Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:22 AM EDT

PDB ID	:	1E9R
Title	:	Bacterial conjugative coupling protein TrwBdeltaN70. Trigonal form in complex with sulphate.
Authors	:	Gomis-Rueth, F.X.; Moncalian, G.; Cabezon, E.; de la Cruz, F.; Coll, M.
Deposited on	:	2000-10-26
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

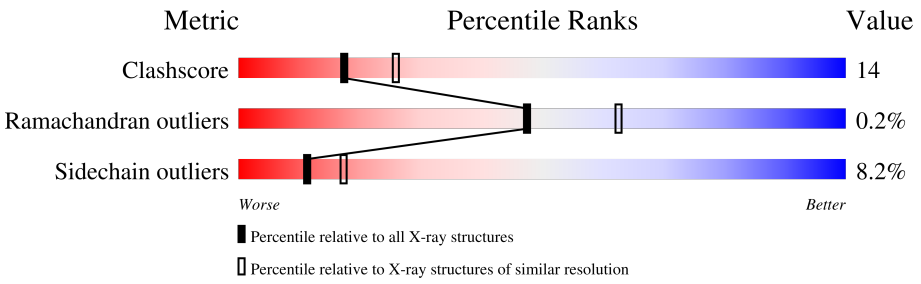
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	68% 24% • •
1	B	437	69% 24% • •
1	D	437	65% 27% • 5%
1	E	437	71% 21% • •
1	F	437	68% 24% • 5%
1	G	437	68% 24% • 5%

2 Entry composition (i)

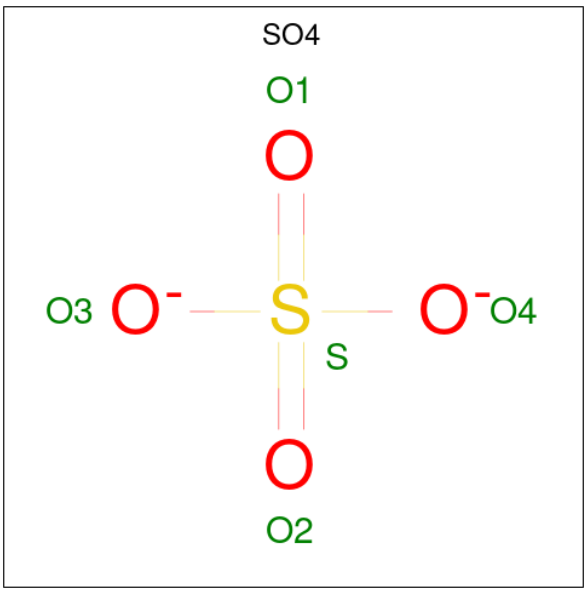
There are 3 unique types of molecules in this entry. The entry contains 20718 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3292	2081	590	611	10	0	0	0
1	B	422	3311	2093	593	615	10	0	0	0
1	D	415	3254	2059	581	604	10	0	0	0
1	E	419	3285	2076	589	610	10	0	0	0
1	F	416	3265	2065	585	605	10	0	0	0
1	G	417	3274	2070	587	607	10	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0
			Total	O	S		
2	E	1	5	4	1	0	0
			Total	O	S		
2	F	1	5	4	1	0	0
			Total	O	S		
2	F	1	5	4	1	0	0
			Total	O	S		
2	F	1	5	4	1	0	0
			Total	O	S		
2	G	1	5	4	1	0	0
			Total	O	S		
2	G	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	201	201	201	0	0
			Total	O		
3	B	174	174	174	0	0
			Total	O		
3	D	148	148	148	0	0
			Total	O		
3	E	122	122	122	0	0
			Total	O		
3	F	133	133	133	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	G	184	184	184	0	0

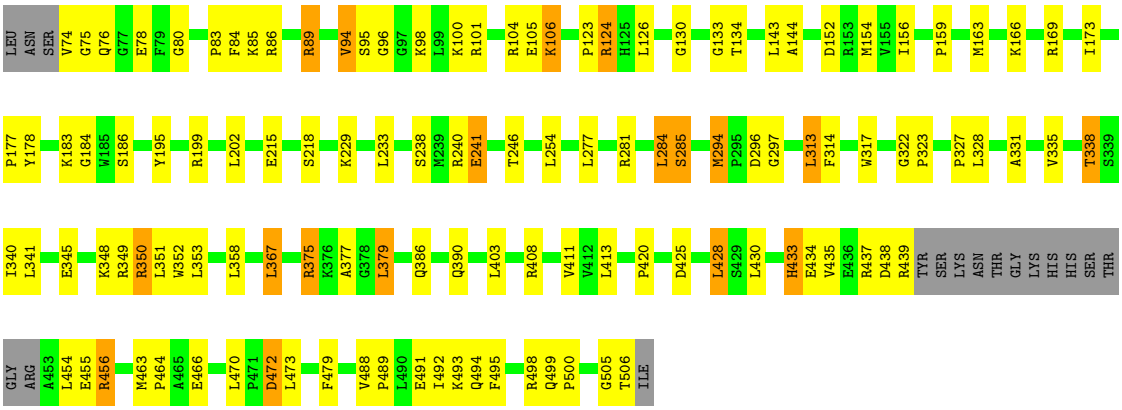
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

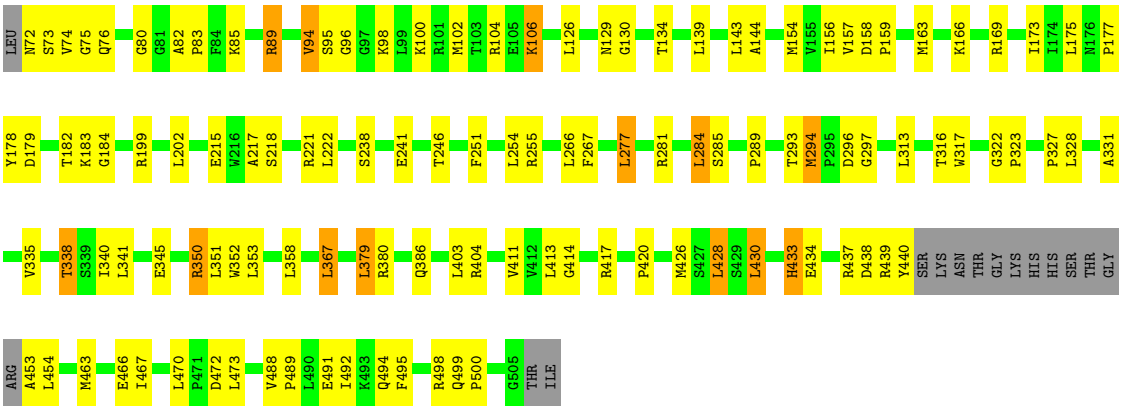
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain A:



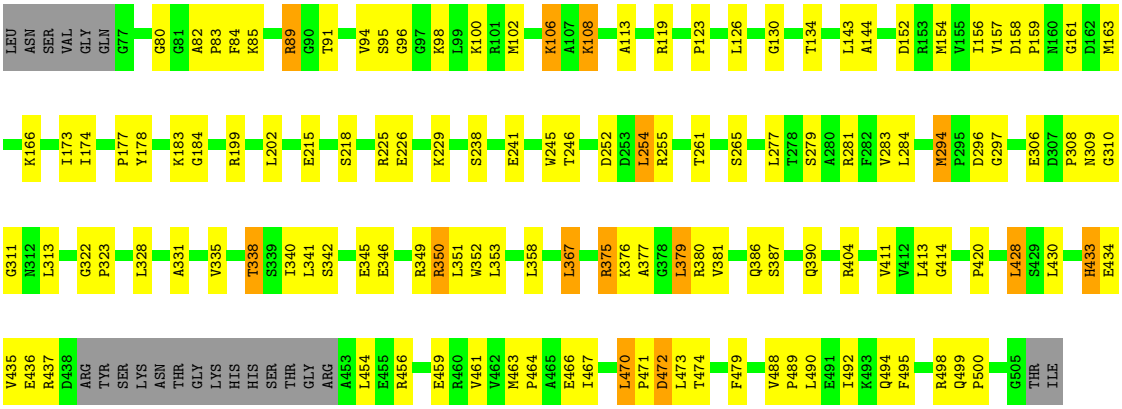
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain B:



