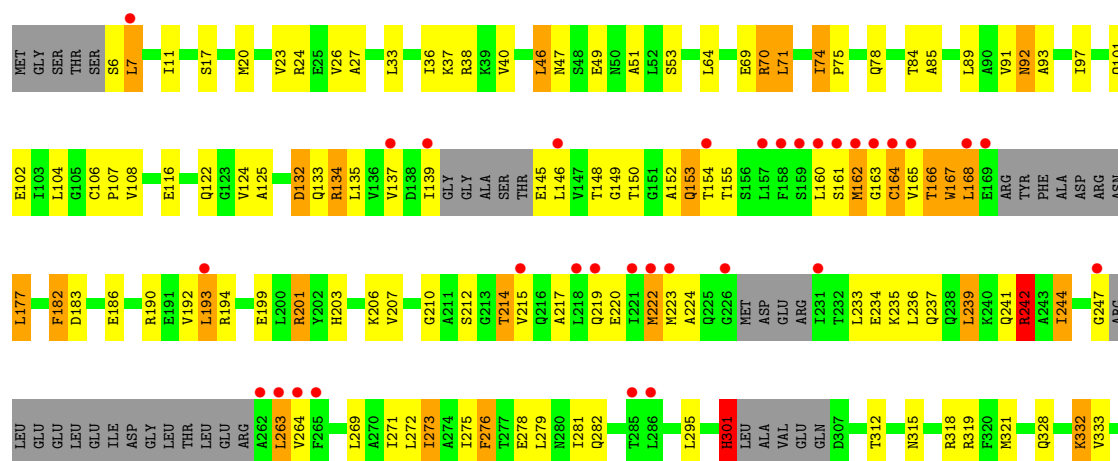




• Molecule 1: Guanosine-5'-triphosphate,3'-diphosphate pyrophosphatase



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.83Å 162.51Å 165.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 2.48 29.46 – 2.48	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.46-2.48) 96.0 (29.46-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.48Å)	Xtriage
Refinement program	PHENIX (dev_3352: ???)	Depositor
R, R_{free}	0.225 , 0.274 0.230 , 0.274	Depositor DCC
R_{free} test set	999 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.53	0/3865	0.71	0/5236
1	B	0.45	0/3847	0.70	1/5210 (0.0%)
1	C	0.55	0/3822	0.80	3/5176 (0.1%)
1	D	0.54	0/3605	0.79	2/4882 (0.0%)
All	All	0.52	0/15139	0.75	6/20504 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	242	ARG	N-CA-C	-7.48	103.61	112.89
1	C	182	PHE	N-CA-C	-6.54	104.07	111.07
1	B	455	HIS	N-CA-C	-5.61	99.31	108.67
1	C	182	PHE	CA-C-N	5.51	129.09	120.82
1	C	182	PHE	C-N-CA	5.51	129.09	120.82
1	D	301	HIS	CA-C-O	-5.38	111.66	120.80

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	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3787	0	3837	150	0
1	C	3762	0	3814	157	0
1	D	3550	0	3606	137	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
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	512	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 17.

