Full wwPDB X-ray Structure Validation Report (i)

Feb 22, 2024 – 03:17 AM EST

PDB ID	:	4RR2
Title	:	Crystal structure of human primase
Authors	:	Baranovskiy, A.G.; Gu, J.; Suwa, Y.; Babayeva, N.D.; Tahirov, T.H.
Deposited on	:	2014-11-05
Resolution	:	2.65 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:

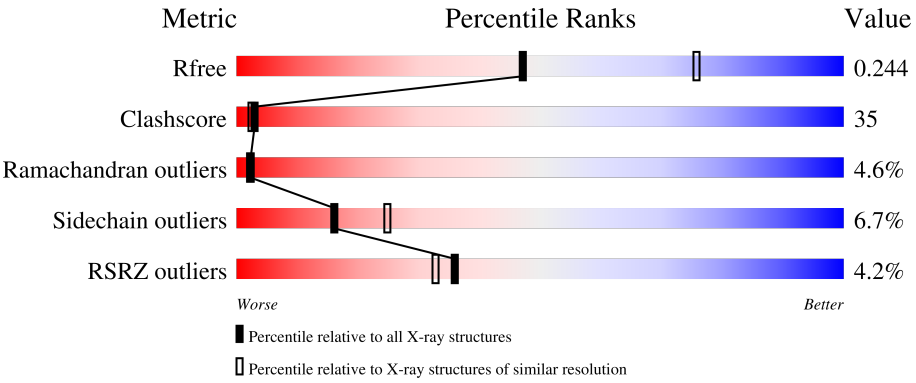
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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% 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	420	% 46% 43% · 7%
1	C	420	% 44% 43% 6% 7%
2	B	509	6% 14% 23% 5% 58%
2	D	509	4% 40% 37% 6% · 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11896 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 DNA primase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3267	2101	566	585	15			
1	C	389	Total	C	N	O	S	0	0	0
			3263	2099	566	583	15			

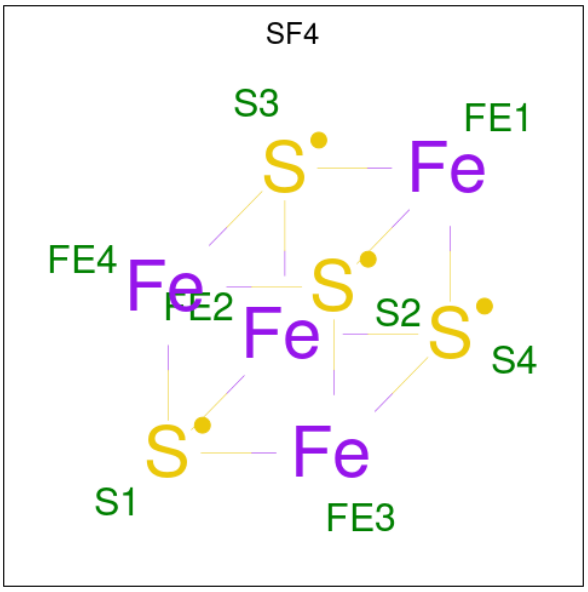
- Molecule 2 is a protein called DNA primase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1755	1133	299	321	2			
2	D	429	Total	C	N	O	S	0	0	0
			3513	2249	608	643	13			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Fe S 8 4 4	0	0

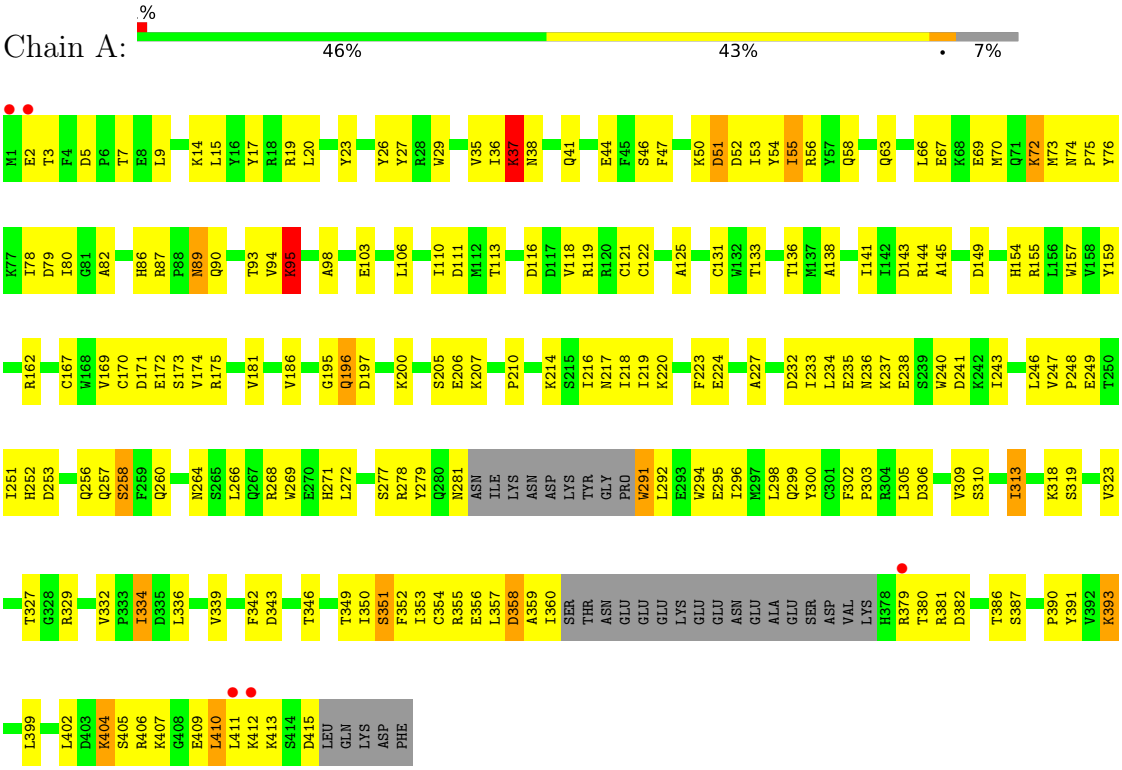
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0
5	B	4	Total O 4 4	0	0
5	C	40	Total O 40 40	0	0
5	D	21	Total O 21 21	0	0

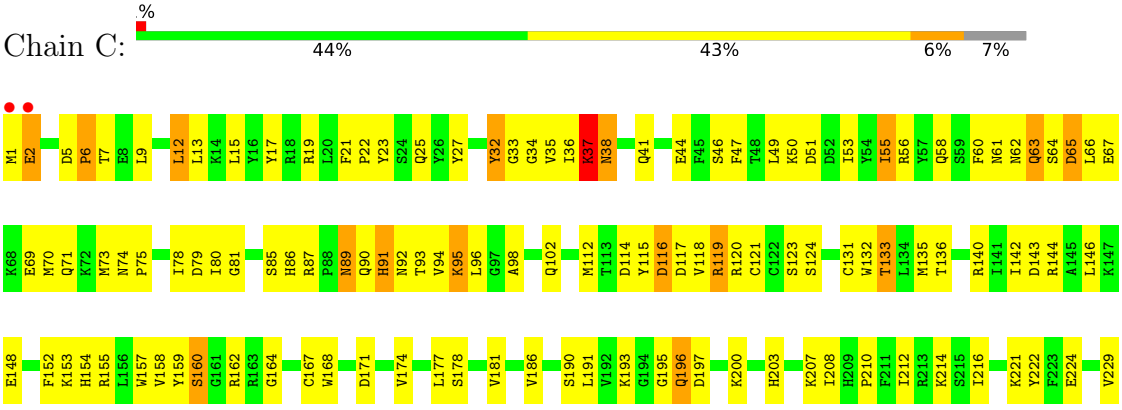
3 Residue-property plots (i)

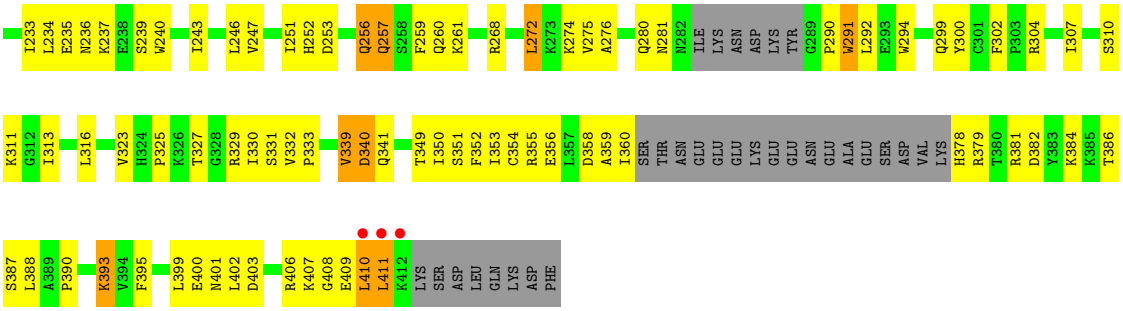
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