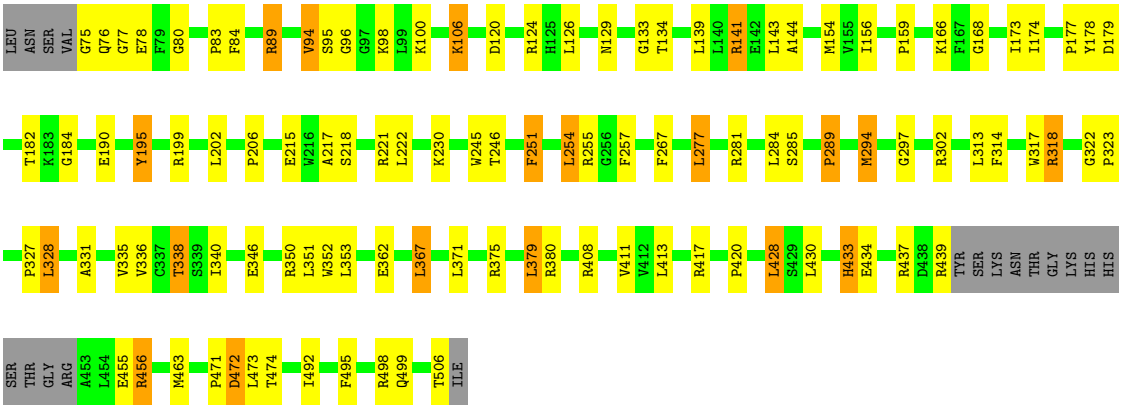
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain D:



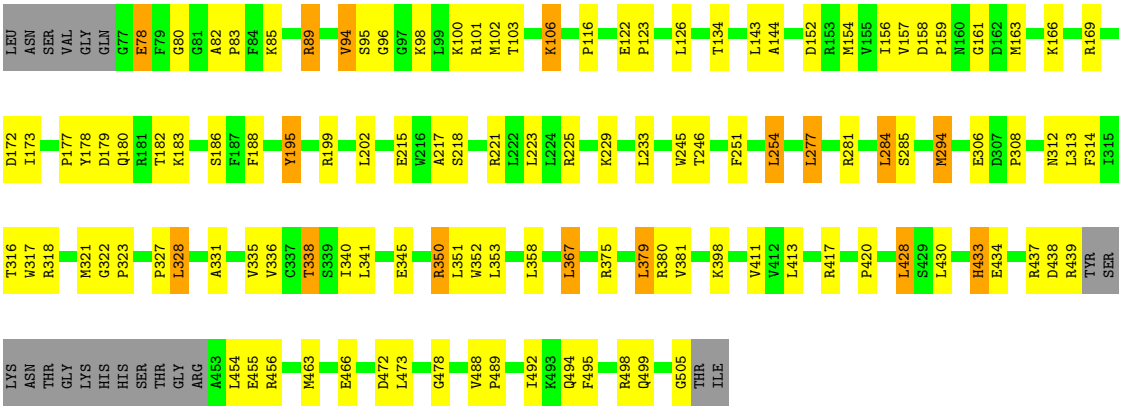
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain E:



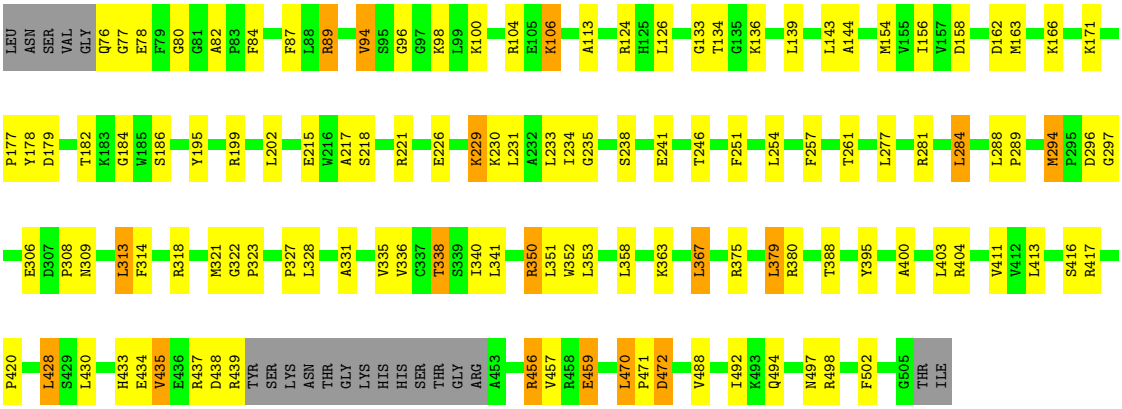
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain F:



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain G:


LEU ASN SER VAL GLY Q76 G77 E78 F79 G80 G81 A82 P83 F84 F87 L88 R89 V94 S95 G96 G97 K98 L99 K100 R104 E105 K106 A113 R124 H125 L126 G133 T134 G135 K136 L139 L143 A144 M154 V155 I156 V157 D158 D162 M163 K166 K171
P177 Y178 D179 T182 K183 G184 W185 S186 Y195 R199 L202 E215 W216 A217 S218 R221 E226 K229 K230 L231 A232 L233 I234 G235 S238 E241 T246 F251 L254 F257 T261 L277 R281 L284 L288 P289 M294 P295 D296 G297
E306 D307 P308 N309 L313 F314 R318 M321 G322 P323 P327 L328 A331 V335 V336 C337 T338 S339 I340 L341 R350 L351 W352 L353 L358 K363 L367 R375 L379 R380 T388 Y395 A400 L403 R404 V411 V412 L413 S416 R417
P420 L428 S429 L430 H433 E434 V435 E436 R437 D438 R439 TYR SER LYS ASN THR GLY LYS HIS HIS SER THR GLY ARG A453 R456 V457 R458 E459 L470 P471 D472 V488 I492 K493 Q494 N497 R498 F502 G505 THR ILE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.30Å 151.30Å 258.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.9 (50.00-2.40)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20718	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

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: SO4

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	0.39	0/3356	0.68	1/4536 (0.0%)
1	B	0.39	0/3376	0.66	0/4563
1	D	0.40	0/3318	0.64	0/4485
1	E	0.40	0/3349	0.67	0/4526
1	F	0.40	0/3329	0.65	0/4499
1	G	0.41	0/3338	0.67	0/4511
All	All	0.40	0/20066	0.66	1/27120 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	195	TYR	Sidechain

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	3292	0	3323	110	0
1	B	3311	0	3336	90	0
1	D	3254	0	3283	107	0
1	E	3285	0	3314	81	0
1	F	3265	0	3296	94	0
1	G	3274	0	3304	107	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	D	20	0	0	0	0
2	E	10	0	0	0	0
2	F	15	0	0	0	0
2	G	10	0	0	0	0
3	A	201	0	0	9	0
3	B	174	0	0	7	0
3	D	148	0	0	2	0
3	E	122	0	0	4	0
3	F	133	0	0	7	0
3	G	184	0	0	9	0
All	All	20718	0	19856	547	0