All (512) 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:HE21	1:D:464[A]:GLN:HA	1.24	1.02
1:D:222:MET:HE3	1:D:235:LYS:HD3	1.39	1.01
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	1.56	0.88
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:C:162:MET:HE3	1:C:189:ALA:HB1	1.58	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:CD1	1:B:160:LEU:CD2	2.57	0.83
1:B:175:ARG:HB2	1:B:175:ARG:CZ	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:O	1:D:168:LEU:HD12	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
1:D:84:THR:HG22	1:D:85:ALA:H	1.48	0.79
1:D:167:TRP:HH2	1:D:192:VAL:HG21	1.47	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: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:C:182:PHE:C	1:C:186:GLU:HG3	2.13	0.74
1:D:168:LEU:HD12	1:D:168:LEU:C	2.13	0.74
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:162:MET:HE3	1:C:189:ALA:CB	2.23	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
1:A:408:VAL:HB	1:A:487:VAL:HG21	1.76	0.67
1:C:157:LEU:HD23	1:C:157:LEU:O	1.95	0.67
1:D:223:MET:HE1	1:D:391:PRO:CB	2.25	0.66
1:B:416:GLN:HG2	1:B:418:ALA:H	1.60	0.66
1:C:222:MET:HE3	1:C:235:LYS:HD3	1.76	0.66
1:C:186:GLU:O	1:C:190:ARG:HG3	1.96	0.66
1:C:233:LEU:HD13	1:C:233:LEU:H	1.60	0.66
1:B:444:ASP:OD1	1:B:445:LEU:HD23	1.96	0.65
1:B:175:ARG:O	1:B:248:ARG:HA	1.96	0.65
1:C:222:MET:HE1	1:C:230:ARG:O	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:20:MET:HE1	1:D:70:ARG:HD2	1.79	0.64
1:D:301:HIS:CD2	1:D:301:HIS:H	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:39:LYS:HD3	1:C:245:HIS:CD2	2.33	0.64
1:B:146:LEU:CD1	1:B:160:LEU:HD23	2.28	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:186:GLU:OE2	1:D:273:ILE:HD11	1.98	0.63
1:D:236:LEU:HD13	1:D:273:ILE:HG22	1.81	0.63
1:D:456:GLU:CD	1:D:456:GLU:H	2.06	0.63
1:A:440:ARG:HB3	1:A:445:LEU:HD23	1.81	0.62
1:C:29:SER:HB3	1:C:315[A]:ASN:CG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:350:ILE:HD12	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
1:C:416:GLN:NE2	2:C:501:CL:CL	2.68	0.61
1:D:464[A]:GLN:HE21	1:D:464[A]:GLN:CA	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:B:146:LEU:CD1	1:B:160:LEU:HD22	2.31	0.60
1:A:57:MET:HE2	1:A:96:PHE:HB2	1.84	0.60
1:A:307:ASP:OD2	1:A:310:SER:HB2	2.01	0.59
1:C:157:LEU:HD23	1:C:157:LEU:C	2.27	0.59
1:D:222:MET:HE1	1:D:235:LYS:HD3	1.81	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:B:250:GLU:CD	1:C:263:LEU:CD1	2.77	0.58
1:D:164:CYS:SG	1:D:264:VAL:HG11	2.44	0.58
1:B:440:ARG:NH2	3:B:603:HOH:O	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:LEU:H	1:B:92:ASN:HB3	1.71	0.56
1:B:149:GLY:HA2	1:B:155:THR:HG23	1.87	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:HD23	1:C:263:LEU:H	1.70	0.55
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:D:222:MET:HE3	1:D:235:LYS:CD	2.26	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: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:HH11	1:C:170:ARG:CG	2.08	0.54
1:D:163:GLY:C	1:D:166:THR:HG23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:182:PHE:C	1:C:186:GLU:CG	2.80	0.53
1:A:384:LEU:O	1:A:394:LYS:NZ	2.37	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
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:N	1:C:263:LEU:CD2	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:61:TRP:O	1:A:65:ARG:HG3	2.10	0.51