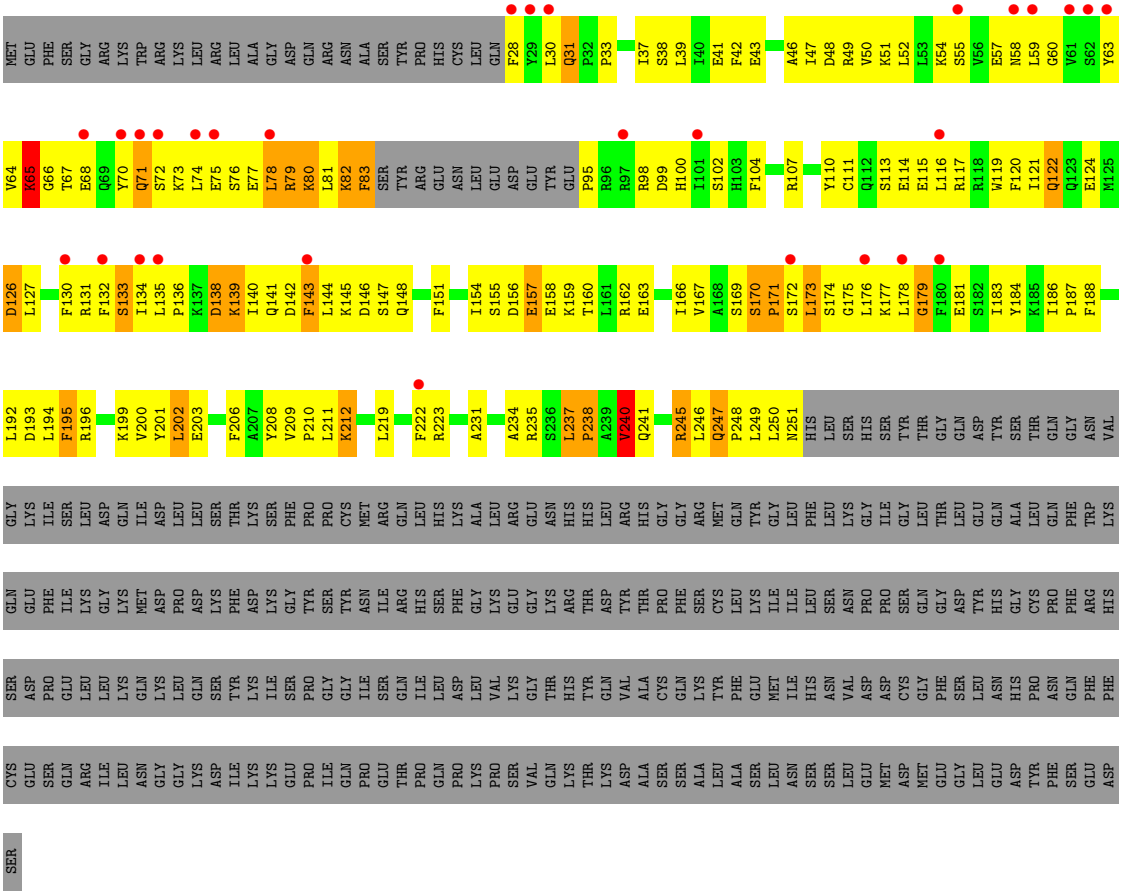
• Molecule 1: DNA primase small subunit





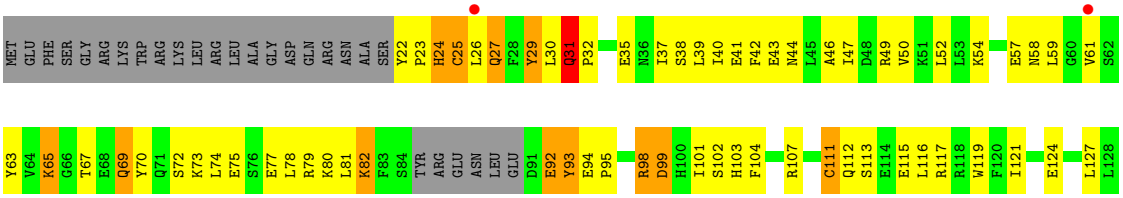
• Molecule 2: DNA primase large subunit

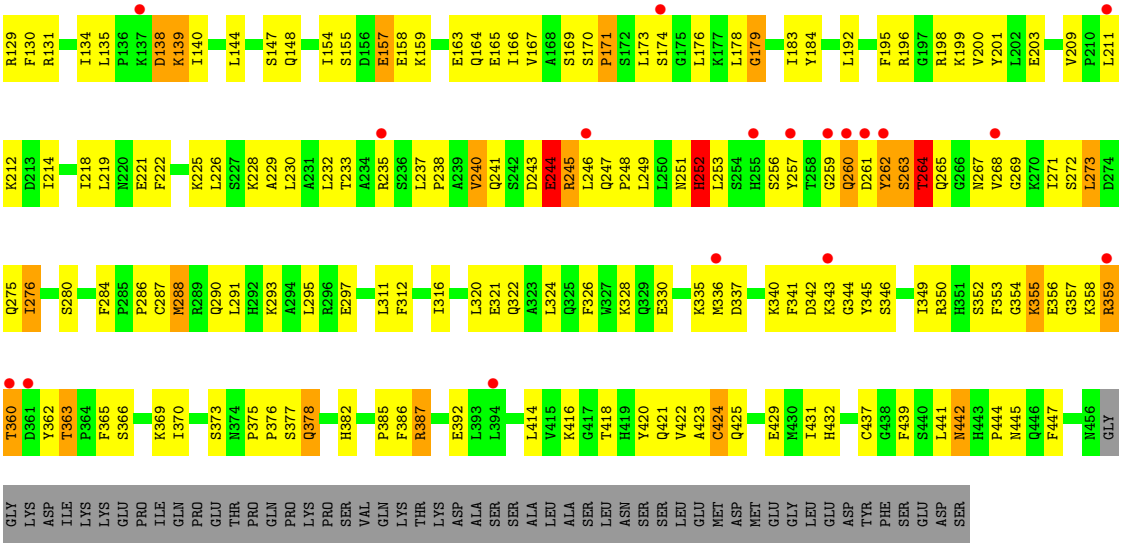
Chain B:



• Molecule 2: DNA primase large subunit

Chain D:




R129 F130 R131 I134 L135 P136 K137 D138 K139 I140 L144 S147 Q148 I154 S155 D156 E157 E158 K159 E163 Q164 E165 I166 V167 A168 S169 S170 P171 S172 L173 S174 G175 L176 K177 L178 G179 I183 Y184 L192 F195 R196 G197 R198 K199 V200 Y201 L202 E203 V209 P210 L211
K212 D213 I214 I218 L219 N220 E221 F222 K225 L226 S227 K228 A229 L230 A231 L232 T233 A234 R235 S236 L237 P238 A239 V240 Q241 S242 D243 E244 R245 L246 Q247 P248 L249 I250 N251 H252 L253 S254 H255 S256 Y257 T258 G259 Q260 D261 Y262 S263 T264 Q265 G266 N267 V268 G269 K270 I271 S272 L273 D274
Q275 I276 S280 F284 P285 P286 C287 M288 R289 Q290 L291 H292 K293 A294 L295 R296 E297 L311 F312 I316 L320 E321 Q322 A323 L324 Q325 F326 W327 K328 Q329 E330 K335 M336 D337 K340 F341 D342 K343 G344 Y345 S346 I349 R350 H351 S352 F353 G354 K355 E356 G357 K358 R359
T360 D361 Y362 T363 P364 F365 S366 K369 I370 S373 N374 P375 P376 S377 Q378 H382 P385 F386 R387 E392 L393 L394 L414 V415 K416 G417 T418 H419 Y420 Q421 V422 A423 C424 Q425 E429 M430 I431 H432 C437 G438 F439 S440 L441 N442 H443 P444 N445 Q446 F447 N456 GLY
GLY LYS ASP ILE LYS LYS GLU PRO ILE GLN PRO GLU THR PRO GLN PRO LYS PRO SER VAL GLN LYS THR LYS ASP ALA SER SER ALA LEU ALA SER LEU ASN SER SER LEU GLU MET ASP MET GLU GLY LEU GLU ASP TYR PHE SER GLU ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.19Å 88.90Å 94.68Å 93.82° 96.57° 111.72°	Depositor
Resolution (Å)	48.48 – 2.65 48.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.5 (48.48-2.65) 88.1 (48.47-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.271 0.206 , 0.244	Depositor DCC
R_{free} test set	3691 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11896	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN

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	0.45	0/3349	0.70	0/4514
1	C	0.49	0/3346	0.74	0/4512
2	B	0.39	0/1787	0.63	0/2402
2	D	0.44	0/3595	0.67	1/4838 (0.0%)
All	All	0.45	0/12077	0.69	1/16266 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	252	HIS	N-CA-C	5.33	125.39	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3267	0	3249	206	0
1	C	3263	0	3243	198	0
2	B	1755	0	1801	184	0
2	D	3513	0	3494	232	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	0	0	0
5	A	23	0	0	11	0
5	B	4	0	0	0	0
5	C	40	0	0	11	0
5	D	21	0	0	3	0
All	All	11896	0	11787	815	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 35.