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

All (547) 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:375:ARG:HH11	1:D:375:ARG:HB3	1.20	1.02
1:D:108:LYS:H	1:D:108:LYS:HD2	1.25	0.98
1:G:350:ARG:HG3	1:G:350:ARG:HH11	1.26	0.98
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.32	0.94
1:A:75:GLY:H	1:A:83:PRO:HB3	1.33	0.93
1:E:177:PRO:HB3	1:E:294:MET:HG2	1.51	0.91
1:D:350:ARG:HB2	1:D:350:ARG:HH11	1.41	0.86
1:A:375:ARG:HH11	1:A:375:ARG:HB3	1.42	0.85
1:G:229:LYS:NZ	1:G:229:LYS:HB3	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:THR:O	1:F:281:ARG:HD2	1.77	0.84
1:F:89:ARG:HD2	1:F:434:GLU:OE1	1.78	0.84
1:E:89:ARG:HD2	1:E:434:GLU:OE1	1.78	0.83
1:G:178:TYR:CE1	1:G:321:MET:HE1	2.16	0.80
1:A:124:ARG:HG3	1:A:124:ARG:NH1	1.90	0.80
1:G:229:LYS:HB3	1:G:229:LYS:HZ2	1.46	0.80
1:D:246:THR:O	1:D:281:ARG:HD2	1.80	0.79
1:G:246:THR:O	1:G:281:ARG:HD2	1.82	0.79
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.66	0.78
1:A:89:ARG:HD2	1:A:434:GLU:OE1	1.84	0.77
1:B:246:THR:O	1:B:281:ARG:HD2	1.84	0.77
1:B:350:ARG:HH11	1:B:350:ARG:HB2	1.50	0.77
1:F:463:MET:SD	1:G:89:ARG:HD3	2.26	0.76
1:A:456:ARG:HD3	1:G:82:ALA:CB	2.16	0.76
1:B:72:ASN:HD21	1:B:438:ASP:HB2	1.51	0.76
1:B:473:LEU:HD11	1:B:492:ILE:HD11	1.68	0.75
1:F:350:ARG:HH11	1:F:350:ARG:HB2	1.49	0.75
1:E:246:THR:O	1:E:281:ARG:HD2	1.85	0.75
1:F:96:GLY:O	1:F:100:LYS:HG3	1.86	0.74
1:B:166:LYS:HD3	1:B:495:PHE:HB2	1.70	0.74
1:D:199:ARG:HE	1:D:338:THR:HG22	1.51	0.74
1:A:246:THR:O	1:A:281:ARG:HD2	1.86	0.74
1:E:154:MET:HE3	1:E:156:ILE:HD11	1.70	0.74
1:D:89:ARG:HD2	1:D:434:GLU:OE1	1.87	0.74
1:G:367:LEU:HD13	1:G:403:LEU:HD11	1.70	0.74
1:D:345:GLU:CD	1:D:345:GLU:H	1.91	0.73
1:G:154:MET:CE	1:G:156:ILE:HD11	2.19	0.73
1:D:375:ARG:HB3	1:D:375:ARG:NH1	2.01	0.73
1:E:473:LEU:HD11	1:E:492:ILE:HD11	1.70	0.73
1:B:73:SER:HA	1:B:76:GLN:HE21	1.54	0.73
1:D:226:GLU:HG3	1:D:261:THR:HB	1.71	0.73
1:G:89:ARG:HD2	1:G:434:GLU:OE1	1.87	0.73
1:A:420:PRO:HB2	1:B:428:LEU:HD13	1.72	0.72
1:G:226:GLU:HG3	1:G:261:THR:HB	1.72	0.72
1:D:350:ARG:HH11	1:D:350:ARG:CB	2.03	0.72
1:F:199:ARG:HE	1:F:338:THR:HG22	1.55	0.71
1:B:94:VAL:HG22	1:B:98:LYS:HD3	1.70	0.71
1:E:350:ARG:HG2	1:E:380:ARG:CZ	2.19	0.71
1:F:345:GLU:CD	1:F:345:GLU:H	1.90	0.71
1:E:463:MET:SD	1:F:89:ARG:HD3	2.31	0.71
1:A:345:GLU:CD	1:A:345:GLU:H	1.94	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:ILE:HD13	1:F:379:LEU:HG	1.73	0.70
1:A:199:ARG:HE	1:A:338:THR:HG22	1.57	0.70
1:B:144:ALA:HB1	1:B:154:MET:HE1	1.72	0.70
1:A:124:ARG:HH11	1:A:124:ARG:CG	2.05	0.70
1:B:154:MET:HB3	1:B:352:TRP:HB2	1.74	0.69
1:F:94:VAL:HG13	1:F:98:LYS:HB3	1.73	0.69
1:F:180:GLN:HB2	1:F:505:GLY:HA2	1.73	0.68
1:A:439:ARG:HA	1:A:439:ARG:NE	2.07	0.68
1:F:78:GLU:HB3	3:F:2004:HOH:O	1.94	0.68
1:D:82:ALA:CB	1:E:456:ARG:HD3	2.23	0.67
1:B:166:LYS:O	1:B:498:ARG:HD2	1.94	0.67
1:G:154:MET:HE3	1:G:156:ILE:HD11	1.77	0.67
1:F:106:LYS:HD2	3:F:2018:HOH:O	1.94	0.67
1:D:199:ARG:HE	1:D:338:THR:CG2	2.07	0.67
1:G:350:ARG:HH11	1:G:350:ARG:CG	2.06	0.66
1:A:463:MET:SD	1:B:89:ARG:HD3	2.36	0.66
1:A:85:LYS:HD2	1:A:454:LEU:HD21	1.77	0.66
1:D:309:ASN:O	1:D:311:GLY:N	2.29	0.65
1:E:94:VAL:HG13	1:E:98:LYS:HB3	1.78	0.65
1:G:195:TYR:HB3	3:G:2061:HOH:O	1.96	0.65
1:E:154:MET:CE	1:E:156:ILE:HD11	2.25	0.65
1:G:106:LYS:HD3	1:G:106:LYS:N	2.11	0.65
1:G:76:GLN:HB3	3:G:2003:HOH:O	1.97	0.65
1:B:340:ILE:HD13	1:B:379:LEU:HG	1.77	0.65
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.78	0.65
1:G:498:ARG:O	1:G:498:ARG:HG2	1.97	0.64
1:B:104:ARG:HD3	3:B:2009:HOH:O	1.96	0.64
1:E:96:GLY:O	1:E:100:LYS:HG3	1.97	0.64
1:F:154:MET:HE3	1:F:156:ILE:HD11	1.78	0.64
1:A:473:LEU:HD11	1:A:492:ILE:HD11	1.79	0.64
1:B:173:ILE:HG23	1:B:183:LYS:HG3	1.80	0.64
1:D:340:ILE:HD13	1:D:379:LEU:HG	1.80	0.64
1:D:463:MET:SD	1:E:89:ARG:HD3	2.37	0.64
1:A:340:ILE:HD13	1:A:379:LEU:HG	1.79	0.63
1:A:96:GLY:O	1:A:100:LYS:HG3	1.99	0.63
1:B:89:ARG:HD2	1:B:434:GLU:OE1	1.99	0.63
1:E:199:ARG:HE	1:E:338:THR:HG22	1.64	0.63
1:G:96:GLY:O	1:G:100:LYS:HG3	1.98	0.63
1:F:154:MET:CE	1:F:156:ILE:HD11	2.29	0.63
1:A:106:LYS:HD3	1:A:106:LYS:N	2.13	0.63
1:D:94:VAL:HG13	1:D:98:LYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:HE	1:B:338:THR:HG22	1.65	0.62
1:G:199:ARG:HE	1:G:338:THR:HG22	1.64	0.62
1:A:89:ARG:HG2	1:G:80:GLY:O	2.00	0.62
1:A:74:VAL:HG22	1:A:74:VAL:O	1.98	0.62
1:D:108:LYS:H	1:D:108:LYS:CD	1.99	0.62
1:A:438:ASP:O	1:A:439:ARG:HG2	1.99	0.61
1:A:456:ARG:NH1	1:G:437:ARG:HD2	2.16	0.61
1:E:134:THR:HB	1:E:413:LEU:HB3	1.82	0.61
1:D:437:ARG:HD2	1:E:456:ARG:NH1	2.15	0.61
1:B:154:MET:CE	1:B:156:ILE:HD11	2.31	0.61
1:D:154:MET:CE	1:D:156:ILE:HD11	2.31	0.61
1:B:144:ALA:HB1	1:B:154:MET:CE	2.31	0.61
1:G:94:VAL:HG22	1:G:98:LYS:HD3	1.81	0.61
1:A:350:ARG:HH11	1:A:350:ARG:HB2	1.66	0.60
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.01	0.60
1:B:85:LYS:HD2	1:B:454:LEU:HD21	1.83	0.60
1:A:154:MET:HB3	1:A:352:TRP:HB2	1.83	0.60
1:D:123:PRO:HB2	1:D:375:ARG:HD3	1.84	0.60