1:A:375[A]:GLN:NE2	3:A:609:HOH:O	2.42	0.51
1:C:390:THR:HG22	1:C:393:GLN:CD	2.36	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:CD2	1:D:7:LEU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:406:ASN:O	1:B:407:PRO:C	2.55	0.50
1:B:9:ALA:HB3	1:B:79:ILE:HG12	1.94	0.50
1:C:20:MET:HE1	1:C:70:ARG:HD2	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:C:57:MET:HE3	1:C:96:PHE:HB2	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:168:LEU:C	1:D:168:LEU:CD1	2.84	0.49
1:B:89:LEU:O	1:B:90:ALA:C	2.55	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
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:425:GLU:HG2	1:A:489:TRP:HZ2	1.77	0.49
1:A:443:ASP:O	1:A:446:VAL:HG22	2.13	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:O	1:D:49:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LEU:HD23	1:D:162:MET:HE2	1.96	0.48
1:A:443:ASP:OD1	1:A:443:ASP:N	2.35	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:53:SER:OG	1:B:55:GLU:OE1	2.20	0.47
1:B:170:ARG:HG3	1:B:171:TYR:CD2	2.49	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
1:A:474:LYS:HE2	1:A:474:LYS:HB3	1.58	0.47
1:B:98:ALA:O	1:B:102:GLU:HG2	2.14	0.47
1:B:236:LEU:HD21	1:B:272:LEU:HD23	1.97	0.47
1:B:262:ALA:HA	1:B:265:PHE:HB2	1.96	0.47
1:B:473:GLY:O	1:B:477:ILE:HG13	2.15	0.47
1:C:20:MET:HE1	1:C:70:ARG:HH11	1.79	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:B:13:LEU:HB2	1:B:83:ALA:HA	1.97	0.47
1:C:164:CYS:HB2	1:C:264:VAL:HG22	1.97	0.47
1:C:197:ALA:HB2	1:C:278:GLU:OE2	2.14	0.47
1:C:305:GLU:CD	1:C:314:ARG:HH22	2.23	0.47
1:D:46:LEU:HD12	1:D:46:LEU:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:429:ARG:HG2	1:B:489:TRP:CE3	2.50	0.46
1:B:466:TRP:CE2	1:B:470:HIS:ND1	2.84	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:HH11	1:D:201:ARG:HB2	1.81	0.46
1:B:52:LEU:H	1:B:92:ASN:CB	2.28	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: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:73:ASP:OD2	1:D:442:ARG:HD3	2.16	0.46
1:C:452:GLN:HG2	1:C:459:THR:O	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: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:HD23	1:B:397:LEU:HA	1.74	0.45
1:B:480:GLU:O	1:B:484:GLN:HG3	2.16	0.45
1:A:322:ILE:HD11	1:A:364:ILE:HB	1.98	0.45
1:A:363:GLU:OE1	1:A:441:ARG:NH2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:HA	1:A:88:ARG:HG2	1.97	0.45
1:B:250:GLU:OE1	1:C:263:LEU:HD11	2.17	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:D:456:GLU:CD	1:D:456:GLU:N	2.75	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:D:190:ARG:O	1:D:194:ARG:HB2	2.17	0.45
1:C:145:GLU:C	1:C:146:LEU:HD12	2.42	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:61:TRP:CZ2	1:B:99:LYS:HB3	2.52	0.44
1:B:106:CYS:HB2	3:B:610:HOH:O	2.18	0.44
1:D:312:THR:OG1	1:D:387:PRO:O	2.35	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:HA	1:D:242:ARG:HD2	1.34	0.44
1:A:382:ARG:HD3	3:A:630:HOH:O	2.18	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: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:A:250:GLU:HB2	1:D:263:LEU:HD13	2.01	0.43
1:D:182:PHE:CE2	1:D:244:ILE:HG12	2.52	0.43
1:B:392:ALA:C	1:B:418:ALA:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:MET:HE3	1:A:57:MET:HB2	1.79	0.43
1:A:422:ARG:HA	1:A:422:ARG:HD3	1.64	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:250:GLU:OE2	1:C:263:LEU:CD1	2.67	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:A:136:VAL:HA	1:A:209:VAL:O	2.19	0.43