All (815) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LYS:HE2	2:D:98:ARG:HD3	1.36	1.07
2:D:117:ARG:HG2	2:D:230:LEU:HD13	1.38	1.05
2:B:68:GLU:HA	2:B:71:GLN:HB3	1.42	1.02
2:B:82:LYS:HG2	2:B:98:ARG:HD3	1.42	1.01
1:C:50:LYS:H	1:C:50:LYS:HD2	1.25	1.00
1:A:95:LYS:H	1:A:95:LYS:HD3	1.27	0.98
2:B:237:LEU:HD13	2:B:241:GLN:HE22	1.25	0.98
2:B:79:ARG:HH11	2:B:79:ARG:HB3	1.27	0.97
1:A:53:ILE:H	1:A:53:ILE:HD12	1.27	0.96
2:B:72:SER:HA	2:B:75:GLU:HG2	1.48	0.96
1:A:37:LYS:HD2	1:A:38:ASN:H	1.28	0.95
2:D:94:GLU:HB3	2:D:95:PRO:HD3	1.49	0.94
2:D:44:ASN:HA	2:D:47:ILE:HD12	1.50	0.92
1:C:233:ILE:HD12	1:C:243:ILE:HD11	1.51	0.91
2:D:43:GLU:O	2:D:47:ILE:HG13	1.70	0.91
1:C:49:LEU:HB3	1:C:50:LYS:HD2	1.53	0.91
1:C:349:THR:HG22	1:C:351:SER:H	1.32	0.91
2:B:154:ILE:CG2	2:B:158:GLU:HB2	2.01	0.91
1:C:379:ARG:HA	5:C:1034:HOH:O	1.72	0.90
1:C:144:ARG:HG2	1:C:144:ARG:HH21	1.36	0.89
2:D:113:SER:HB3	2:D:116:LEU:HG	1.55	0.88
1:C:353:ILE:HB	1:C:386:THR:HG21	1.54	0.88
2:D:262:TYR:HB2	2:D:264:THR:H	1.39	0.88
2:B:170:SER:HB3	2:B:171:PRO:HD2	1.55	0.87
2:D:82:LYS:HE2	2:D:98:ARG:CD	2.04	0.87
1:C:154:HIS:ND1	1:C:402:LEU:HD12	1.89	0.86
1:C:247:VAL:HG22	1:C:292:LEU:HD13	1.57	0.85
1:A:247:VAL:HG22	1:A:292:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LYS:HD2	1:C:38:ASN:H	1.42	0.85
1:C:355:ARG:HG3	1:C:355:ARG:HH11	1.41	0.85
2:D:82:LYS:HG3	2:D:98:ARG:HD3	1.59	0.85
1:C:38:ASN:HB3	1:C:41:GLN:HB2	1.57	0.84
2:B:82:LYS:CG	2:B:98:ARG:HD3	2.06	0.84
2:B:49:ARG:CG	2:B:102:SER:HB3	2.08	0.84
1:A:51:ASP:H	1:A:53:ILE:HD11	1.40	0.84
2:B:154:ILE:HG21	2:B:158:GLU:HB2	1.60	0.84
1:A:353:ILE:HB	1:A:386:THR:HG21	1.60	0.84
1:A:410:LEU:HD23	1:A:411:LEU:N	1.93	0.83
1:C:260:GLN:HB2	5:C:1002:HOH:O	1.77	0.83
1:C:349:THR:HG22	1:C:351:SER:N	1.93	0.82
1:A:232:ASP:OD2	1:A:235:GLU:HB2	1.80	0.82
2:D:67:THR:HG22	2:D:69:GLN:H	1.43	0.81
2:B:113:SER:HB2	2:B:116:LEU:HG	1.62	0.81
2:D:80:LYS:HZ3	2:D:418:THR:HG22	1.45	0.81
1:A:349:THR:HG22	1:A:351:SER:H	1.46	0.81
1:C:36:ILE:HG22	1:C:37:LYS:HG3	1.63	0.81
1:A:379:ARG:HB3	1:A:382:ASP:OD1	1.80	0.80
1:A:327:THR:OG1	1:A:329:ARG:HG2	1.81	0.80
1:A:38:ASN:HB3	1:A:41:GLN:HB2	1.64	0.79
1:C:276:ALA:O	1:C:280:GLN:HG2	1.82	0.78
1:A:37:LYS:CD	1:A:38:ASN:H	1.96	0.78
1:A:172:GLU:HA	1:A:175:ARG:NH1	1.99	0.78
2:D:425:GLN:O	2:D:429:GLU:HG3	1.85	0.78
1:A:51:ASP:H	1:A:53:ILE:CD1	1.97	0.77
1:A:235:GLU:HG2	1:A:236:ASN:ND2	1.99	0.77
2:D:170:SER:HB3	2:D:171:PRO:HD2	1.66	0.77
1:A:260:GLN:HA	1:A:260:GLN:NE2	2.00	0.77
2:D:155:SER:OG	2:D:157:GLU:HB2	1.85	0.77
2:D:421:GLN:O	2:D:425:GLN:HG3	1.83	0.77
2:B:247:GLN:N	2:B:247:GLN:HE21	1.83	0.77
1:C:353:ILE:HB	1:C:386:THR:CG2	2.13	0.77
1:C:349:THR:CG2	1:C:351:SER:HB3	2.16	0.76
2:B:144:LEU:O	2:B:147:SER:HB3	1.86	0.76
2:B:59:LEU:HD21	2:B:73:LYS:HG2	1.66	0.75
2:D:82:LYS:CE	2:D:98:ARG:HD3	2.16	0.75
2:B:199:LYS:O	2:B:200:VAL:HG13	1.87	0.75
1:C:46:SER:HB3	1:C:79:ASP:HB2	1.69	0.75
2:B:46:ALA:O	2:B:50:VAL:HG23	1.86	0.75
2:D:273:LEU:HD11	2:D:326:PHE:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ASN:OD1	1:C:64:SER:HB3	1.87	0.74
1:A:386:THR:HG22	1:A:387:SER:N	2.01	0.74
1:A:407:LYS:HG3	1:A:411:LEU:HD12	1.67	0.74
2:B:171:PRO:HG2	2:B:173:LEU:HB2	1.68	0.74
1:C:95:LYS:HD3	1:C:98:ALA:HB2	1.67	0.74
1:A:334:ILE:HD12	1:A:342:PHE:CE2	2.22	0.74
1:A:349:THR:HG22	1:A:351:SER:N	2.02	0.73
1:C:85:SER:HA	1:C:102:GLN:NE2	2.03	0.73
1:C:144:ARG:HG2	1:C:144:ARG:NH2	2.00	0.73
2:B:30:LEU:HG	2:B:31:GLN:HG3	1.70	0.73
2:D:80:LYS:NZ	2:D:418:THR:HG22	2.04	0.73
2:B:238:PRO:HA	2:B:241:GLN:HG2	1.70	0.73
2:D:320:LEU:HD11	2:D:350:ARG:HA	1.70	0.73
1:C:55:ILE:HD12	1:C:58:GLN:NE2	2.04	0.72
2:D:77:GLU:CD	2:D:418:THR:HG21	2.09	0.72
2:B:113:SER:H	2:B:116:LEU:HD12	1.54	0.72
2:B:173:LEU:HD23	2:B:173:LEU:O	1.90	0.72
2:B:151:PHE:HB3	2:B:186:ILE:HG22	1.72	0.72
2:B:163:GLU:O	2:B:167:VAL:HG23	1.90	0.72
1:A:196:GLN:HG2	1:A:196:GLN:O	1.88	0.72
1:A:247:VAL:HG22	1:A:292:LEU:HD21	1.71	0.71
1:C:393:LYS:HE3	1:C:393:LYS:HA	1.72	0.71
1:A:355:ARG:HG3	1:A:355:ARG:HH11	1.56	0.71
2:D:265:GLN:HA	2:D:265:GLN:HE21	1.56	0.71
2:D:418:THR:HG22	2:D:418:THR:O	1.91	0.71
1:C:51:ASP:HB2	1:C:53:ILE:HD13	1.72	0.71
1:C:355:ARG:HG3	1:C:355:ARG:NH1	2.06	0.70
2:D:25:CYS:HB3	2:D:131:ARG:HD3	1.73	0.70
2:B:50:VAL:O	2:B:54:LYS:HB2	1.90	0.70
2:B:240:VAL:HG13	2:B:246:LEU:CD1	2.21	0.70
2:D:358:LYS:HG3	2:D:363:THR:OG1	1.92	0.70
1:A:5:ASP:OD1	1:A:7:THR:HB	1.90	0.70
2:B:110:TYR:HB3	2:B:116:LEU:HB3	1.74	0.70
2:D:178:LEU:HD11	2:D:183:ILE:HD11	1.72	0.70
1:C:386:THR:HG22	1:C:387:SER:N	2.07	0.70
1:C:89:ASN:HD22	1:C:89:ASN:C	1.95	0.69
1:C:299:GLN:O	1:C:304:ARG:NH2	2.26	0.69
1:C:73:MET:HG3	5:C:1033:HOH:O	1.92	0.69
1:C:49:LEU:HD13	1:C:50:LYS:NZ	2.08	0.69
1:C:386:THR:HG22	1:C:388:LEU:H	1.57	0.69
2:D:268:VAL:HG12	2:D:269:GLY:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HE2	1:A:241:ASP:OD1	1.93	0.69
2:D:358:LYS:HE3	2:D:360:THR:HA	1.74	0.69
2:B:163:GLU:HG3	2:B:178:LEU:HB2	1.74	0.68
2:D:199:LYS:O	2:D:200:VAL:HG13	1.92	0.68
1:A:118:VAL:HG13	1:A:300:TYR:CD2	2.28	0.68
2:D:24:HIS:CE1	2:D:92:GLU:HB2	2.28	0.68
2:D:92:GLU:HG2	2:D:93:TYR:H	1.59	0.68
1:C:120:ARG:NH2	1:C:235:GLU:OE1	2.25	0.68
2:D:30:LEU:HG	2:D:31:GLN:HG3	1.74	0.68
2:B:95:PRO:N	2:B:98:ARG:HD2	2.08	0.68
2:B:184:TYR:HE1	2:B:211:LEU:HB2	1.58	0.68
2:B:49:ARG:HG3	2:B:102:SER:HB3	1.75	0.68
2:B:77:GLU:HA	2:B:80:LYS:HE3	1.75	0.68
2:B:212:LYS:HD3	2:B:212:LYS:C	2.14	0.67
1:A:29:TRP:HB2	1:A:399:LEU:HD21	1.77	0.67
2:B:151:PHE:CB	2:B:186:ILE:HG22	2.24	0.67
1:A:393:LYS:HA	1:A:393:LYS:HE3	1.77	0.66
1:C:207:LYS:NZ	2:D:167:VAL:O	2.28	0.66
2:D:30:LEU:HD12	2:D:31:GLN:H	1.59	0.66
1:A:359:ALA:O	1:A:360:ILE:HD13	1.95	0.66
2:B:238:PRO:HA	2:B:241:GLN:CG	2.25	0.66
2:D:244:GLU:O	2:D:247:GLN:HG2	1.94	0.66
1:A:353:ILE:HB	1:A:386:THR:CG2	2.26	0.66
2:D:63:TYR:OH	2:D:73:LYS:NZ	2.26	0.66
2:B:156:ASP:HA	2:B:159:LYS:HB2	1.77	0.66
1:A:37:LYS:HD2	1:A:38:ASN:N	2.09	0.65
1:A:247:VAL:HG13	1:A:248:PRO:HD2	1.78	0.65
2:B:72:SER:HA	2:B:75:GLU:CG	2.26	0.65
2:D:26:LEU:HD12	2:D:135:LEU:HD12	1.78	0.65
1:A:224:GLU:OE2	1:C:381:ARG:HD2	1.96	0.65
2:D:107:ARG:O	2:D:111:CYS:HB3	1.96	0.65
1:C:349:THR:CG2	1:C:351:SER:H	2.07	0.65
1:C:237:LYS:HA	1:C:240:TRP:CE2	2.31	0.65
1:C:37:LYS:HB2	1:C:38:ASN:HD22	1.63	0.64
1:C:112:MET:HG3	1:C:119:ARG:NH1	2.11	0.64
1:C:191:LEU:HD11	1:C:212:ILE:HG12	1.78	0.64
2:D:271:ILE:HD13	2:D:316:ILE:HD12	1.79	0.64
2:D:163:GLU:O	2:D:167:VAL:HG23	1.98	0.64
1:A:266:LEU:HD13	1:C:384:LYS:HD3	1.79	0.64
2:B:79:ARG:HH11	2:B:79:ARG:CB	2.07	0.64
2:D:42:PHE:HE2	2:D:249:LEU:HD13	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:O	2:B:82:LYS:CB	2.45	0.64
2:D:268:VAL:HG12	2:D:269:GLY:O	1.97	0.64
2:D:29:TYR:HE2	2:D:99:ASP:OD1	1.81	0.63
2:D:214:ILE:O	2:D:218:ILE:HG13	1.98	0.63
1:C:410:LEU:HG	1:C:411:LEU:HD23	1.81	0.63
2:D:173:LEU:HD23	2:D:174:SER:O	1.98	0.63
2:D:243:ASP:OD1	2:D:245:ARG:HD2	1.99	0.63
1:A:260:GLN:HA	1:A:260:GLN:HE21	1.63	0.63
2:D:421:GLN:NE2	2:D:441:LEU:O	2.31	0.63
2:B:130:PHE:CZ	2:B:134:ILE:HD11	2.34	0.62
2:D:293:LYS:O	2:D:297:GLU:HG3	1.99	0.62
2:D:365:PHE:HE1	2:D:369:LYS:HZ3	1.47	0.62
2:D:268:VAL:HG12	2:D:269:GLY:H	1.64	0.62
2:D:337:ASP:HB3	2:D:340:LYS:CB	2.28	0.62
2:D:337:ASP:HB3	2:D:340:LYS:HB2	1.81	0.62
1:C:234:LEU:CD2	1:C:243:ILE:HD12	2.30	0.62
1:C:25:GLN:OE1	1:C:25:GLN:N	2.31	0.62
2:D:261:ASP:HB2	2:D:442:ASN:HD21	1.64	0.62
2:D:265:GLN:HA	2:D:265:GLN:NE2	2.15	0.62
2:B:37:ILE:HB	2:B:41:GLU:HG3	1.82	0.61
2:B:131:ARG:O	2:B:135:LEU:HG	2.00	0.61
1:C:349:THR:HG21	1:C:351:SER:HB3	1.81	0.61
2:D:37:ILE:HB	2:D:41:GLU:HB3	1.83	0.61
1:C:118:VAL:CG1	5:C:1032:HOH:O	2.49	0.61
2:B:64:VAL:C	2:B:66:GLY:H	2.04	0.61
2:D:39:LEU:HB3	2:D:43:GLU:OE1	2.01	0.61
2:D:178:LEU:O	2:D:179:GLY:O	2.17	0.61
2:D:290:GLN:NE2	2:D:385:PRO:HG3	2.16	0.61
2:D:387:ARG:HD2	2:D:420:TYR:CZ	2.35	0.61
2:D:26:LEU:HD12	2:D:135:LEU:CD1	2.31	0.61
1:A:53:ILE:HD12	1:A:53:ILE:N	2.09	0.61
1:C:181:VAL:HG21	5:C:1023:HOH:O	2.01	0.61
1:C:9:LEU:HD11	1:C:325:PRO:HA	1.83	0.61
1:A:233:ILE:HD12	1:A:243:ILE:HD11	1.83	0.61
2:B:192:LEU:O	2:B:196:ARG:HG2	2.01	0.61
1:C:290:PRO:O	1:C:291:TRP:HB2	2.00	0.61
2:D:82:LYS:CG	2:D:98:ARG:HD3	2.29	0.61
2:D:176:LEU:HB3	5:D:1108:HOH:O	2.00	0.61
1:C:190:SER:O	2:D:198:ARG:NH2	2.33	0.61
1:A:402:LEU:HA	5:A:919:HOH:O	2.01	0.60
1:A:55:ILE:HD12	1:A:58:GLN:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:VAL:O	2:B:66:GLY:N	2.32	0.60
2:B:169:SER:OG	2:B:201:TYR:HB2	2.00	0.60
2:B:75:GLU:HB3	2:B:130:PHE:HZ	1.64	0.60
2:B:75:GLU:HB2	2:B:79:ARG:HH21	1.65	0.60
1:A:247:VAL:CG2	1:A:292:LEU:HD11	2.28	0.60
2:B:178:LEU:HD21	2:B:183:ILE:HD12	1.84	0.60
2:D:246:LEU:HD23	2:D:249:LEU:HD12	1.83	0.60
2:D:44:ASN:HA	2:D:47:ILE:CD1	2.30	0.60
2:D:147:SER:O	2:D:148:GLN:HB2	2.00	0.60
1:A:103:GLU:HG2	1:A:175:ARG:O	2.01	0.60
2:D:113:SER:HB3	2:D:116:LEU:CG	2.31	0.59