1:F:177:PRO:HB3	1:F:294:MET:HG2	1.84	0.60
1:D:177:PRO:HB3	1:D:294:MET:HE2	1.84	0.60
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.84	0.60
1:A:154:MET:CE	1:A:156:ILE:HD11	2.32	0.60
1:F:126:LEU:HD11	1:F:411:VAL:HG23	1.84	0.60
1:D:134:THR:HB	1:D:413:LEU:HB3	1.84	0.59
1:F:82:ALA:CB	1:G:456:ARG:HD3	2.32	0.59
1:G:134:THR:HB	1:G:413:LEU:HB3	1.84	0.59
1:B:293:THR:HG21	3:B:2098:HOH:O	2.02	0.59
1:G:439:ARG:HB2	1:G:439:ARG:NH1	2.18	0.59
1:A:199:ARG:HE	1:A:338:THR:CG2	2.16	0.59
1:A:456:ARG:HD3	1:G:82:ALA:HB2	1.83	0.59
1:E:318:ARG:NH2	1:F:341:LEU:O	2.36	0.59
1:D:173:ILE:HG23	1:D:183:LYS:HG3	1.85	0.58
1:G:439:ARG:HB2	1:G:439:ARG:HH11	1.66	0.58
1:F:169:ARG:HD3	1:F:172:ASP:OD2	2.04	0.58
1:G:154:MET:HE2	1:G:156:ILE:HD11	1.85	0.58
1:B:215:GLU:O	1:B:218:SER:HB3	2.03	0.58
1:G:340:ILE:HD13	1:G:379:LEU:HG	1.84	0.58
1:E:498:ARG:O	1:E:499:GLN:HB2	2.04	0.58
1:G:178:TYR:CD1	1:G:321:MET:HE1	2.38	0.58
1:D:106:LYS:HD3	1:D:106:LYS:N	2.19	0.58
1:F:199:ARG:HE	1:F:338:THR:CG2	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:HD3	1:B:106:LYS:N	2.19	0.57
1:A:390:GLN:HG3	3:B:2132:HOH:O	2.02	0.57
1:F:166:LYS:HD2	1:F:495:PHE:HB2	1.85	0.57
1:G:215:GLU:O	1:G:218:SER:HB3	2.04	0.57
1:D:82:ALA:HB2	1:E:456:ARG:HD3	1.85	0.57
1:D:473:LEU:HD11	1:D:492:ILE:HD11	1.85	0.57
1:E:177:PRO:HG2	1:E:178:TYR:CD1	2.39	0.57
1:E:498:ARG:O	1:E:498:ARG:HG2	2.02	0.57
1:B:327:PRO:HG2	3:B:2107:HOH:O	2.03	0.57
1:B:350:ARG:HH11	1:B:350:ARG:CB	2.18	0.57
1:F:246:THR:HB	1:F:284:LEU:HD23	1.86	0.57
1:B:134:THR:HB	1:B:413:LEU:HB3	1.86	0.57
1:D:494:GLN:HA	1:D:494:GLN:NE2	2.19	0.57
1:D:166:LYS:HD2	1:D:495:PHE:HB2	1.87	0.56
1:G:94:VAL:HG13	1:G:98:LYS:HB3	1.86	0.56
1:F:223:LEU:HD23	1:F:284:LEU:HD22	1.88	0.56
1:A:493:LYS:NZ	3:A:2191:HOH:O	2.37	0.56
1:B:106:LYS:HD3	1:B:106:LYS:H	1.69	0.56
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.86	0.56
1:D:108:LYS:HD2	1:D:108:LYS:N	2.07	0.56
1:A:94:VAL:HG13	1:A:98:LYS:HB3	1.86	0.56
1:D:470:LEU:HD23	1:D:471:PRO:HD2	1.88	0.56
1:E:433:HIS:HD2	1:E:433:HIS:O	1.89	0.56
1:G:162:ASP:HB2	3:G:2042:HOH:O	2.05	0.56
1:E:206:PRO:HG2	1:E:362:GLU:OE1	2.06	0.56
1:G:171:LYS:HE3	1:G:309:ASN:O	2.06	0.56
1:G:322:GLY:N	1:G:323:PRO:HD2	2.21	0.56
1:B:72:ASN:ND2	1:B:438:ASP:HB2	2.20	0.56
1:B:417:ARG:NH1	1:D:479:PHE:O	2.39	0.56
1:A:350:ARG:HH11	1:A:350:ARG:CG	2.20	0.56
1:D:499:GLN:HG2	1:D:500:PRO:HD2	1.88	0.55
1:B:322:GLY:N	1:B:323:PRO:HD2	2.21	0.55
1:B:331:ALA:O	1:B:335:VAL:HG23	2.06	0.55
1:D:358:LEU:HD11	1:D:367:LEU:HD11	1.88	0.55
1:E:199:ARG:HE	1:E:338:THR:CG2	2.20	0.55
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.88	0.55
1:F:350:ARG:HH11	1:F:350:ARG:CB	2.16	0.55
1:F:498:ARG:O	1:F:499:GLN:HB2	2.07	0.55
1:G:177:PRO:HG2	1:G:178:TYR:CD1	2.42	0.55
1:D:106:LYS:HD3	1:D:106:LYS:H	1.71	0.55
1:B:238:SER:HB3	1:B:241:GLU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:ARG:HE	1:G:338:THR:CG2	2.20	0.55
1:B:367:LEU:HD13	1:B:403:LEU:HD11	1.90	0.54
1:A:173:ILE:HG23	1:A:183:LYS:HG3	1.89	0.54
1:D:83:PRO:O	1:D:437:ARG:HD3	2.07	0.54
1:E:331:ALA:O	1:E:335:VAL:HG23	2.07	0.54
1:A:106:LYS:HD3	1:A:106:LYS:H	1.71	0.54
1:D:177:PRO:CA	1:D:294:MET:HE2	2.36	0.54
1:F:154:MET:CB	1:F:352:TRP:HB2	2.35	0.54
1:B:154:MET:HE2	1:B:156:ILE:HD11	1.89	0.54
1:D:331:ALA:O	1:D:335:VAL:HG23	2.08	0.54
1:D:350:ARG:HH11	1:D:350:ARG:CG	2.19	0.54
1:F:225:ARG:O	1:F:229:LYS:HB2	2.08	0.54
1:D:154:MET:HE3	1:D:156:ILE:HD11	1.87	0.54
1:F:313:LEU:HD23	1:F:314:PHE:N	2.23	0.54
1:A:134:THR:HB	1:A:413:LEU:HB3	1.90	0.54
1:B:80:GLY:O	1:D:89:ARG:HG2	2.08	0.54
1:G:439:ARG:NH1	1:G:439:ARG:CB	2.70	0.54
1:A:240:ARG:HG2	3:A:2097:HOH:O	2.07	0.54
1:A:425:ASP:HB2	3:A:2169:HOH:O	2.08	0.54
1:E:139:LEU:HD23	1:E:139:LEU:O	2.07	0.53
1:F:134:THR:HB	1:F:413:LEU:HB3	1.89	0.53
1:E:184:GLY:HA3	1:E:297:GLY:HA3	1.89	0.53
1:E:327:PRO:HG2	3:E:2070:HOH:O	2.08	0.53
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.90	0.53
1:G:306:GLU:O	1:G:308:PRO:HD3	2.08	0.53
1:D:177:PRO:CB	1:D:294:MET:HE2	2.38	0.53
1:F:438:ASP:O	1:F:439:ARG:HB2	2.07	0.53
1:F:179:ASP:O	1:F:182:THR:HG22	2.09	0.53
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.91	0.53
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.89	0.53
1:F:379:LEU:HD13	1:F:381:VAL:HG23	1.91	0.53
1:B:222:LEU:HD23	1:B:267:PHE:CZ	2.44	0.53
1:E:106:LYS:HD3	1:E:106:LYS:N	2.23	0.53
1:G:439:ARG:O	1:G:439:ARG:HG3	2.09	0.53
1:A:106:LYS:H	1:A:106:LYS:CD	2.22	0.53
1:A:177:PRO:HG2	1:A:178:TYR:CD1	2.44	0.53
1:D:488:VAL:HG13	1:D:489:PRO:HD2	1.90	0.53
1:D:85:LYS:HD2	1:D:454:LEU:HD21	1.91	0.52
1:A:375:ARG:HB3	1:A:375:ARG:NH1	2.20	0.52
1:B:463:MET:HB2	1:B:466:GLU:HG3	1.91	0.52
1:G:350:ARG:HG3	1:G:350:ARG:NH1	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLY:O	1:A:76:GLN:HB2	2.08	0.52
1:D:238:SER:HB3	1:D:241:GLU:HB2	1.92	0.52
1:E:75:GLY:HA3	1:E:84:PHE:CE1	2.44	0.52
1:E:322:GLY:N	1:E:323:PRO:HD2	2.24	0.52
1:D:499:GLN:CG	1:D:500:PRO:HD2	2.39	0.52
1:G:226:GLU:CG	1:G:261:THR:HB	2.40	0.52