1:B:101:GLN:CD	1:B:108:VAL:H	2.27	0.43
1:B:262:ALA:HA	1:B:265:PHE:CB	2.49	0.43
1:C:194:ARG:HD2	1:C:194:ARG:HA	1.79	0.43
1:B:100:ALA:O	1:B:104:LEU:HG	2.19	0.43
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:A:440:ARG:HA	1:A:440:ARG:HD3	1.73	0.43
1:C:46:LEU:HD21	1:C:89:LEU:HD11	2.01	0.43
1:C:222:MET:HE2	1:C:228:ASP:O	2.19	0.43
1:D:92:ASN:O	1:D:93:ALA:C	2.61	0.43
1:D:380:LEU:HD23	1:D:380:LEU:HA	1.86	0.43
1:A:415:GLN:HE21	1:A:415:GLN:HB3	1.55	0.42
1:D:84:THR:HG23	1:D:116:GLU:OE1	2.19	0.42
1:D:223:MET:HE1	1:D:391:PRO:C	2.44	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:HB2	1:D:201:ARG:NH1	2.34	0.42
1:A:61:TRP:CZ2	1:A:99:LYS:HD3	2.54	0.42
1:A:449:MET:HG2	1:A:462:LEU:HD23	2.00	0.42
1:B:97:ILE:HG22	1:B:101:GLN:HE22	1.84	0.42
1:B:321:MET:HE2	1:B:321:MET:HB3	1.86	0.42
1:C:193:LEU:HD21	1:C:275:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:36:ILE:HD13	1:D:36:ILE:HA	1.83	0.42
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.93	0.42
1:B:57:MET:HE2	1:B:57:MET:HB2	1.95	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:61:TRP:CE3	1:B:99:LYS:HD3	2.55	0.42
1:B:308:ILE:O	1:B:311:ARG:N	2.52	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:D:409:ASP:OD1	1:D:409:ASP:C	2.63	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:HE21	1:D:153:GLN:HA	1.85	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:HE21	1:C:219:GLN:HA	1.85	0.42
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:308:ILE:O	1:B:309:ARG:C	2.64	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:B:444:ASP:C	1:B:445:LEU:HD23	2.45	0.41
1:C:30:ILE:CG1	1:C:300:LEU:HD21	2.48	0.41
1:C:319:ARG:HG2	1:D:321:MET:HE2	2.02	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:D:332:LYS:HG3	1:D:333:VAL:N	2.34	0.41
1:A:11:ILE:HD12	1:A:67:PHE:CD2	2.55	0.41
1:A:30:ILE:HG21	1:A:30:ILE:HD13	1.68	0.41
1:A:363:GLU:CD	1:A:441:ARG:NH2	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:ASN:HD21	1:A:49:GLU:HB2	1.85	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD12	1.86	0.41
1:B:89:LEU:HD12	1:B:89:LEU:HA	1.72	0.41
1:C:38:ARG:HD2	1:C:67:PHE:CE1	2.55	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: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:39:LYS:HB3	1:A:39:LYS:HE2	1.91	0.41
1:A:385:ASP:O	1:A:386:LEU:HD23	2.21	0.41
1:A:470:HIS:HB3	1:B:69:GLU:OE2	2.21	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: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: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:13:LEU:HD12	1:B:83:ALA:HB2	2.02	0.40
1:B:160:LEU:HD11	1:B:196:VAL:HG11	2.02	0.40
1:B:250:GLU:CD	1:C:263:LEU:HD12	2.46	0.40
1:C:38:ARG:HD2	1:C:67:PHE:HE1	1.86	0.40
1:C:187:LYS:O	1:C:191:GLU:HG3	2.21	0.40
1:C:229:GLU:OE1	1:C:390:THR:OG1	2.37	0.40
1:D:443:ASP:O	1:D:446:VAL:HG13	2.22	0.40
1:B:53:SER:O	1:B:57:MET:HE2	2.21	0.40
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:30:ILE:HD13	1:C:300:LEU:HD11	2.03	0.40
1:C:190:ARG:O	1:C:194:ARG:N	2.55	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/494 (98%)	463 (96%)	18 (4%)	1 (0%)	43	61
1	B	477/494 (97%)	448 (94%)	26 (6%)	3 (1%)	21	35
1	C	475/494 (96%)	449 (94%)	25 (5%)	1 (0%)	43	61
1	D	443/494 (90%)	419 (95%)	22 (5%)	2 (0%)	24	40
All	All	1877/1976 (95%)	1779 (95%)	91 (5%)	7 (0%)	30	46