2:D:140:ILE:O	2:D:144:LEU:HG	2.00	0.59
1:A:237:LYS:HA	1:A:240:TRP:CE2	2.38	0.59
1:A:336:LEU:O	1:A:339:VAL:HG23	2.02	0.59
1:C:49:LEU:HD13	1:C:50:LYS:HZ2	1.67	0.59
1:C:216:ILE:HD13	1:C:294:TRP:CD2	2.37	0.59
1:C:407:LYS:O	1:C:411:LEU:HB2	2.01	0.59
1:A:386:THR:HG22	1:A:387:SER:H	1.68	0.59
2:B:247:GLN:HE21	2:B:247:GLN:CA	2.14	0.59
2:B:113:SER:HB2	2:B:116:LEU:CG	2.31	0.59
2:D:444:PRO:O	2:D:447:PHE:HB3	2.01	0.59
2:B:30:LEU:HD12	2:B:31:GLN:H	1.66	0.59
2:B:68:GLU:CA	2:B:71:GLN:HB3	2.27	0.59
1:A:35:VAL:HG12	1:A:35:VAL:O	2.03	0.59
2:B:114:GLU:OE1	2:B:117:ARG:HD3	2.03	0.59
1:A:266:LEU:CD1	1:C:384:LYS:HD3	2.32	0.59
2:B:75:GLU:O	2:B:79:ARG:NE	2.35	0.59
1:A:181:VAL:HG21	5:A:903:HOH:O	2.02	0.58
1:C:234:LEU:HD21	1:C:243:ILE:HD12	1.85	0.58
2:D:69:GLN:O	2:D:73:LYS:HG3	2.03	0.58
1:A:110:ILE:HD13	1:A:138:ALA:HB1	1.85	0.58
1:C:33:GLY:O	1:C:35:VAL:N	2.36	0.58
2:D:24:HIS:NE2	2:D:92:GLU:HB3	2.18	0.58
2:D:293:LYS:HE2	2:D:297:GLU:OE2	2.03	0.58
1:A:19:ARG:NH1	1:A:379:ARG:HH11	2.00	0.58
1:C:195:GLY:O	1:C:197:ASP:N	2.36	0.58
2:B:82:LYS:HB2	2:B:82:LYS:NZ	2.19	0.58
1:A:247:VAL:HG22	1:A:292:LEU:CD1	2.29	0.58
2:B:81:LEU:O	2:B:82:LYS:HB2	2.03	0.58
2:B:240:VAL:HG13	2:B:246:LEU:HD12	1.85	0.58
2:D:418:THR:HG23	2:D:420:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:TYR:CE1	2:D:203:GLU:HB2	2.39	0.58
1:C:37:LYS:CD	1:C:38:ASN:H	2.12	0.58
1:C:19:ARG:CZ	1:C:379:ARG:HD2	2.33	0.57
2:D:22:TYR:HB2	2:D:24:HIS:NE2	2.19	0.57
2:D:22:TYR:HB2	2:D:24:HIS:CD2	2.39	0.57
1:C:410:LEU:HG	1:C:411:LEU:N	2.18	0.57
2:D:442:ASN:C	2:D:442:ASN:HD22	2.06	0.57
1:C:216:ILE:HD13	1:C:294:TRP:CG	2.40	0.57
2:B:144:LEU:HB3	2:B:151:PHE:CE2	2.40	0.57
1:A:35:VAL:O	1:A:36:ILE:HD13	2.04	0.57
1:A:141:ILE:HG21	1:A:302:PHE:CE2	2.39	0.57
2:D:358:LYS:HG2	2:D:360:THR:N	2.20	0.57
1:C:349:THR:HG22	1:C:351:SER:HB3	1.86	0.57
1:A:247:VAL:HG13	1:A:292:LEU:HD21	1.87	0.57
1:A:19:ARG:HH12	1:A:379:ARG:HH11	1.53	0.56
1:A:195:GLY:O	1:A:197:ASP:N	2.39	0.56
1:A:386:THR:CG2	1:A:387:SER:N	2.68	0.56
2:B:72:SER:CA	2:B:75:GLU:HG2	2.29	0.56
2:B:104:PHE:CE1	2:B:107:ARG:NH1	2.73	0.56
2:B:64:VAL:HG12	2:B:65:LYS:H	1.69	0.56
1:C:329:ARG:HG3	5:C:1036:HOH:O	2.03	0.56
2:D:130:PHE:CE2	2:D:134:ILE:HD11	2.40	0.56
2:D:192:LEU:HD12	2:D:192:LEU:O	2.05	0.56
2:D:342:ASP:HA	2:D:346:SER:HB2	1.86	0.56
2:D:24:HIS:CE1	2:D:92:GLU:CB	2.89	0.56
2:D:77:GLU:OE1	2:D:418:THR:HG21	2.05	0.56
2:B:33:PRO:HD3	2:B:104:PHE:CD2	2.41	0.56
2:D:287:CYS:SG	2:D:288:MET:N	2.79	0.56
1:C:144:ARG:NH2	1:C:148:GLU:HB2	2.20	0.56
2:D:22:TYR:HB3	2:D:23:PRO:HD2	1.88	0.56
1:A:343:ASP:CG	1:A:346:THR:HG23	2.25	0.56
1:A:355:ARG:HG3	1:A:355:ARG:NH1	2.20	0.56
1:A:38:ASN:HA	1:A:41:GLN:OE1	2.05	0.56
1:A:260:GLN:HE21	1:A:260:GLN:CA	2.17	0.56
1:A:19:ARG:HH12	1:A:379:ARG:NH1	2.03	0.55
1:C:51:ASP:HB2	1:C:53:ILE:CD1	2.36	0.55
1:C:379:ARG:HB3	1:C:382:ASP:OD2	2.06	0.55
2:B:59:LEU:HD13	2:B:74:LEU:HB2	1.88	0.55
1:C:38:ASN:HA	1:C:41:GLN:OE1	2.05	0.55
1:A:111:ASP:OD2	1:A:113:THR:HG23	2.05	0.55
1:A:9:LEU:HD23	1:A:76:TYR:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LYS:HE2	1:C:246:LEU:O	2.07	0.55
1:C:38:ASN:HD22	1:C:38:ASN:N	2.05	0.55
1:C:61:ASN:HB2	1:C:65:ASP:OD1	2.07	0.55
1:A:172:GLU:HA	1:A:175:ARG:CZ	2.36	0.55
2:D:32:PRO:HA	2:D:104:PHE:CE1	2.42	0.55
2:D:262:TYR:N	2:D:262:TYR:CD2	2.74	0.55
1:A:402:LEU:HB3	1:A:406:ARG:HH21	1.72	0.55
2:B:54:LYS:O	2:B:57:GLU:HB3	2.07	0.55
2:B:58:ASN:C	2:B:60:GLY:H	2.10	0.55
1:C:21:PHE:O	1:C:23:TYR:N	2.35	0.55
2:D:245:ARG:O	2:D:248:PRO:HD2	2.07	0.55
2:D:65:LYS:H	2:D:65:LYS:HD2	1.72	0.54
2:D:437:CYS:HB2	2:D:439:PHE:CE2	2.42	0.54
1:C:36:ILE:CG2	1:C:37:LYS:HG3	2.36	0.54
1:A:409:GLU:O	1:A:413:LYS:HB2	2.07	0.54
2:B:64:VAL:HG12	2:B:65:LYS:N	2.23	0.54
2:B:154:ILE:N	2:B:154:ILE:HD12	2.21	0.54
2:B:192:LEU:O	2:B:192:LEU:HD23	2.07	0.54
2:B:194:LEU:HD13	2:B:200:VAL:HG11	1.90	0.54
2:B:237:LEU:HB3	2:B:241:GLN:NE2	2.23	0.54
2:B:166:ILE:HD13	2:B:183:ILE:HD13	1.88	0.54
1:C:12:LEU:CD1	1:C:351:SER:HA	2.36	0.54
1:A:14:LYS:HG2	1:A:74:ASN:ND2	2.22	0.54
2:B:47:ILE:O	2:B:51:LYS:HG3	2.08	0.54
1:C:50:LYS:O	1:C:53:ILE:HD13	2.08	0.54
1:C:112:MET:HG3	1:C:119:ARG:CZ	2.37	0.54
1:C:193:LYS:HE2	5:C:1013:HOH:O	2.08	0.54
2:D:261:ASP:HB2	2:D:442:ASN:OD1	2.07	0.54
1:A:302:PHE:CD2	1:A:303:PRO:HD2	2.43	0.54
2:D:129:ARG:HG2	2:D:219:LEU:HD11	1.89	0.54
1:A:51:ASP:N	1:A:53:ILE:CD1	2.68	0.54
1:C:50:LYS:H	1:C:50:LYS:CD	2.04	0.54
1:C:81:GLY:CA	1:C:316:LEU:HD23	2.38	0.54
1:A:233:ILE:HG13	1:A:234:LEU:HG	1.90	0.54
1:C:280:GLN:HE22	1:C:290:PRO:CD	2.21	0.54
1:A:66:LEU:CD1	1:A:70:MET:HE3	2.38	0.54
1:A:272:LEU:HD12	1:A:272:LEU:O	2.08	0.54
2:D:54:LYS:O	2:D:57:GLU:HB3	2.08	0.54
2:B:141:GLN:HE21	2:B:145:LYS:HE3	1.73	0.53
1:C:153:LYS:HE2	1:C:153:LYS:HA	1.90	0.53
2:B:78:LEU:HD23	2:B:79:ARG:HH22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:CYS:SG	1:A:131:CYS:HB3	2.47	0.53
1:A:224:GLU:HB2	5:A:907:HOH:O	2.08	0.53
1:A:247:VAL:HG22	1:A:292:LEU:CD2	2.38	0.53
1:A:292:LEU:O	1:A:296:ILE:HG13	2.09	0.53
1:A:412:LYS:O	1:A:412:LYS:HG2	2.08	0.53
2:D:94:GLU:OE2	2:D:94:GLU:HA	2.07	0.53
2:D:358:LYS:CE	2:D:360:THR:HA	2.37	0.53
1:A:306:ASP:HB3	1:A:309:VAL:HG23	1.90	0.53
2:B:75:GLU:HB3	2:B:130:PHE:CZ	2.44	0.53
2:D:273:LEU:HD13	2:D:322:GLN:HB3	1.90	0.53
1:C:67:GLU:O	1:C:71:GLN:HG3	2.09	0.53
2:D:163:GLU:CD	2:D:178:LEU:HB3	2.28	0.53
2:D:424:CYS:HB3	2:D:441:LEU:HD23	1.89	0.53
1:C:257:GLN:O	1:C:261:LYS:HG3	2.08	0.53
2:D:358:LYS:HG2	2:D:360:THR:H	1.74	0.53
1:A:118:VAL:HG11	1:A:300:TYR:O	2.08	0.53
2:B:237:LEU:CD1	2:B:241:GLN:HE22	2.10	0.53
1:C:401:ASN:N	1:C:401:ASN:HD22	2.05	0.53
2:D:261:ASP:HB2	2:D:442:ASN:ND2	2.23	0.53
1:A:402:LEU:CA	5:A:919:HOH:O	2.57	0.53
1:C:118:VAL:HG12	5:C:1032:HOH:O	2.09	0.53
2:D:264:THR:OG1	2:D:265:GLN:N	2.42	0.53
2:D:121:ILE:HG12	2:D:226:LEU:HD23	1.91	0.53
2:D:280:SER:HA	2:D:284:PHE:CD2	2.45	0.52
1:A:238:GLU:HG2	1:A:238:GLU:O	2.09	0.52
2:B:59:LEU:HD21	2:B:73:LYS:CG	2.38	0.52
1:C:33:GLY:C	1:C:35:VAL:H	2.12	0.52
1:C:400:GLU:O	1:C:403:ASP:N	2.42	0.52
2:D:192:LEU:HA	2:D:195:PHE:CE2	2.43	0.52
2:B:235:ARG:NH1	2:B:235:ARG:HG2	2.25	0.52
2:D:263:SER:OG	2:D:445:ASN:HB2	2.10	0.52
1:A:237:LYS:HD2	1:A:240:TRP:HE1	1.75	0.52
2:B:39:LEU:HD23	2:B:39:LEU:O	2.09	0.52
2:B:49:ARG:NH2	2:B:124:GLU:OE1	2.42	0.52
2:B:201:TYR:CE1	2:B:203:GLU:HB2	2.45	0.52
1:C:89:ASN:C	1:C:89:ASN:ND2	2.62	0.52
2:D:74:LEU:HD12	2:D:74:LEU:O	2.08	0.52
1:A:53:ILE:H	1:A:53:ILE:CD1	2.06	0.52
2:B:140:ILE:O	2:B:143:PHE:HD1	1.93	0.52
1:A:356:GLU:O	1:A:360:ILE:HG12	2.09	0.52
1:A:413:LYS:C	1:A:415:ASP:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLU:O	1:C:2:GLU:HG2	2.09	0.52
2:D:263:SER:CB	2:D:445:ASN:HB3	2.40	0.52
2:B:117:ARG:NH2	2:B:231:ALA:HA	2.25	0.52
2:D:113:SER:H	2:D:116:LEU:HD12	1.74	0.52
1:C:19:ARG:NH2	1:C:379:ARG:NH2	2.57	0.52
1:C:132:TRP:CZ3	1:C:135:MET:HG3	2.45	0.52
2:B:136:PRO:O	2:B:140:ILE:HG13	2.09	0.52
2:B:71:GLN:HG2	2:B:72:SER:N	2.24	0.51
1:C:44:GLU:OE1	1:C:56:ARG:HG2	2.10	0.51
2:D:94:GLU:HB3	2:D:95:PRO:CD	2.31	0.51
2:D:311:LEU:CD1	2:D:363:THR:H	2.23	0.51
1:A:118:VAL:CG1	1:A:118:VAL:O	2.57	0.51
1:C:1:MET:HB3	5:C:1011:HOH:O	2.09	0.51
1:C:86:HIS:CD2	1:C:94:VAL:HG11	2.45	0.51
1:A:20:LEU:HD13	1:A:353:ILE:HD12	1.91	0.51
2:B:195:PHE:CD1	2:B:195:PHE:C	2.83	0.51
2:D:49:ARG:HB2	2:D:102:SER:HB2	1.91	0.51
2:D:237:LEU:HD12	2:D:240:VAL:HG12	1.92	0.51
1:A:19:ARG:NH1	1:A:379:ARG:NH1	2.58	0.51
1:A:349:THR:CG2	1:A:351:SER:H	2.21	0.51
2:B:192:LEU:HD23	2:B:192:LEU:C	2.31	0.51
2:D:268:VAL:CG1	2:D:269:GLY:N	2.73	0.51
1:C:47:PHE:CE1	1:C:78:ILE:HG23	2.45	0.51
1:C:81:GLY:HA3	1:C:316:LEU:HD23	1.92	0.51
1:C:208:ILE:HD11	1:C:291:TRP:CD1	2.46	0.51
1:A:27:TYR:HB2	1:A:63:GLN:HG3	1.92	0.51
1:C:280:GLN:NE2	1:C:290:PRO:HD2	2.25	0.51
1:C:395:PHE:O	1:C:399:LEU:HG	2.10	0.51
2:D:247:GLN:O	2:D:251:ASN:HB2	2.11	0.51
1:A:251:ILE:HG22	1:A:251:ILE:O	2.10	0.51
2:B:237:LEU:HD22	2:B:241:GLN:NE2	2.26	0.51
1:A:79:ASP:OD2	1:A:318:LYS:HA	2.11	0.51
2:B:52:LEU:HD22	2:B:83:PHE:CE1	2.46	0.51
2:B:49:ARG:C	2:B:51:LYS:N	2.63	0.51
2:D:252:HIS:HD2	2:D:257:TYR:HE2	1.59	0.51
1:C:386:THR:CG2	1:C:387:SER:N	2.72	0.51
1:A:44:GLU:OE1	1:A:56:ARG:NE	2.40	0.50
2:B:38:SER:OG	2:B:41:GLU:HG2	2.11	0.50
2:B:72:SER:HA	2:B:75:GLU:OE2	2.11	0.50
2:B:126:ASP:N	2:B:126:ASP:OD2	2.44	0.50
2:B:237:LEU:N	2:B:238:PRO:CD	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:HIS:ND1	1:C:402:LEU:CD1	2.70	0.50
1:A:89:ASN:HD22	1:A:90:GLN:N	2.09	0.50
1:C:178:SER:OG	1:C:181:VAL:HG23	2.12	0.50
2:D:252:HIS:CB	2:D:256:SER:HB2	2.42	0.50
1:A:248:PRO:HG3	1:A:279:TYR:CE2	2.46	0.50
1:A:402:LEU:HD23	5:A:919:HOH:O	2.10	0.50
2:B:95:PRO:CA	2:B:98:ARG:HD2	2.42	0.50
2:B:219:LEU:O	2:B:222:PHE:HB3	2.11	0.50
1:C:155:ARG:HG3	1:C:155:ARG:HH11	1.75	0.50
2:D:352:SER:HA	2:D:362:TYR:CD2	2.46	0.50
1:A:334:ILE:HD13	1:A:334:ILE:N	2.26	0.50
1:A:172:GLU:CA	1:A:175:ARG:NH1	2.74	0.50