1:D:404:ARG:NH1	3:D:2119:HOH:O	2.41	0.52
1:G:144:ALA:HB1	1:G:154:MET:CE	2.40	0.52
1:A:144:ALA:HB1	1:A:154:MET:CE	2.40	0.52
1:E:294:MET:HG3	1:E:328:LEU:HD11	1.92	0.52
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.91	0.51
1:A:331:ALA:O	1:A:335:VAL:HG23	2.10	0.51
1:B:106:LYS:H	1:B:106:LYS:CD	2.23	0.51
1:B:246:THR:HB	1:B:284:LEU:HD23	1.92	0.51
1:A:177:PRO:HB3	1:A:294:MET:HG2	1.92	0.51
1:F:322:GLY:N	1:F:323:PRO:HD2	2.25	0.51
1:A:154:MET:HE3	1:A:156:ILE:HD11	1.92	0.51
1:A:456:ARG:HH11	1:G:437:ARG:HD2	1.75	0.51
1:A:177:PRO:HA	1:A:294:MET:HE1	1.93	0.51
1:B:498:ARG:O	1:B:499:GLN:HB2	2.11	0.51
1:E:340:ILE:HD13	1:E:379:LEU:HG	1.93	0.51
1:F:173:ILE:HG23	1:F:183:LYS:HG3	1.91	0.51
1:A:144:ALA:HB1	1:A:154:MET:HE1	1.92	0.51
1:G:124:ARG:HE	1:G:375:ARG:HH12	1.58	0.51
1:A:166:LYS:HD2	1:A:495:PHE:HB2	1.92	0.51
1:F:98:LYS:O	1:F:101:ARG:HB2	2.11	0.51
1:F:245:TRP:O	1:F:254:LEU:HG	2.11	0.51
1:D:433:HIS:HD2	1:D:433:HIS:O	1.94	0.51
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.92	0.50
1:D:158:ASP:OD2	1:D:161:GLY:HA2	2.11	0.50
1:F:437:ARG:HD2	1:G:456:ARG:NH1	2.26	0.50
1:F:473:LEU:CD1	1:F:492:ILE:HD11	2.41	0.50
1:B:411:VAL:HG12	1:B:413:LEU:CD1	2.42	0.50
1:B:414:GLY:HA2	1:B:467:ILE:HG23	1.93	0.50
1:B:420:PRO:HB2	1:D:428:LEU:HD13	1.94	0.50
1:F:177:PRO:HG2	1:F:178:TYR:CD1	2.47	0.50
1:B:96:GLY:O	1:B:100:LYS:HG3	2.12	0.50
1:B:499:GLN:HG2	1:B:500:PRO:HD2	1.93	0.50
1:D:464:PRO:HD2	3:D:2135:HOH:O	2.11	0.50
1:E:375:ARG:HG2	1:E:375:ARG:HH11	1.75	0.50
1:E:420:PRO:HB2	1:F:428:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:PHE:HB3	1:D:437:ARG:HG3	1.93	0.50
1:G:439:ARG:CZ	1:G:439:ARG:HB3	2.42	0.50
1:A:184:GLY:HA3	1:A:297:GLY:HA3	1.93	0.50
1:A:488:VAL:HG13	1:A:489:PRO:HD2	1.94	0.50
1:F:331:ALA:O	1:F:335:VAL:HG23	2.12	0.50
1:A:123:PRO:HB2	1:A:375:ARG:HG3	1.92	0.50
1:G:133:GLY:O	1:G:472:ASP:OD2	2.29	0.50
1:G:388:THR:HG22	3:G:2129:HOH:O	2.12	0.50
1:D:91:THR:HB	1:D:461:VAL:HG21	1.94	0.49
1:E:352:TRP:CE2	1:E:380:ARG:HD3	2.47	0.49
1:F:144:ALA:HB1	1:F:154:MET:CE	2.41	0.49
1:A:89:ARG:HG2	1:G:80:GLY:C	2.32	0.49
1:B:437:ARG:HD2	1:D:456:ARG:NH1	2.27	0.49
1:F:103:THR:OG1	1:F:116:PRO:HG2	2.12	0.49
1:F:488:VAL:HG13	1:F:489:PRO:HD2	1.95	0.49
1:B:173:ILE:HG23	1:B:183:LYS:CG	2.41	0.49
1:F:106:LYS:H	1:F:106:LYS:CD	2.25	0.49
1:G:106:LYS:CD	1:G:106:LYS:H	2.26	0.49
1:A:322:GLY:N	1:A:323:PRO:HD2	2.27	0.49
1:G:331:ALA:O	1:G:335:VAL:HG23	2.12	0.49
1:A:154:MET:HE2	1:A:156:ILE:HD11	1.95	0.49
1:E:106:LYS:HD3	1:E:106:LYS:H	1.77	0.49
1:E:336:VAL:O	1:E:340:ILE:HG23	2.12	0.49
1:G:400:ALA:O	1:G:404:ARG:HG3	2.13	0.49
1:A:411:VAL:HG12	1:A:413:LEU:CD1	2.43	0.48
1:E:76:GLN:C	1:E:78:GLU:H	2.16	0.48
1:F:327:PRO:HG2	3:F:2089:HOH:O	2.13	0.48
1:D:225:ARG:O	1:D:229:LYS:HB2	2.12	0.48
1:D:414:GLY:HA2	1:D:467:ILE:CG2	2.43	0.48
1:D:346:GLU:HB2	1:D:349:ARG:NH2	2.28	0.48
1:E:84:PHE:HB3	1:E:437:ARG:HG3	1.94	0.48
1:E:251:PHE:CE1	1:E:277:LEU:HD13	2.47	0.48
1:B:154:MET:HE3	1:B:156:ILE:HD11	1.96	0.48
1:A:195:TYR:HB3	3:G:2051:HOH:O	2.13	0.48
1:A:375:ARG:HH11	1:A:375:ARG:CB	2.22	0.48
1:E:80:GLY:O	1:F:89:ARG:HG2	2.13	0.48
1:B:199:ARG:HE	1:B:338:THR:CG2	2.25	0.48
1:E:471:PRO:HG2	1:E:474:THR:OG1	2.14	0.48
1:F:98:LYS:O	1:F:102:MET:HG3	2.14	0.48
1:D:96:GLY:O	1:D:100:LYS:HG3	2.14	0.48
1:E:94:VAL:HG22	1:E:98:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:MET:HE2	3:B:2157:HOH:O	2.14	0.48
1:D:113:ALA:HA	1:D:490:LEU:HD23	1.95	0.48
1:D:144:ALA:HB1	1:D:154:MET:CE	2.44	0.48
1:E:83:PRO:O	1:E:437:ARG:HD3	2.14	0.48
1:G:87:PHE:HA	1:G:435:VAL:HG12	1.96	0.48
1:A:350:ARG:HH11	1:A:350:ARG:CB	2.26	0.48
1:A:494:GLN:HA	1:A:494:GLN:NE2	2.29	0.47
1:G:126:LEU:HD11	1:G:411:VAL:HG23	1.96	0.47
1:B:340:ILE:HG13	1:B:341:LEU:N	2.29	0.47
1:D:106:LYS:H	1:D:106:LYS:CD	2.24	0.47
1:D:352:TRP:CE2	1:D:380:ARG:HD3	2.50	0.47
1:F:158:ASP:O	1:F:316:THR:HA	2.14	0.47
1:A:169:ARG:HG2	1:A:498:ARG:NH2	2.28	0.47
1:F:134:THR:HA	1:F:472:ASP:OD1	2.13	0.47
1:B:440:TYR:CD1	1:B:440:TYR:N	2.82	0.47
1:B:179:ASP:O	1:B:182:THR:HG22	2.15	0.47
1:B:463:MET:SD	1:D:89:ARG:HD3	2.55	0.47
1:D:80:GLY:O	1:E:89:ARG:HG2	2.15	0.47
1:F:94:VAL:HG13	1:F:95:SER:N	2.29	0.47
1:A:83:PRO:O	1:A:437:ARG:HD3	2.14	0.47
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.79	0.47
1:B:129:ASN:OD1	1:B:426:MET:SD	2.72	0.47
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.79	0.47
1:E:230:LYS:HD3	1:E:257:PHE:CZ	2.50	0.47
1:F:85:LYS:HD2	1:F:454:LEU:HD21	1.97	0.47
1:F:95:SER:HA	3:F:2004:HOH:O	2.14	0.47
1:D:411:VAL:HG12	1:D:413:LEU:CD1	2.44	0.47
1:F:82:ALA:HB2	1:G:456:ARG:HD3	1.96	0.47
1:D:144:ALA:HB1	1:D:154:MET:HE1	1.97	0.47
1:F:195:TYR:CZ	1:F:199:ARG:HD2	2.50	0.47
1:G:78:GLU:HA	3:G:2004:HOH:O	2.15	0.47
1:B:177:PRO:HB3	1:B:294:MET:HG2	1.97	0.47
1:D:437:ARG:HD2	1:E:456:ARG:HH11	1.79	0.47
1:A:358:LEU:HD11	1:A:367:LEU:HD11	1.96	0.46
1:B:281:ARG:NH2	1:D:265:SER:HB3	2.30	0.46
1:D:94:VAL:HG13	1:D:95:SER:N	2.30	0.46
1:E:215:GLU:O	1:E:218:SER:HB3	2.15	0.46