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

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%)	360 (89%)	44 (11%)	6	11
1	B	403/410 (98%)	328 (81%)	75 (19%)	1	2
1	C	399/410 (97%)	333 (84%)	66 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	378/410 (92%)	308 (82%)	70 (18%)	1	2
All	All	1584/1640 (97%)	1329 (84%)	255 (16%)	2	4

All (255) 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	77	SER
1	A	89	LEU
1	A	97	ILE
1	A	101	GLN
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	170	ARG
1	A	206	LYS
1	A	209	VAL
1	A	212	SER
1	A	219	GLN
1	A	248	ARG
1	A	249	LEU
1	A	250	GLU
1	A	252	LEU
1	A	263	LEU
1	A	281	ILE
1	A	306	GLN
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	436	ILE
1	A	440	ARG

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Mol	Chain	Res	Type
1	A	443	ASP
1	A	444	ASP
1	A	445	LEU
1	A	457	LEU
1	A	461	THR
1	A	464	GLN
1	A	468	THR
1	A	476	ILE
1	B	23	VAL
1	B	35	ARG
1	B	42	LEU
1	B	48	SER
1	B	53	SER
1	B	55	GLU
1	B	57	MET
1	B	71	LEU
1	B	86	THR
1	B	87	LEU
1	B	88	ARG
1	B	89	LEU
1	B	101	GLN
1	B	104	LEU
1	B	110	VAL
1	B	124	VAL
1	B	135	LEU
1	B	148	THR
1	B	154	THR
1	B	160	LEU
1	B	169	GLU
1	B	170	ARG
1	B	175	ARG
1	B	177	LEU
1	B	181	ASN
1	B	182	PHE
1	B	187	LYS
1	B	192	VAL
1	B	196	VAL
1	B	202	TYR
1	B	214	THR
1	B	215	VAL
1	B	219	GLN
1	B	222	MET

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Mol	Chain	Res	Type
1	B	227	MET
1	B	238	GLN
1	B	241	GLN
1	B	244	ILE
1	B	249	LEU
1	B	252	LEU
1	B	253	GLU
1	B	258	THR
1	B	259	LEU
1	B	263	LEU
1	B	273	ILE
1	B	276	PHE
1	B	282	GLN
1	B	284	MET
1	B	291	LEU
1	B	306	GLN
1	B	307	ASP
1	B	308	ILE
1	B	318	ARG
1	B	319	ARG
1	B	328	GLN
1	B	342	GLU
1	B	345	TRP
1	B	356	ILE
1	B	390	THR
1	B	396	LEU
1	B	401	LEU
1	B	413	LEU
1	B	415	GLN
1	B	416	GLN
1	B	417	ASN
1	B	423	VAL
1	B	440	ARG
1	B	444	ASP
1	B	452	GLN
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

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Mol	Chain	Res	Type
1	C	23	VAL
1	C	26	VAL
1	C	30	ILE
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	104	LEU
1	C	115	GLU
1	C	124	VAL
1	C	134	ARG
1	C	135	LEU
1	C	156	SER
1	C	161	SER
1	C	166	THR
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	227	MET
1	C	229	GLU
1	C	233	LEU
1	C	234	GLU
1	C	237	GLN
1	C	238	GLN
1	C	242	ARG
1	C	258	THR
1	C	259	LEU
1	C	260	GLU
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	264	VAL
1	C	267	SER
1	C	271	ILE
1	C	296	VAL
1	C	300	LEU
1	C	304	VAL
1	C	310	SER
1	C	314	ARG
1	C	318	ARG
1	C	325	ASP
1	C	372	GLN
1	C	401	LEU
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	461	THR
1	C	464	GLN
1	C	468	THR
1	C	487	VAL
1	C	493	VAL
1	D	6	SER
1	D	7	LEU
1	D	17	SER
1	D	23	VAL
1	D	33	LEU
1	D	37	LYS
1	D	40	VAL
1	D	46	LEU
1	D	53	SER
1	D	70	ARG
1	D	71	LEU
1	D	74	ILE
1	D	89	LEU
1	D	91	VAL
1	D	92	ASN
1	D	102	GLU
1	D	122	GLN
1	D	124	VAL
1	D	132	ASP

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Mol	Chain	Res	Type
1	D	134	ARG
1	D	135	LEU
1	D	145	GLU
1	D	148	THR
1	D	153	GLN
1	D	154	THR
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
1	D	182	PHE
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	244	ILE
1	D	263	LEU
1	D	273	ILE
1	D	276	PHE
1	D	281	ILE
1	D	282	GLN
1	D	295	LEU
1	D	301	HIS
1	D	328	GLN
1	D	332	LYS
1	D	343	ASN
1	D	346	HIS
1	D	352	ARG
1	D	375	GLN
1	D	395	LYS
1	D	411	SER
1	D	413	LEU
1	D	416	GLN