2:B:144:LEU:HB3	2:B:151:PHE:CZ	2.47	0.50
2:B:237:LEU:HD13	2:B:241:GLN:NE2	2.09	0.50
2:D:46:ALA:O	2:D:50:VAL:HG23	2.12	0.50
1:A:200:LYS:NZ	1:A:295:GLU:OE2	2.37	0.50
1:C:210:PRO:O	1:C:214:LYS:HG3	2.12	0.50
1:C:329:ARG:CG	5:C:1036:HOH:O	2.59	0.50
2:D:70:TYR:CD1	2:D:70:TYR:C	2.85	0.50
2:D:265:GLN:HB3	2:D:356:GLU:HA	1.93	0.50
2:B:120:PHE:O	2:B:124:GLU:HB2	2.11	0.50
1:C:80:ILE:HB	1:C:168:TRP:HH2	1.77	0.50
1:A:154:HIS:ND1	1:A:402:LEU:HD23	2.27	0.49
1:C:154:HIS:N	1:C:154:HIS:CD2	2.79	0.49
2:D:311:LEU:HD13	2:D:363:THR:H	1.77	0.49
1:A:118:VAL:O	1:A:118:VAL:HG12	2.11	0.49
2:D:43:GLU:O	2:D:47:ILE:CG1	2.53	0.49
2:D:268:VAL:CG1	2:D:269:GLY:H	2.23	0.49
1:A:113:THR:HA	1:A:116:ASP:OD1	2.11	0.49
1:A:186:VAL:HG21	1:A:310:SER:HB2	1.93	0.49
1:A:217:ASN:O	1:A:220:LYS:HB2	2.12	0.49
2:B:68:GLU:O	2:B:72:SER:N	2.45	0.49
2:D:365:PHE:N	5:D:1105:HOH:O	2.38	0.49
2:B:49:ARG:HG2	2:B:102:SER:HB3	1.93	0.49
2:D:49:ARG:HD3	2:D:102:SER:OG	2.11	0.49
2:D:243:ASP:O	2:D:247:GLN:NE2	2.35	0.49
2:D:288:MET:HG3	2:D:312:PHE:CD2	2.48	0.49
2:B:74:LEU:O	2:B:74:LEU:HD23	2.12	0.49
2:D:286:PRO:O	2:D:290:GLN:HB2	2.13	0.49
1:A:232:ASP:CG	1:A:235:GLU:HB2	2.32	0.49
1:A:278:ARG:HG2	1:A:278:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASN:N	1:C:38:ASN:ND2	2.61	0.49
1:C:15:LEU:HD23	1:C:354:CYS:SG	2.53	0.49
2:D:113:SER:OG	2:D:115:GLU:HB2	2.12	0.49
2:D:221:GLU:OE1	2:D:225:LYS:HE3	2.13	0.49
2:D:272:SER:H	2:D:275:GLN:NE2	2.10	0.49
1:A:349:THR:CG2	1:A:351:SER:HB3	2.43	0.49
1:C:91:HIS:ND1	1:C:92:ASN:N	2.61	0.49
2:D:237:LEU:HB3	2:D:238:PRO:HD3	1.95	0.49
2:D:82:LYS:CG	2:D:82:LYS:O	2.60	0.49
1:A:118:VAL:HG11	1:A:300:TYR:HA	1.95	0.49
1:C:143:ASP:OD1	1:C:155:ARG:NE	2.42	0.48
1:C:191:LEU:HD12	1:C:302:PHE:CE2	2.47	0.48
2:D:57:GLU:O	2:D:61:VAL:HG23	2.13	0.48
2:D:337:ASP:HB3	2:D:340:LYS:HB3	1.94	0.48
1:A:170:CYS:O	1:A:175:ARG:NH1	2.45	0.48
1:A:247:VAL:HG22	1:A:292:LEU:CG	2.43	0.48
1:C:339:VAL:O	1:C:341:GLN:N	2.46	0.48
2:D:103:HIS:HE1	2:D:124:GLU:HG2	1.77	0.48
2:D:164:GLN:HE22	2:D:176:LEU:HD22	1.77	0.48
1:A:402:LEU:N	5:A:919:HOH:O	2.46	0.48
2:B:138:ASP:OD2	2:B:138:ASP:N	2.43	0.48
2:B:145:LYS:O	2:B:147:SER:N	2.46	0.48
2:B:235:ARG:HG2	2:B:235:ARG:HH11	1.77	0.48
1:C:60:PHE:HB3	1:C:65:ASP:HB2	1.95	0.48
2:D:219:LEU:O	2:D:222:PHE:HB3	2.13	0.48
2:D:229:ALA:O	2:D:233:THR:HG23	2.12	0.48
2:D:259:GLY:O	2:D:260:GLN:HG2	2.13	0.48
2:D:320:LEU:HD13	2:D:353:PHE:CD1	2.47	0.48
2:B:119:TRP:O	2:B:122:GLN:HB3	2.14	0.48
2:D:335:LYS:HD2	2:D:335:LYS:N	2.28	0.48
1:A:386:THR:CG2	1:A:387:SER:H	2.27	0.48
1:C:381:ARG:NH1	1:C:384:LYS:NZ	2.61	0.48
2:D:418:THR:O	2:D:418:THR:CG2	2.61	0.48
1:A:210:PRO:O	1:A:214:LYS:HG3	2.13	0.48
2:B:64:VAL:C	2:B:66:GLY:N	2.65	0.48
2:B:115:GLU:O	2:B:119:TRP:HB2	2.14	0.48
2:D:324:LEU:HD23	2:D:349:ILE:HG21	1.95	0.48
2:B:104:PHE:HE1	2:B:107:ARG:NH1	2.12	0.48
2:D:35:GLU:OE2	2:D:101:ILE:HD11	2.13	0.48
1:A:216:ILE:HD13	1:A:294:TRP:CD2	2.49	0.48
1:C:95:LYS:HD3	1:C:98:ALA:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TYR:CD2	2:B:116:LEU:HD22	2.49	0.48
1:C:69:GLU:O	1:C:73:MET:HG2	2.14	0.48
2:D:117:ARG:CG	2:D:230:LEU:HD13	2.27	0.47
2:D:424:CYS:HB3	2:D:441:LEU:CD2	2.44	0.47
1:A:133:THR:O	1:A:136:THR:HB	2.13	0.47
1:C:116:ASP:CG	1:C:124:SER:OG	2.53	0.47
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.79	0.47
2:B:132:PHE:O	2:B:133:SER:C	2.53	0.47
2:D:155:SER:C	2:D:157:GLU:N	2.67	0.47
2:B:178:LEU:HD11	2:B:183:ILE:HD11	1.96	0.47
2:D:288:MET:CG	2:D:312:PHE:CD2	2.97	0.47
1:A:41:GLN:HB3	1:A:87:ARG:NH1	2.29	0.47
2:B:110:TYR:HA	2:B:116:LEU:HD13	1.97	0.47
2:D:32:PRO:HG3	2:D:104:PHE:HE1	1.79	0.47
2:D:129:ARG:HE	2:D:219:LEU:HD13	1.79	0.47
2:B:111:CYS:O	2:B:234:ALA:HB2	2.14	0.47
2:D:94:GLU:CB	2:D:95:PRO:HD3	2.33	0.47
1:A:69:GLU:OE2	1:A:72:LYS:HE3	2.14	0.47
1:A:145:ALA:O	1:A:149:ASP:HB2	2.15	0.47
2:B:155:SER:C	2:B:157:GLU:N	2.68	0.47
1:C:280:GLN:HE22	1:C:290:PRO:HD2	1.80	0.47
1:C:360:ILE:HG22	1:C:360:ILE:O	2.15	0.47
2:D:72:SER:HA	2:D:75:GLU:HG2	1.97	0.47
2:D:80:LYS:NZ	2:D:418:THR:CG2	2.76	0.47
2:D:362:TYR:O	2:D:363:THR:OG1	2.29	0.47
2:B:37:ILE:HB	2:B:41:GLU:CB	2.45	0.47
2:D:262:TYR:HB2	2:D:264:THR:N	2.20	0.47
2:B:37:ILE:HB	2:B:41:GLU:CG	2.43	0.47
1:C:160:SER:OG	1:C:164:GLY:O	2.32	0.47
2:D:24:HIS:O	2:D:25:CYS:C	2.53	0.47
2:D:159:LYS:HE3	2:D:183:ILE:HD12	1.97	0.47
1:A:15:LEU:HD23	1:A:354:CYS:HB3	1.97	0.47
2:D:166:ILE:HG21	2:D:183:ILE:HD13	1.97	0.47
1:A:159:TYR:HB2	1:A:334:ILE:HD11	1.97	0.46
2:B:202:LEU:HA	2:B:206:PHE:O	2.15	0.46
1:C:65:ASP:OD2	1:C:65:ASP:N	2.48	0.46
1:C:140:ARG:HD3	5:C:1025:HOH:O	2.14	0.46
1:C:158:VAL:HG12	1:C:159:TYR:N	2.30	0.46
1:C:390:PRO:O	1:C:393:LYS:HB3	2.15	0.46
2:D:431:ILE:HG13	2:D:432:HIS:ND1	2.28	0.46
1:A:47:PHE:CE1	1:A:78:ILE:HG23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:HA	1:A:252:HIS:CD2	2.51	0.46
2:B:145:LYS:C	2:B:147:SER:N	2.67	0.46
1:C:118:VAL:HG11	1:C:300:TYR:O	2.15	0.46
2:D:263:SER:CB	2:D:445:ASN:CB	2.93	0.46
2:D:359:ARG:HB2	2:D:362:TYR:HB2	1.97	0.46
1:A:402:LEU:HB3	1:A:406:ARG:NH2	2.30	0.46
2:B:141:GLN:O	2:B:145:LYS:HG3	2.14	0.46
2:D:200:VAL:HG12	2:D:209:VAL:HG12	1.98	0.46
1:A:214:LYS:NZ	5:A:914:HOH:O	2.47	0.46
1:A:379:ARG:O	1:A:381:ARG:N	2.47	0.46
1:A:249:GLU:HG2	1:A:252:HIS:CE1	2.50	0.46
2:B:58:ASN:C	2:B:60:GLY:N	2.68	0.46
2:B:65:LYS:HE3	2:B:65:LYS:O	2.15	0.46
1:C:95:LYS:H	1:C:95:LYS:HG3	1.46	0.46
1:C:171:ASP:OD2	1:C:171:ASP:N	2.48	0.46
2:B:170:SER:HB3	2:B:171:PRO:CD	2.35	0.46
1:A:260:GLN:NE2	1:A:260:GLN:CA	2.68	0.46
1:A:323:VAL:HG21	1:A:350:ILE:HD12	1.98	0.46
2:D:29:TYR:HB3	2:D:104:PHE:HE2	1.80	0.46
1:A:41:GLN:CD	1:A:41:GLN:H	2.18	0.46
1:A:66:LEU:HG	1:A:70:MET:CE	2.46	0.46
2:B:39:LEU:O	2:B:43:GLU:HB2	2.15	0.46
2:B:175:GLY:O	2:B:176:LEU:HD23	2.16	0.46
1:C:162:ARG:HG3	1:C:327:THR:CG2	2.46	0.46
1:C:196:GLN:O	1:C:196:GLN:HG2	2.16	0.46
1:C:200:LYS:HG2	1:C:203:HIS:CE1	2.51	0.46
2:D:184:TYR:N	2:D:184:TYR:CD1	2.83	0.46
2:D:288:MET:HG2	2:D:312:PHE:CG	2.50	0.46
1:C:152:PHE:CE1	1:C:174:VAL:HG22	2.51	0.46
2:D:263:SER:HB3	2:D:445:ASN:HB3	1.97	0.46
1:A:157:TRP:CZ3	1:A:167:CYS:HB2	2.51	0.46
1:A:235:GLU:HG2	1:A:236:ASN:HD21	1.78	0.46
1:A:336:LEU:HA	1:A:339:VAL:HG22	1.98	0.46
2:B:238:PRO:C	2:B:240:VAL:H	2.19	0.46
1:C:90:GLN:O	1:C:93:THR:HB	2.15	0.46
1:A:334:ILE:CD1	1:A:342:PHE:CE2	2.97	0.45
1:A:404:LYS:O	1:A:405:SER:C	2.54	0.45
1:A:407:LYS:O	1:A:411:LEU:HB2	2.15	0.45
2:B:49:ARG:NH1	2:B:99:ASP:OD2	2.49	0.45
1:C:381:ARG:HH11	1:C:384:LYS:HZ2	1.64	0.45
2:D:78:LEU:HD11	2:D:127:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:O	1:A:268:ARG:HG3	2.17	0.45
2:B:49:ARG:CD	2:B:102:SER:HB3	2.46	0.45
2:B:199:LYS:O	2:B:200:VAL:CG1	2.62	0.45
1:C:89:ASN:O	1:C:90:GLN:HG3	2.15	0.45
2:D:342:ASP:HA	2:D:346:SER:CB	2.47	0.45
2:B:48:ASP:O	2:B:51:LYS:HB2	2.15	0.45
2:B:172:SER:O	2:B:174:SER:N	2.49	0.45
1:C:5:ASP:OD1	1:C:7:THR:OG1	2.25	0.45
1:C:160:SER:OG	1:C:164:GLY:C	2.55	0.45
2:D:47:ILE:HG13	2:D:47:ILE:H	1.59	0.45
2:D:251:ASN:HB3	2:D:252:HIS:ND1	2.31	0.45
1:A:327:THR:CB	1:A:329:ARG:HG2	2.47	0.45
2:B:113:SER:HB2	2:B:116:LEU:CD1	2.47	0.45
1:C:66:LEU:HD12	1:C:66:LEU:HA	1.81	0.45
1:C:115:TYR:C	1:C:117:ASP:H	2.20	0.45
2:D:336:MET:HG3	5:D:1111:HOH:O	2.16	0.45
2:D:343:LYS:O	2:D:343:LYS:HG2	2.17	0.45
2:B:38:SER:H	2:B:41:GLU:HG3	1.81	0.45
1:C:153:LYS:N	1:C:171:ASP:OD1	2.36	0.45
2:D:265:GLN:CB	2:D:356:GLU:HA	2.46	0.45
1:A:73:MET:HG3	5:A:922:HOH:O	2.16	0.45
2:B:28:PHE:CG	2:B:28:PHE:O	2.70	0.45
2:B:247:GLN:CA	2:B:247:GLN:NE2	2.79	0.45
1:C:50:LYS:HD2	1:C:50:LYS:N	2.10	0.45
1:C:140:ARG:HG2	1:C:140:ARG:NH1	2.31	0.45
2:D:272:SER:HB2	2:D:275:GLN:HG3	1.99	0.45
2:D:375:PRO:HA	2:D:376:PRO:HD2	1.82	0.45
1:A:26:TYR:OH	1:A:80:ILE:HD11	2.16	0.45
1:A:237:LYS:HE3	1:A:256:GLN:OE1	2.17	0.45
2:B:171:PRO:C	2:B:173:LEU:H	2.18	0.45
2:B:247:GLN:N	2:B:248:PRO:CD	2.80	0.45
1:C:12:LEU:HD13	1:C:351:SER:HA	1.97	0.45
2:D:82:LYS:HG3	2:D:98:ARG:CD	2.37	0.45
2:D:414:LEU:HD13	2:D:422:VAL:HG12	1.97	0.45
1:A:258:SER:HB3	1:A:271:HIS:ND1	2.31	0.45
1:A:302:PHE:CG	1:A:303:PRO:HD2	2.52	0.45
1:C:224:GLU:O	1:C:229:VAL:HG23	2.17	0.45
2:D:57:GLU:OE1	2:D:119:TRP:NE1	2.48	0.45
2:B:177:LYS:C	2:B:179:GLY:H	2.20	0.45
1:C:19:ARG:NH2	1:C:379:ARG:HH21	2.13	0.45
2:D:65:LYS:HD2	2:D:65:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HD3	1:A:382:ASP:OD2	2.16	0.44
2:B:49:ARG:O	2:B:51:LYS:N	2.50	0.44
2:B:181:GLU:OE2	2:B:210:PRO:HB2	2.16	0.44
1:C:272:LEU:HD12	1:C:272:LEU:O	2.17	0.44
1:C:349:THR:HG22	1:C:351:SER:CA	2.47	0.44
2:D:192:LEU:O	2:D:196:ARG:HG2	2.16	0.44
2:D:354:GLY:HA3	2:D:359:ARG:NH1	2.32	0.44
2:B:49:ARG:HH22	2:B:124:GLU:CD	2.19	0.44
2:D:265:GLN:HB3	2:D:355:LYS:O	2.16	0.44
2:D:295:LEU:HG	2:D:330:GLU:HG2	1.99	0.44
1:C:56:ARG:HG2	1:C:56:ARG:O	2.16	0.44
2:D:154:ILE:HB	2:D:158:GLU:HB2	1.99	0.44
1:A:332:VAL:HB	1:A:391:TYR:CD2	2.52	0.44