1:A:124:ARG:NH2	1:G:472:ASP:CG	2.69	0.46
1:G:106:LYS:HD3	1:G:106:LYS:H	1.76	0.46
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.96	0.46
1:A:246:THR:HB	1:A:284:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:O	1:A:499:GLN:HB2	2.15	0.46
1:E:313:LEU:HD23	1:E:314:PHE:N	2.29	0.46
1:A:101:ARG:HD2	3:A:2013:HOH:O	2.16	0.46
1:D:154:MET:HE2	1:D:156:ILE:HD11	1.97	0.46
1:F:251:PHE:CE1	1:F:277:LEU:HD13	2.51	0.46
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.98	0.46
1:G:492:ILE:O	1:G:492:ILE:HG22	2.15	0.46
1:A:215:GLU:O	1:A:218:SER:HB3	2.16	0.46
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.98	0.46
1:F:420:PRO:HB2	1:G:428:LEU:HD13	1.98	0.46
1:A:238:SER:HB3	1:A:241:GLU:HB2	1.98	0.46
1:A:428:LEU:HD13	1:G:420:PRO:HB2	1.98	0.46
1:D:119:ARG:HH12	1:D:350:ARG:HE	1.64	0.46
1:E:94:VAL:CG2	1:E:98:LYS:HG2	2.46	0.46
1:A:433:HIS:HD2	1:A:433:HIS:O	1.99	0.46
1:B:154:MET:CB	1:B:352:TRP:HB2	2.43	0.46
1:E:506:THR:HB	3:E:2122:HOH:O	2.15	0.46
1:D:379:LEU:HD13	1:D:381:VAL:HG23	1.97	0.45
1:F:494:GLN:NE2	1:F:494:GLN:HA	2.32	0.45
1:A:464:PRO:HD2	3:B:2144:HOH:O	2.15	0.45
1:D:322:GLY:N	1:D:323:PRO:HD2	2.31	0.45
1:G:457:VAL:HG12	1:G:459:GLU:HG2	1.98	0.45
1:A:313:LEU:HD23	1:A:314:PHE:N	2.31	0.45
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.52	0.45
1:D:279:SER:O	1:D:283:VAL:HG23	2.16	0.45
1:D:349:ARG:HD2	1:D:377:ALA:O	2.16	0.45
1:D:472:ASP:O	1:D:473:LEU:HB2	2.17	0.45
1:F:80:GLY:O	1:G:89:ARG:HG2	2.15	0.45
1:F:83:PRO:O	1:F:437:ARG:HD3	2.16	0.45
1:B:439:ARG:HG3	1:B:453:ALA:O	2.17	0.45
1:G:84:PHE:HA	1:G:437:ARG:HG2	1.98	0.45
1:G:233:LEU:C	1:G:235:GLY:H	2.20	0.45
1:D:245:TRP:O	1:D:254:LEU:HG	2.17	0.45
1:F:455:GLU:HG3	1:F:455:GLU:O	2.16	0.45
1:B:404:ARG:NH1	3:B:2133:HOH:O	2.47	0.45
1:G:113:ALA:O	1:G:488:VAL:HG11	2.17	0.45
1:A:130:GLY:O	1:A:386:GLN:HA	2.17	0.45
1:F:186:SER:OG	1:F:188:PHE:HB2	2.16	0.45
1:F:223:LEU:HD23	1:F:284:LEU:CD2	2.47	0.45
1:G:411:VAL:HG12	1:G:413:LEU:CD1	2.47	0.45
1:A:159:PRO:HG3	1:A:317:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:O	1:G:417:ARG:NH1	2.50	0.44
1:E:166:LYS:HD2	1:E:495:PHE:HB2	1.98	0.44
1:F:323:PRO:HG2	3:F:2086:HOH:O	2.17	0.44
1:B:472:ASP:O	1:B:473:LEU:HB2	2.17	0.44
1:D:177:PRO:HG2	1:D:178:TYR:CD1	2.52	0.44
1:D:255:ARG:HH11	1:D:255:ARG:HG3	1.82	0.44
1:G:144:ALA:HB1	1:G:154:MET:HE1	1.98	0.44
1:G:439:ARG:CB	1:G:439:ARG:CZ	2.95	0.44
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.98	0.44
1:D:306:GLU:O	1:D:308:PRO:HD3	2.17	0.44
1:E:159:PRO:HG3	1:E:317:TRP:CH2	2.52	0.44
1:A:80:GLY:O	1:B:89:ARG:HG2	2.18	0.44
1:D:98:LYS:O	1:D:102:MET:HG3	2.17	0.44
1:E:106:LYS:H	1:E:106:LYS:CD	2.28	0.44
1:E:346:GLU:OE1	1:E:346:GLU:HA	2.17	0.44
1:A:84:PHE:HB3	1:A:437:ARG:HG3	2.00	0.44
1:B:158:ASP:O	1:B:316:THR:HA	2.18	0.44
1:F:169:ARG:NH1	1:F:172:ASP:OD1	2.51	0.44
1:G:136:LYS:HG2	1:G:413:LEU:HD22	2.00	0.44
1:B:169:ARG:HE	1:B:169:ARG:HB2	1.56	0.44
1:E:433:HIS:O	1:E:433:HIS:CD2	2.70	0.44
1:F:157:VAL:O	1:F:159:PRO:HD3	2.18	0.44
1:F:321:MET:HA	3:F:2086:HOH:O	2.17	0.44
1:G:104:ARG:HG2	1:G:104:ARG:HH11	1.83	0.44
1:B:76:GLN:HG2	1:B:83:PRO:HB3	1.99	0.44
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.86	0.44
1:B:433:HIS:HD2	1:B:433:HIS:O	2.01	0.44
1:D:215:GLU:O	1:D:218:SER:HB3	2.18	0.44
1:D:420:PRO:HB2	1:E:428:LEU:HD13	2.00	0.44
1:G:363:LYS:HG3	1:G:395:TYR:CD2	2.52	0.44
1:A:499:GLN:HG2	1:A:500:PRO:HD2	2.00	0.44
1:G:321:MET:HE3	1:G:321:MET:HB3	1.78	0.44
1:A:124:ARG:NH2	1:G:472:ASP:OD2	2.45	0.43
1:A:438:ASP:O	1:A:439:ARG:CB	2.66	0.43
1:D:386:GLN:HG3	1:D:387:SER:N	2.33	0.43
1:F:328:LEU:O	1:F:331:ALA:HB3	2.17	0.43
1:A:84:PHE:CB	1:A:435:VAL:CG1	2.96	0.43
1:E:230:LYS:NZ	1:E:257:PHE:O	2.38	0.43
1:A:340:ILE:HG13	1:A:341:LEU:N	2.33	0.43
1:B:494:GLN:HA	1:B:494:GLN:NE2	2.34	0.43
1:F:379:LEU:HD13	1:F:381:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:ALA:O	1:G:221:ARG:HG3	2.19	0.43
1:G:327:PRO:HG2	3:G:2106:HOH:O	2.17	0.43
1:F:159:PRO:HG3	1:F:317:TRP:CH2	2.53	0.43
1:A:84:PHE:CG	1:A:435:VAL:HG11	2.54	0.43
1:D:350:ARG:CG	1:D:350:ARG:NH1	2.81	0.43
1:F:306:GLU:O	1:F:308:PRO:HD3	2.18	0.43
1:A:349:ARG:HD2	1:A:377:ALA:O	2.19	0.43
1:A:463:MET:HB2	1:A:466:GLU:HG3	2.01	0.43
1:E:168:GLY:O	1:E:498:ARG:HD2	2.18	0.43
1:G:238:SER:HB3	1:G:241:GLU:HB2	1.99	0.43
1:G:336:VAL:O	1:G:340:ILE:HG23	2.19	0.43
1:A:472:ASP:O	1:A:473:LEU:HB2	2.18	0.43
1:D:471:PRO:HG2	1:D:474:THR:OG1	2.19	0.43
1:F:217:ALA:O	1:F:221:ARG:HG3	2.17	0.43
1:D:130:GLY:O	1:D:386:GLN:HA	2.19	0.43
1:E:154:MET:CB	1:E:352:TRP:HB2	2.47	0.43
1:E:173:ILE:HG22	1:E:174:ILE:N	2.34	0.43
1:F:318:ARG:NH1	3:F:2085:HOH:O	2.52	0.43
1:A:327:PRO:HG2	3:A:2137:HOH:O	2.19	0.42
1:A:505:GLY:O	1:A:506:THR:HB	2.19	0.42
1:B:139:LEU:C	1:B:139:LEU:HD23	2.39	0.42
1:B:358:LEU:HD11	1:B:367:LEU:HD11	2.01	0.42
1:F:144:ALA:HB1	1:F:154:MET:HE3	2.00	0.42
1:B:157:VAL:O	1:B:159:PRO:HD3	2.19	0.42
1:D:156:ILE:HG22	1:D:158:ASP:HB2	2.01	0.42
1:F:350:ARG:HH11	1:F:350:ARG:CG	2.32	0.42