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Mol	Chain	Res	Type
1	D	442	ARG
1	D	446	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	50	ASN
1	A	181	ASN
1	A	203	HIS
1	A	219	GLN
1	A	238	GLN
1	A	315	ASN
1	A	415	GLN
1	A	452	GLN
1	A	464	GLN
1	A	482	GLN
1	A	488	HIS
1	B	19	HIS
1	B	78	GLN
1	B	153	GLN
1	B	343	ASN
1	B	375	GLN
1	B	415	GLN
1	B	454	ASN
1	C	16	ASN
1	C	31	GLN
1	C	219	GLN
1	C	225	GLN
1	C	237	GLN
1	C	245	HIS
1	C	336	ASN
1	C	346	HIS
1	C	372	GLN
1	C	375	GLN

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Mol	Chain	Res	Type
1	C	406	ASN
1	C	417	ASN
1	C	470	HIS
1	C	482	GLN
1	C	488	HIS
1	D	16	ASN
1	D	19	HIS
1	D	122	GLN
1	D	126	HIS
1	D	133	GLN
1	D	153	GLN
1	D	179	GLN
1	D	203	HIS
1	D	219	GLN
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 oligosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	485/494 (98%)	-0.15	1 (0%) 91 90	29, 70, 94, 115	1 (0%)
1	B	483/494 (97%)	0.29	6 (1%) 76 74	30, 94, 142, 165	0
1	C	477/494 (96%)	0.21	19 (3%) 42 38	23, 76, 148, 176	4 (0%)
1	D	454/494 (91%)	0.25	33 (7%) 21 18	32, 73, 165, 188	1 (0%)
All	All	1899/1976 (96%)	0.15	59 (3%) 51 48	23, 77, 148, 188	6 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	221	ILE	4.7
1	B	444	ASP	4.5
1	D	219	GLN	4.0
1	C	157	LEU	3.8
1	D	218	LEU	3.8
1	D	164	CYS	3.7
1	C	173	ALA	3.7
1	C	304	VAL	3.5
1	D	137	VAL	3.5
1	D	163	GLY	3.4
1	D	7	LEU	3.2
1	D	226	GLY	3.2
1	C	243	ALA	3.1
1	D	262	ALA	3.0
1	C	177	LEU	3.0
1	D	231	ILE	2.9
1	D	159	SER	2.9
1	D	165	VAL	2.9
1	D	223	MET	2.9
1	D	139	ILE	2.8
1	D	222	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	158	PHE	2.8
1	B	451	LEU	2.7
1	C	142	ALA	2.7
1	B	302	LEU	2.7
1	C	52	LEU	2.7
1	D	169	GLU	2.7
1	C	223[A]	MET	2.6
1	D	263	LEU	2.6
1	C	192	VAL	2.6
1	C	263	LEU	2.5
1	C	152	ALA	2.5
1	C	248	ARG	2.5
1	D	168	LEU	2.5
1	C	264	VAL	2.5
1	D	162	MET	2.5
1	D	215	VAL	2.4
1	D	285	THR	2.4
1	B	252	LEU	2.4
1	D	160	LEU	2.4
1	D	464[A]	GLN	2.4
1	C	139	ILE	2.3
1	C	151	GLY	2.3
1	C	146	LEU	2.3
1	C	193	LEU	2.3
1	C	27	ALA	2.2
1	B	279	LEU	2.2
1	A	437	PHE	2.2
1	D	157	LEU	2.2
1	D	161	SER	2.1
1	B	389	PHE	2.1
1	D	247	GLY	2.1
1	D	193	LEU	2.1
1	D	264	VAL	2.1
1	D	146	LEU	2.1
1	D	154	THR	2.1
1	D	265	PHE	2.0
1	D	286	LEU	2.0
1	C	148	THR	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 [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	501	1/1	0.83	0.10	115,115,115,115	0
2	CL	D	502	1/1	0.83	0.13	109,109,109,109	0
2	CL	C	502	1/1	0.91	0.09	90,90,90,90	0
2	CL	A	501	1/1	0.92	0.18	95,95,95,95	0
2	CL	A	502	1/1	0.93	0.07	81,81,81,81	0
2	CL	C	501	1/1	0.93	0.16	92,92,92,92	0
2	CL	D	501	1/1	0.96	0.05	77,77,77,77	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.