2:B:42:PHE:CZ	2:B:249:LEU:HD22	2.52	0.44
2:B:117:ARG:O	2:B:121:ILE:HG13	2.18	0.44
2:D:248:PRO:HB3	2:D:253:LEU:HB2	1.99	0.44
1:A:73:MET:O	1:A:74:ASN:C	2.56	0.44
2:B:75:GLU:HB2	2:B:79:ARG:NH2	2.32	0.44
2:B:201:TYR:HD1	2:B:208:TYR:HD2	1.64	0.44
1:C:191:LEU:HD21	1:C:212:ILE:HD11	1.98	0.44
2:D:82:LYS:CD	2:D:98:ARG:HD3	2.47	0.44
2:D:192:LEU:HD12	2:D:192:LEU:C	2.38	0.44
2:D:418:THR:HG23	2:D:420:TYR:CZ	2.52	0.44
1:A:205:SER:O	1:A:206:GLU:C	2.54	0.44
1:C:27:TYR:CD1	1:C:63:GLN:HB2	2.52	0.44
2:D:263:SER:OG	2:D:445:ASN:CB	2.65	0.44
1:A:144:ARG:CZ	1:A:214:LYS:HD2	2.47	0.44
1:C:87:ARG:HD3	1:C:90:GLN:NE2	2.33	0.44
1:A:253:ASP:O	1:A:257:GLN:HG3	2.18	0.44
2:B:249:LEU:C	2:B:251:ASN:H	2.21	0.44
1:C:35:VAL:O	1:C:35:VAL:HG12	2.16	0.44
2:D:232:LEU:O	2:D:235:ARG:HB3	2.17	0.44
1:A:125:ALA:HB1	1:A:162:ARG:NH1	2.33	0.44
1:A:80:ILE:HG13	1:A:319:SER:HB2	1.99	0.43
1:C:259:PHE:HA	1:C:268:ARG:HG2	2.00	0.43
2:D:392:GLU:OE2	2:D:392:GLU:HA	2.16	0.43
1:C:19:ARG:HH21	1:C:379:ARG:NH2	2.15	0.43
2:D:52:LEU:CD1	2:D:78:LEU:HD12	2.48	0.43
2:D:82:LYS:HE2	2:D:98:ARG:NE	2.32	0.43
2:D:420:TYR:O	2:D:423:ALA:HB3	2.17	0.43
1:A:409:GLU:OE1	5:A:920:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG23	2:B:158:GLU:OE1	2.18	0.43
2:D:42:PHE:CE2	2:D:249:LEU:HD13	2.49	0.43
2:B:113:SER:O	2:B:116:LEU:HB2	2.18	0.43
2:B:141:GLN:HA	2:B:144:LEU:HD12	2.00	0.43
2:B:200:VAL:HG11	2:B:209:VAL:CG1	2.48	0.43
1:C:49:LEU:HD13	1:C:50:LYS:HZ1	1.78	0.43
2:D:75:GLU:O	2:D:79:ARG:HB2	2.18	0.43
2:D:112:GLN:HE21	2:D:112:GLN:HB2	1.56	0.43
1:A:82:ALA:HB2	1:A:313:ILE:O	2.18	0.43
1:A:237:LYS:HA	1:A:240:TRP:NE1	2.33	0.43
2:B:37:ILE:HD12	2:B:41:GLU:CB	2.49	0.43
2:B:158:GLU:HB3	2:B:162:ARG:NH2	2.33	0.43
1:C:323:VAL:HG21	1:C:350:ILE:HD12	2.01	0.43
2:D:173:LEU:HD23	2:D:173:LEU:C	2.38	0.43
2:D:366:SER:O	2:D:370:ILE:HG13	2.18	0.43
1:A:66:LEU:HD11	1:A:70:MET:CE	2.48	0.43
1:A:248:PRO:HD2	1:A:292:LEU:CD2	2.49	0.43
1:C:5:ASP:HA	1:C:6:PRO:HD2	1.79	0.43
1:C:33:GLY:C	1:C:35:VAL:N	2.71	0.43
1:C:37:LYS:CG	1:C:38:ASN:H	2.31	0.43
1:C:177:LEU:HD22	1:C:181:VAL:HG11	2.01	0.43
1:A:19:ARG:HD2	1:A:357:LEU:HD21	2.01	0.43
2:B:132:PHE:CE2	2:B:219:LEU:HD21	2.53	0.43
1:C:132:TRP:O	1:C:135:MET:N	2.52	0.43
1:A:95:LYS:HE2	1:A:98:ALA:CB	2.48	0.43
1:A:410:LEU:HD23	1:A:411:LEU:CA	2.49	0.43
2:B:42:PHE:CE2	2:B:249:LEU:HD22	2.54	0.43
2:B:134:ILE:O	2:B:135:LEU:C	2.55	0.43
1:C:133:THR:O	1:C:136:THR:HB	2.19	0.43
2:D:81:LEU:O	2:D:82:LYS:CB	2.66	0.43
1:A:154:HIS:CD2	5:A:919:HOH:O	2.71	0.43
1:A:246:LEU:HD12	1:A:296:ILE:HG23	2.01	0.43
1:A:358:ASP:C	1:A:360:ILE:H	2.22	0.43
1:C:74:ASN:N	1:C:75:PRO:HD3	2.33	0.43
1:A:278:ARG:HH11	1:A:278:ARG:CG	2.32	0.43
1:A:291:TRP:HA	1:A:291:TRP:CE3	2.53	0.43
1:A:334:ILE:HD12	1:A:342:PHE:CD2	2.51	0.43
2:B:237:LEU:N	2:B:238:PRO:HD2	2.33	0.43
1:C:13:LEU:HD22	1:C:17:TYR:CE2	2.54	0.43
1:C:94:VAL:HG12	1:C:98:ALA:HB3	2.00	0.43
1:C:251:ILE:HG23	1:C:275:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:O	1:A:218:ILE:C	2.56	0.42
2:B:82:LYS:HB2	2:B:82:LYS:HZ2	1.84	0.42
1:C:66:LEU:HG	1:C:70:MET:HE3	1.99	0.42
2:D:245:ARG:H	2:D:245:ARG:HG3	1.57	0.42
2:D:291:LEU:HD21	2:D:382:HIS:HA	2.00	0.42
2:D:386:PHE:HE2	2:D:424:CYS:SG	2.42	0.42
1:C:157:TRP:CE3	1:C:167:CYS:HB2	2.54	0.42
1:C:353:ILE:CB	1:C:386:THR:CG2	2.93	0.42
1:A:90:GLN:O	1:A:93:THR:HB	2.20	0.42
1:C:200:LYS:HD2	1:C:246:LEU:HB3	2.02	0.42
2:D:265:GLN:NE2	2:D:265:GLN:CA	2.80	0.42
1:A:106:LEU:HB3	1:A:169:VAL:HB	2.01	0.42
1:A:118:VAL:HG21	1:A:299:GLN:O	2.20	0.42
2:B:37:ILE:HD12	2:B:41:GLU:HB2	2.01	0.42
1:C:36:ILE:HG22	1:C:37:LYS:N	2.32	0.42
1:A:95:LYS:HD3	1:A:95:LYS:N	2.12	0.42
1:A:359:ALA:C	1:A:360:ILE:HD13	2.40	0.42
1:C:356:GLU:OE1	1:C:387:SER:N	2.48	0.42
1:C:378:HIS:O	1:C:379:ARG:HG3	2.19	0.42
2:D:27:GLN:HE21	2:D:27:GLN:HB3	1.57	0.42
2:D:67:THR:CG2	2:D:69:GLN:HE21	2.32	0.42
1:A:54:TYR:CE2	1:A:56:ARG:HB2	2.55	0.42
1:A:412:LYS:O	1:A:415:ASP:OD1	2.37	0.42
2:B:49:ARG:NH2	2:B:124:GLU:OE2	2.53	0.42
1:C:32:TYR:O	1:C:406:ARG:NE	2.53	0.42
1:C:186:VAL:HG21	1:C:310:SER:HB2	2.01	0.42
1:C:381:ARG:NH1	1:C:384:LYS:HZ2	2.18	0.42
2:D:341:PHE:O	2:D:345:TYR:N	2.53	0.42
2:D:441:LEU:HD12	2:D:441:LEU:HA	1.79	0.42
1:A:224:GLU:HG3	1:A:266:LEU:CD2	2.50	0.42
2:B:154:ILE:HG23	2:B:158:GLU:HB2	1.98	0.42
1:C:140:ARG:NE	1:C:222:TYR:OH	2.53	0.42
1:C:155:ARG:HG3	1:C:155:ARG:NH1	2.35	0.42
1:C:280:GLN:OE1	1:C:292:LEU:HG	2.20	0.42
2:D:416:LYS:HE2	2:D:416:LYS:HB3	1.85	0.42
1:A:66:LEU:HG	1:A:70:MET:HE3	2.01	0.42
1:A:269:TRP:CZ3	1:A:272:LEU:HD23	2.54	0.42
2:B:159:LYS:O	2:B:163:GLU:N	2.53	0.42
2:D:271:ILE:CD1	2:D:316:ILE:HD12	2.47	0.42
2:D:58:ASN:O	2:D:59:LEU:C	2.58	0.42
2:D:170:SER:HB3	2:D:171:PRO:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:SER:C	2:D:375:PRO:HD3	2.40	0.42
1:A:51:ASP:O	1:A:52:ASP:CB	2.68	0.42
1:A:247:VAL:CG2	1:A:292:LEU:HD21	2.47	0.42
1:A:390:PRO:O	1:A:393:LYS:HB3	2.18	0.42
1:C:114:ASP:O	1:C:304:ARG:HD2	2.20	0.42
1:C:236:ASN:HB2	1:C:239:SER:H	1.85	0.42
1:C:307:ILE:O	1:C:311:LYS:HB3	2.20	0.42
1:C:330:ILE:O	1:C:332:VAL:HG13	2.19	0.42
2:D:50:VAL:O	2:D:54:LYS:HB2	2.20	0.42
2:D:173:LEU:HD23	2:D:173:LEU:O	2.20	0.42
1:A:46:SER:HB3	1:A:79:ASP:HB2	2.01	0.41
1:A:277:SER:O	1:A:281:ASN:ND2	2.53	0.41
2:B:39:LEU:HD12	2:B:245:ARG:HD3	2.01	0.41
2:B:95:PRO:HA	2:B:98:ARG:HD2	2.02	0.41
2:B:148:GLN:NE2	2:B:148:GLN:HA	2.35	0.41
2:B:65:LYS:O	2:B:65:LYS:HG3	2.20	0.41
2:B:79:ARG:H	2:B:79:ARG:HG2	1.65	0.41
2:D:247:GLN:N	2:D:248:PRO:CD	2.83	0.41
2:D:49:ARG:HH11	2:D:124:GLU:CD	2.23	0.41
2:D:138:ASP:OD2	2:D:138:ASP:N	2.53	0.41
1:A:171:ASP:O	1:A:174:VAL:N	2.53	0.41
1:A:349:THR:HG22	1:A:352:PHE:H	1.86	0.41
2:B:110:TYR:CB	2:B:116:LEU:HB3	2.45	0.41
2:B:201:TYR:CZ	2:B:203:GLU:HB2	2.56	0.41
1:C:257:GLN:HE21	1:C:257:GLN:HB3	1.53	0.41
1:C:349:THR:HG22	1:C:352:PHE:H	1.85	0.41
2:D:237:LEU:HG	2:D:241:GLN:HG3	2.01	0.41
1:A:86:HIS:CG	1:A:94:VAL:HG21	2.56	0.41
1:A:415:ASP:OD1	1:A:415:ASP:C	2.59	0.41
2:B:43:GLU:O	2:B:47:ILE:HG13	2.21	0.41
2:B:51:LYS:O	2:B:55:SER:N	2.53	0.41
1:C:313:ILE:HG12	1:C:313:ILE:O	2.21	0.41
1:C:358:ASP:C	1:C:360:ILE:H	2.23	0.41
2:D:377:SER:O	2:D:378:GLN:C	2.58	0.41
1:C:158:VAL:HG12	1:C:159:TYR:O	2.21	0.41
1:A:2:GLU:HG2	1:A:3:THR:N	2.33	0.41
1:A:35:VAL:O	1:A:35:VAL:CG1	2.68	0.41
1:A:223:PHE:O	1:A:227:ALA:HB3	2.21	0.41
2:B:192:LEU:C	2:B:192:LEU:CD2	2.89	0.41
1:C:121:CYS:SG	1:C:131:CYS:HB3	2.61	0.41
1:A:23:TYR:CG	1:A:67:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:C	2:B:51:LYS:H	2.24	0.41
2:B:78:LEU:HD23	2:B:79:ARG:NH2	2.35	0.41
2:B:113:SER:N	2:B:116:LEU:HD12	2.30	0.41
2:B:139:LYS:HD3	2:B:142:ASP:OD2	2.21	0.41
2:B:141:GLN:NE2	2:B:145:LYS:HE3	2.33	0.41
1:C:233:ILE:HD12	1:C:243:ILE:CD1	2.35	0.41
1:C:349:THR:HG22	1:C:351:SER:CB	2.50	0.41
1:A:143:ASP:CG	1:A:155:ARG:HE	2.24	0.41
1:A:234:LEU:HD21	1:A:243:ILE:HD12	2.03	0.41
1:A:237:LYS:HE2	1:A:241:ASP:CG	2.40	0.41
1:A:313:ILE:O	1:A:313:ILE:CG1	2.68	0.41
1:A:409:GLU:O	1:A:413:LYS:N	2.49	0.41
2:B:74:LEU:HD13	2:B:130:PHE:CD1	2.56	0.41
1:C:142:ILE:HB	1:C:157:TRP:HH2	1.86	0.41
2:D:135:LEU:HB3	2:D:139:LYS:HB3	2.03	0.41
2:D:200:VAL:HG12	2:D:209:VAL:CG1	2.51	0.41
1:A:171:ASP:HB2	1:A:174:VAL:CG2	2.51	0.41
1:A:237:LYS:CD	1:A:256:GLN:OE1	2.69	0.41
1:A:305:LEU:HA	5:A:918:HOH:O	2.20	0.41
1:A:413:LYS:C	1:A:415:ASP:N	2.74	0.41
2:B:30:LEU:O	2:B:31:GLN:HB2	2.21	0.41
2:B:178:LEU:HD12	2:B:178:LEU:HA	1.91	0.41
1:A:343:ASP:OD2	1:A:346:THR:HG23	2.22	0.40
2:B:222:PHE:O	2:B:223:ARG:C	2.58	0.40
1:C:339:VAL:C	1:C:341:GLN:N	2.74	0.40
2:D:58:ASN:O	2:D:61:VAL:N	2.55	0.40
2:D:275:GLN:O	2:D:276:ILE:C	2.60	0.40
2:D:328:LYS:HA	2:D:341:PHE:CE1	2.56	0.40
1:A:413:LYS:HE2	1:A:413:LYS:HB3	1.91	0.40
1:C:146:LEU:O	1:C:152:PHE:HB2	2.20	0.40
2:D:30:LEU:O	2:D:31:GLN:CB	2.70	0.40
2:D:38:SER:C	2:D:40:ILE:N	2.73	0.40
2:D:358:LYS:HE3	2:D:360:THR:CA	2.48	0.40
1:A:17:TYR:CE2	1:A:75:PRO:HD2	2.57	0.40
1:A:36:ILE:HG22	1:A:37:LYS:HG3	2.03	0.40
1:A:219:ILE:HD12	1:A:298:LEU:HD23	2.03	0.40
1:A:306:ASP:HB3	1:A:309:VAL:CG2	2.50	0.40
2:D:92:GLU:O	2:D:95:PRO:HD2	2.21	0.40
2:D:259:GLY:C	2:D:260:GLN:HG2	2.42	0.40
1:A:51:ASP:O	1:A:52:ASP:HB3	2.21	0.40
2:B:76:SER:O	2:B:80:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LYS:C	2:B:147:SER:H	2.25	0.40
1:C:36:ILE:CG2	1:C:37:LYS:N	2.84	0.40
1:C:251:ILE:HD13	1:C:251:ILE:HA	1.93	0.40
2:D:184:TYR:CZ	2:D:211:LEU:HD13	2.56	0.40
2:B:49:ARG:HD3	2:B:102:SER:HB3	2.02	0.40
2:B:127:LEU:HG	2:B:131:ARG:HH11	1.87	0.40
1:C:256:GLN:HE21	1:C:256:GLN:HB2	1.53	0.40
2:D:212:LYS:H	2:D:212:LYS:HG3	1.63	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	383/420 (91%)	331 (86%)	45 (12%)	7 (2%)	8	12
1	C	383/420 (91%)	327 (85%)	36 (9%)	20 (5%)	2	1
2	B	209/509 (41%)	156 (75%)	37 (18%)	16 (8%)	1	0
2	D	425/509 (84%)	346 (81%)	58 (14%)	21 (5%)	2	2
All	All	1400/1858 (75%)	1160 (83%)	176 (13%)	64 (5%)	2	2