1:A:124:ARG:NH1	3:A:2027:HOH:O	2.41	0.42
1:D:173:ILE:HG22	1:D:174:ILE:N	2.34	0.42
1:D:340:ILE:HG13	1:D:341:LEU:N	2.33	0.42
1:D:435:VAL:CG1	1:D:436:GLU:N	2.82	0.42
1:E:255:ARG:HG3	1:E:255:ARG:HH11	1.84	0.42
1:B:82:ALA:CB	1:D:456:ARG:HD3	2.49	0.42
1:B:217:ALA:O	1:B:221:ARG:HG3	2.19	0.42
1:B:251:PHE:CE1	1:B:277:LEU:HD13	2.54	0.42
1:E:433:HIS:CD2	1:E:433:HIS:C	2.92	0.42
1:D:173:ILE:HG23	1:D:183:LYS:CG	2.46	0.42
1:E:217:ALA:O	1:E:221:ARG:HG3	2.19	0.42
1:G:231:LEU:HD23	1:G:234:ILE:HD11	2.02	0.42
1:A:84:PHE:CB	1:A:435:VAL:HG11	2.49	0.42
1:E:126:LEU:HD11	1:E:411:VAL:HG23	2.01	0.42
1:G:156:ILE:HG22	1:G:158:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:THR:HB	1:G:284:LEU:HD23	2.01	0.42
1:G:494:GLN:HA	1:G:494:GLN:NE2	2.35	0.42
1:A:74:VAL:HG13	1:A:84:PHE:O	2.20	0.42
1:D:390:GLN:HG3	3:E:2088:HOH:O	2.19	0.42
1:D:433:HIS:CD2	1:D:459:GLU:HG3	2.55	0.42
1:E:94:VAL:HG13	1:E:95:SER:N	2.35	0.42
1:F:380:ARG:HG3	1:F:380:ARG:HH11	1.84	0.42
1:A:124:ARG:HH21	1:G:472:ASP:CG	2.23	0.42
1:E:179:ASP:O	1:E:182:THR:HG22	2.19	0.42
1:A:94:VAL:HG13	1:A:95:SER:N	2.35	0.42
1:A:173:ILE:HG23	1:A:183:LYS:CG	2.50	0.42
1:D:199:ARG:NH2	1:D:342:SER:OG	2.48	0.42
1:G:166:LYS:HD3	1:G:497:ASN:HD22	1.83	0.42
1:G:470:LEU:HD23	1:G:471:PRO:HD2	2.02	0.42
1:A:229:LYS:HB3	3:A:2091:HOH:O	2.20	0.41
1:B:350:ARG:HH11	1:B:350:ARG:CG	2.33	0.41
1:G:233:LEU:HD23	1:G:233:LEU:HA	1.85	0.41
1:A:455:GLU:O	1:A:455:GLU:HG3	2.20	0.41
1:B:130:GLY:O	1:B:386:GLN:HA	2.20	0.41
1:B:159:PRO:HG3	1:B:317:TRP:CH2	2.55	0.41
1:B:491:GLU:H	1:B:491:GLU:HG2	1.64	0.41
1:E:455:GLU:O	1:E:455:GLU:HG3	2.19	0.41
1:G:318:ARG:NE	1:G:502:PHE:CD2	2.87	0.41
1:G:340:ILE:HG13	1:G:341:LEU:N	2.34	0.41
1:D:414:GLY:HA2	1:D:467:ILE:HG23	2.02	0.41
1:F:433:HIS:HD2	1:F:433:HIS:O	2.02	0.41
1:D:84:PHE:HA	1:D:437:ARG:HG2	2.01	0.41
1:D:84:PHE:CB	1:D:437:ARG:HG3	2.50	0.41
1:E:124:ARG:HB3	1:E:408:ARG:HB2	2.02	0.41
1:F:82:ALA:O	1:F:437:ARG:NH1	2.53	0.41
1:G:162:ASP:O	1:G:166:LYS:HG2	2.21	0.41
1:G:352:TRP:CE2	1:G:380:ARG:HD3	2.56	0.41
1:B:352:TRP:CE2	1:B:380:ARG:HD3	2.54	0.41
1:G:472:ASP:HB2	3:G:2167:HOH:O	2.20	0.41
1:D:252:ASP:O	1:D:255:ARG:HB2	2.19	0.41
1:G:437:ARG:HH22	1:G:459:GLU:CD	2.24	0.41
1:A:408:ARG:HA	1:G:416:SER:OG	2.21	0.41
1:A:439:ARG:HA	1:A:439:ARG:CZ	2.50	0.41
1:F:122:GLU:HB2	1:F:123:PRO:HD3	2.02	0.41
1:G:139:LEU:C	1:G:139:LEU:HD23	2.40	0.41
1:G:358:LEU:HD11	1:G:367:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:HA	3:A:2051:HOH:O	2.19	0.41
1:D:498:ARG:O	1:D:499:GLN:HB2	2.19	0.41
1:E:133:GLY:O	1:E:472:ASP:OD2	2.37	0.41
1:E:367:LEU:HD22	1:E:371:LEU:CD1	2.51	0.41
1:F:336:VAL:O	1:F:340:ILE:HG23	2.19	0.41
1:F:472:ASP:O	1:F:473:LEU:HB2	2.21	0.41
1:G:288:LEU:N	1:G:289:PRO:CD	2.84	0.41
1:A:133:GLY:O	1:A:472:ASP:OD2	2.39	0.41
1:B:94:VAL:CG2	1:B:98:LYS:HD3	2.47	0.41
1:B:94:VAL:HG13	1:B:95:SER:N	2.35	0.41
1:G:106:LYS:N	1:G:106:LYS:CD	2.76	0.41
1:G:230:LYS:HD3	1:G:257:PHE:CE2	2.56	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.88	0.41
1:A:499:GLN:CG	1:A:500:PRO:HD2	2.52	0.41
1:B:74:VAL:HG12	1:B:75:GLY:N	2.35	0.41
1:E:177:PRO:HA	1:E:294:MET:HE2	2.02	0.41
1:E:417:ARG:HD3	1:F:478:GLY:O	2.21	0.41
1:F:158:ASP:OD2	1:F:161:GLY:HA2	2.21	0.41
1:F:358:LEU:HD11	1:F:367:LEU:HD11	2.03	0.41
1:F:437:ARG:HD2	1:G:456:ARG:HH11	1.85	0.41
1:A:285:SER:HB2	1:B:266:LEU:HD11	2.03	0.40
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.90	0.40
1:B:488:VAL:HG13	1:B:489:PRO:HD2	2.03	0.40
1:D:463:MET:HB2	1:D:466:GLU:HG3	2.03	0.40
1:E:144:ALA:HB1	1:E:154:MET:CE	2.51	0.40
1:F:233:LEU:HD23	1:F:233:LEU:HA	1.87	0.40
1:G:104:ARG:HD2	3:G:2022:HOH:O	2.21	0.40
1:B:379:LEU:HD22	1:B:380:ARG:N	2.35	0.40
1:E:141:ARG:HH11	1:E:141:ARG:HG2	1.86	0.40
1:E:245:TRP:O	1:E:254:LEU:HG	2.21	0.40
3:E:2080:HOH:O	1:F:398:LYS:HG3	2.20	0.40
1:F:169:ARG:NH1	1:F:312:ASN:ND2	2.70	0.40
1:F:215:GLU:O	1:F:218:SER:HB3	2.22	0.40
1:G:179:ASP:O	1:G:182:THR:HG22	2.21	0.40
1:G:313:LEU:HD23	1:G:314:PHE:N	2.36	0.40
1:A:100:LYS:O	1:A:104:ARG:HB2	2.22	0.40
1:A:105:GLU:HB2	3:A:2017:HOH:O	2.21	0.40
1:E:84:PHE:HA	1:E:437:ARG:HG2	2.02	0.40
1:E:411:VAL:HG12	1:E:413:LEU:CD1	2.51	0.40
1:F:411:VAL:HG12	1:F:413:LEU:CD1	2.51	0.40
1:A:498:ARG:O	1:A:498:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:LEU:HD22	1:D:380:ARG:N	2.37	0.40
1:A:491:GLU:H	1:A:491:GLU:HG2	1.66	0.40
1:D:157:VAL:O	1:D:159:PRO:HD3	2.21	0.40
1:D:433:HIS:CD2	1:D:433:HIS:C	2.95	0.40
1:E:222:LEU:HD23	1:E:267:PHE:CZ	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	416/437 (95%)	398 (96%)	18 (4%)	0	100	100
1	B	418/437 (96%)	400 (96%)	17 (4%)	1 (0%)	47	62
1	D	411/437 (94%)	391 (95%)	19 (5%)	1 (0%)	47	62
1	E	415/437 (95%)	396 (95%)	17 (4%)	2 (0%)	29	41
1	F	412/437 (94%)	397 (96%)	15 (4%)	0	100	100
1	G	413/437 (94%)	395 (96%)	17 (4%)	1 (0%)	47	62
All	All	2485/2622 (95%)	2377 (96%)	103 (4%)	5 (0%)	47	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	310	GLY
1	B	289	PRO
1	E	77	GLY
1	G	77	GLY
1	E	289	PRO

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	349/364 (96%)	317 (91%)	32 (9%)	9 13
1	B	351/364 (96%)	326 (93%)	25 (7%)	14 23
1	D	345/364 (95%)	318 (92%)	27 (8%)	12 19
1	E	348/364 (96%)	319 (92%)	29 (8%)	11 17
1	F	346/364 (95%)	319 (92%)	27 (8%)	12 19
1	G	347/364 (95%)	316 (91%)	31 (9%)	9 14
All	All	2086/2184 (96%)	1915 (92%)	171 (8%)	11 17

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	89	ARG
1	A	94	VAL
1	A	106	LYS
1	A	124	ARG
1	A	143	LEU
1	A	152	ASP
1	A	163	MET
1	A	202	LEU
1	A	241	GLU
1	A	254	LEU
1	A	277	LEU
1	A	284	LEU
1	A	285	SER
1	A	294	MET
1	A	296	ASP
1	A	313	LEU
1	A	328	LEU
1	A	338	THR
1	A	348	LYS
1	A	350	ARG
1	A	351	LEU

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Mol	Chain	Res	Type
1	A	353	LEU
1	A	367	LEU
1	A	375	ARG
1	A	379	LEU
1	A	428	LEU
1	A	430	LEU
1	A	433	HIS
1	A	456	ARG
1	A	470	LEU
1	A	472	ASP
1	B	89	ARG
1	B	94	VAL
1	B	106	LYS
1	B	143	LEU
1	B	163	MET
1	B	202	LEU
1	B	254	LEU
1	B	277	LEU
1	B	284	LEU
1	B	285	SER
1	B	294	MET
1	B	296	ASP
1	B	313	LEU
1	B	328	LEU
1	B	338	THR
1	B	345	GLU
1	B	350	ARG
1	B	351	LEU
1	B	353	LEU
1	B	367	LEU
1	B	379	LEU
1	B	428	LEU
1	B	430	LEU
1	B	433	HIS
1	B	470	LEU
1	D	89	ARG
1	D	106	LYS
1	D	108	LYS
1	D	143	LEU
1	D	152	ASP
1	D	163	MET
1	D	202	LEU

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Mol	Chain	Res	Type
1	D	254	LEU
1	D	277	LEU
1	D	284	LEU
1	D	294	MET
1	D	296	ASP
1	D	313	LEU
1	D	328	LEU
1	D	338	THR
1	D	350	ARG
1	D	351	LEU
1	D	353	LEU
1	D	367	LEU
1	D	375	ARG
1	D	376	LYS
1	D	379	LEU
1	D	428	LEU
1	D	430	LEU
1	D	433	HIS
1	D	470	LEU
1	D	472	ASP
1	E	89	ARG
1	E	94	VAL
1	E	106	LYS
1	E	120	ASP
1	E	129	ASN
1	E	141	ARG
1	E	143	LEU
1	E	195	TYR
1	E	202	LEU
1	E	251	PHE
1	E	254	LEU
1	E	277	LEU
1	E	284	LEU
1	E	285	SER
1	E	289	PRO
1	E	294	MET
1	E	318	ARG
1	E	328	LEU
1	E	338	THR
1	E	351	LEU
1	E	353	LEU
1	E	367	LEU

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Mol	Chain	Res	Type
1	E	379	LEU
1	E	428	LEU
1	E	430	LEU
1	E	433	HIS
1	E	439	ARG
1	E	456	ARG
1	E	472	ASP
1	F	78	GLU
1	F	89	ARG
1	F	94	VAL
1	F	106	LYS
1	F	143	LEU
1	F	152	ASP
1	F	163	MET
1	F	195	TYR
1	F	202	LEU
1	F	254	LEU
1	F	277	LEU
1	F	284	LEU
1	F	285	SER
1	F	294	MET
1	F	328	LEU
1	F	338	THR
1	F	350	ARG
1	F	351	LEU
1	F	353	LEU
1	F	367	LEU
1	F	375	ARG
1	F	379	LEU
1	F	417	ARG
1	F	428	LEU
1	F	430	LEU
1	F	433	HIS
1	F	456	ARG
1	G	89	ARG
1	G	94	VAL
1	G	106	LYS
1	G	143	LEU
1	G	163	MET
1	G	186	SER
1	G	202	LEU
1	G	229	LYS

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Mol	Chain	Res	Type
1	G	251	PHE
1	G	254	LEU
1	G	277	LEU
1	G	284	LEU
1	G	294	MET
1	G	296	ASP
1	G	313	LEU
1	G	328	LEU
1	G	338	THR
1	G	350	ARG
1	G	351	LEU
1	G	353	LEU
1	G	367	LEU
1	G	379	LEU
1	G	428	LEU
1	G	430	LEU
1	G	433	HIS
1	G	435	VAL
1	G	438	ASP
1	G	456	ARG
1	G	459	GLU
1	G	470	LEU
1	G	472	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	494	GLN
1	A	497	ASN
1	A	499	GLN
1	B	76	GLN
1	B	129	ASN
1	B	494	GLN
1	B	497	ASN
1	B	499	GLN
1	D	433	HIS
1	D	494	GLN
1	D	497	ASN
1	D	499	GLN
1	E	129	ASN
1	E	433	HIS
1	E	494	GLN

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Mol	Chain	Res	Type
1	E	497	ASN
1	E	499	GLN
1	F	129	ASN
1	F	494	GLN
1	F	497	ASN
1	F	499	GLN
1	G	76	GLN
1	G	494	GLN
1	G	497	ASN
1	G	499	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)

15 ligands are 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	SO4	E	602	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	B	602	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	D	603	-	4,4,4	0.43	0	6,6,6	0.08	0
2	SO4	B	601	-	4,4,4	0.33	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	604	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	F	602	-	4,4,4	0.36	0	6,6,6	0.13	0
2	SO4	F	601	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	F	603	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	E	601	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	D	601	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	G	601	-	4,4,4	0.36	0	6,6,6	0.22	0
2	SO4	D	602	-	4,4,4	0.39	0	6,6,6	0.12	0
2	SO4	A	601	-	4,4,4	0.43	0	6,6,6	0.11	0
2	SO4	A	602	-	4,4,4	0.42	0	6,6,6	0.11	0
2	SO4	G	602	-	4,4,4	0.37	0	6,6,6	0.25	0

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.