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	50	LYS
1	A	95	LYS
1	A	196	GLN
1	A	380	THR
2	B	82	LYS
2	B	173	LEU

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Mol	Chain	Res	Type
1	C	37	LYS
1	C	196	GLN
2	D	25	CYS
2	D	179	GLY
2	D	264	THR
2	D	267	ASN
2	B	179	GLY
1	C	32	TYR
1	C	34	GLY
1	C	63	GLN
1	C	252	HIS
1	C	281	ASN
1	C	340	ASP
1	C	410	LEU
2	D	24	HIS
2	D	93	TYR
2	D	171	PRO
2	D	252	HIS
2	D	276	ILE
1	A	404	LYS
2	B	71	GLN
2	B	122	GLN
2	B	146	ASP
2	B	157	GLU
2	B	171	PRO
1	C	96	LEU
1	C	409	GLU
1	C	411	LEU
2	D	29	TYR
2	D	157	GLU
2	D	263	SER
2	D	273	LEU
2	D	355	LYS
2	D	360	THR
2	B	67	THR
2	B	78	LEU
2	B	100	HIS
2	B	133	SER
2	B	170	SER
2	B	240	VAL
2	B	250	LEU
1	C	22	PRO

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Mol	Chain	Res	Type
1	C	116	ASP
1	C	133	THR
1	C	253	ASP
1	C	291	TRP
1	A	410	LEU
2	B	65	LYS
1	C	359	ALA
2	D	244	GLU
2	D	260	GLN
2	D	357	GLY
1	C	6	PRO
2	D	31	GLN
1	C	408	GLY
2	D	344	GLY
2	D	363	THR

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	364/393 (93%)	347 (95%)	17 (5%)	26	40
1	C	363/393 (92%)	341 (94%)	22 (6%)	18	29
2	B	194/459 (42%)	171 (88%)	23 (12%)	5	7
2	D	389/459 (85%)	363 (93%)	26 (7%)	16	25
All	All	1310/1704 (77%)	1222 (93%)	88 (7%)	16	25

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	51	ASP
1	A	55	ILE
1	A	72	LYS
1	A	89	ASN
1	A	95	LYS

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Mol	Chain	Res	Type
1	A	119	ARG
1	A	122	CYS
1	A	173	SER
1	A	207	LYS
1	A	258	SER
1	A	291	TRP
1	A	313	ILE
1	A	334	ILE
1	A	351	SER
1	A	358	ASP
1	A	393	LYS
2	B	31	GLN
2	B	63	TYR
2	B	65	LYS
2	B	70	TYR
2	B	79	ARG
2	B	80	LYS
2	B	83	PHE
2	B	126	ASP
2	B	138	ASP
2	B	139	LYS
2	B	143	PHE
2	B	160	THR
2	B	187	PRO
2	B	188	PHE
2	B	193	ASP
2	B	195	PHE
2	B	202	LEU
2	B	212	LYS
2	B	237	LEU
2	B	238	PRO
2	B	240	VAL
2	B	245	ARG
2	B	247	GLN
1	C	2	GLU
1	C	12	LEU
1	C	37	LYS
1	C	38	ASN
1	C	55	ILE
1	C	65	ASP
1	C	89	ASN
1	C	91	HIS

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Mol	Chain	Res	Type
1	C	95	LYS
1	C	119	ARG
1	C	123	SER
1	C	160	SER
1	C	221	LYS
1	C	256	GLN
1	C	257	GLN
1	C	272	LEU
1	C	274	LYS
1	C	331	SER
1	C	333	PRO
1	C	339	VAL
1	C	340	ASP
1	C	393	LYS
2	D	27	GLN
2	D	31	GLN
2	D	65	LYS
2	D	69	GLN
2	D	82	LYS
2	D	92	GLU
2	D	98	ARG
2	D	99	ASP
2	D	111	CYS
2	D	138	ASP
2	D	139	LYS
2	D	165	GLU
2	D	169	SER
2	D	228	LYS
2	D	240	VAL
2	D	244	GLU
2	D	245	ARG
2	D	262	TYR
2	D	264	THR
2	D	288	MET
2	D	321	GLU
2	D	359	ARG
2	D	378	GLN
2	D	387	ARG
2	D	424	CYS
2	D	442	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	71	GLN
1	A	74	ASN
1	A	86	HIS
1	A	89	ASN
1	A	90	GLN
1	A	92	ASN
1	A	166	HIS
1	A	236	ASN
1	A	260	GLN
1	A	281	ASN
1	A	337	GLN
1	A	378	HIS
1	A	401	ASN
2	B	31	GLN
2	B	44	ASN
2	B	58	ASN
2	B	69	GLN
2	B	123	GLN
2	B	141	GLN
2	B	148	GLN
2	B	150	GLN
2	B	164	GLN
2	B	241	GLN
2	B	247	GLN
1	C	31	ASN
1	C	38	ASN
1	C	58	GLN
1	C	86	HIS
1	C	89	ASN
1	C	90	GLN
1	C	102	GLN
1	C	166	HIS
1	C	203	HIS
1	C	236	ASN
1	C	257	GLN
1	C	260	GLN
1	C	267	GLN
1	C	271	HIS
1	C	280	GLN
1	C	337	GLN
1	C	341	GLN
1	C	401	ASN

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Mol	Chain	Res	Type
2	D	27	GLN
2	D	31	GLN
2	D	69	GLN
2	D	71	GLN
2	D	100	HIS
2	D	112	GLN
2	D	141	GLN
2	D	150	GLN
2	D	164	GLN
2	D	260	GLN
2	D	265	GLN
2	D	267	ASN
2	D	275	GLN
2	D	290	GLN
2	D	298	ASN
2	D	329	GLN
2	D	351	HIS
2	D	396	GLN
2	D	399	GLN
2	D	442	ASN

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	SF4	D	1000	2	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	D	1000	2	-	-	0/6/5/5

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	389/420 (92%)	-0.05	5 (1%) 77 75	13, 42, 78, 100	0
1	C	389/420 (92%)	-0.07	5 (1%) 77 75	14, 37, 75, 95	0
2	B	213/509 (41%)	0.61	29 (13%) 3 2	23, 77, 100, 109	0
2	D	429/509 (84%)	0.11	20 (4%) 31 28	15, 61, 95, 107	0
All	All	1420/1858 (76%)	0.09	59 (4%) 36 33	13, 50, 93, 109	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	29	TYR	9.1
1	C	1	MET	6.8
2	D	361	ASP	6.7
1	A	1	MET	6.7
2	B	74	LEU	6.5
2	B	62	SER	5.9
1	C	411	LEU	5.5
2	D	261	ASP	5.5
2	B	132	PHE	5.4
2	D	360	THR	5.0
2	B	61	VAL	4.9
2	B	58	ASN	4.5
2	B	178	LEU	4.5
2	B	97	ARG	4.1
1	A	411	LEU	3.8
1	C	412	LYS	3.8
2	B	180	PHE	3.8
2	B	78	LEU	3.7
1	A	2	GLU	3.7
2	B	130	PHE	3.6
2	B	134	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	75	GLU	3.6
1	C	2	GLU	3.5
2	B	70	TYR	3.5
2	B	68	GLU	3.4
2	D	359	ARG	3.4
2	B	63	TYR	3.4
2	B	30	LEU	3.3
2	D	262	TYR	3.2
2	D	336	MET	3.2
2	B	172	SER	3.1
2	D	26	LEU	3.1
2	D	268	VAL	2.9
2	D	174	SER	2.8
2	B	143	PHE	2.7
2	B	59	LEU	2.7
2	D	61	VAL	2.7
2	B	55	SER	2.6
2	B	222	PHE	2.6
2	D	260	GLN	2.6
2	B	72	SER	2.6
1	C	410	LEU	2.6
2	D	255	HIS	2.5
2	B	28	PHE	2.4
2	B	71	GLN	2.3
2	B	116	LEU	2.3
2	B	135	LEU	2.3
2	B	101	ILE	2.2
1	A	379	ARG	2.2
2	D	394	LEU	2.2
1	A	412	LYS	2.1
2	D	257	TYR	2.1
2	B	176	LEU	2.1
2	D	343	LYS	2.1
2	D	259	GLY	2.1
2	D	235	ARG	2.0
2	D	246	LEU	2.0
2	D	137	LYS	2.0
2	D	211	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^{th} 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^2)	Q<0.9
3	ZN	A	800	1/1	0.98	0.19	34,34,34,34	0
4	SF4	D	1000	8/8	0.98	0.21	17,26,32,38	0
3	ZN	C	900	1/1	1.00	0.21	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.