Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 08:03 AM EST

PDB ID	:	4JT5
Title	:	mTORdeltaN-mLST8-pp242 complex
Authors	:	Pavletich, N.P.; Yang, H.
Deposited on	:	2013-03-22
Resolution	:	3.45 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:

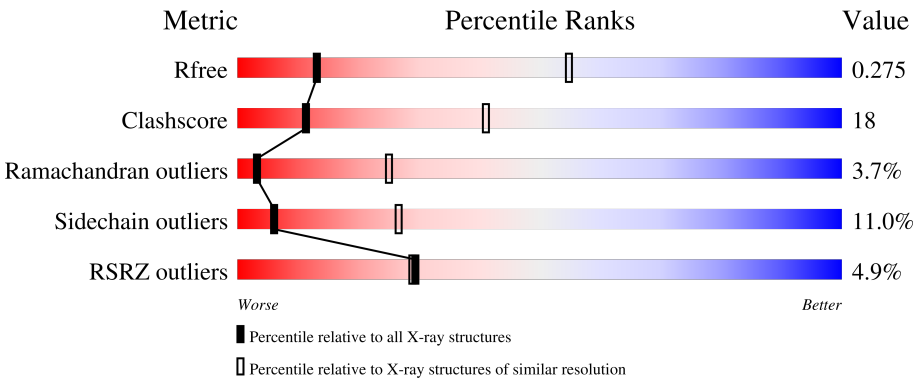
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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% 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	1174	7% 56% 29% • 10%
1	B	1174	4% 55% 29% 5% 10%
2	C	326	4% 48% 40% 9% • •
2	D	326	% 46% 41% 9% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22143 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1058	8608	5472	1521	1552	63	0	0	0
1	A	1054	8577	5451	1517	1546	63	0	0	0

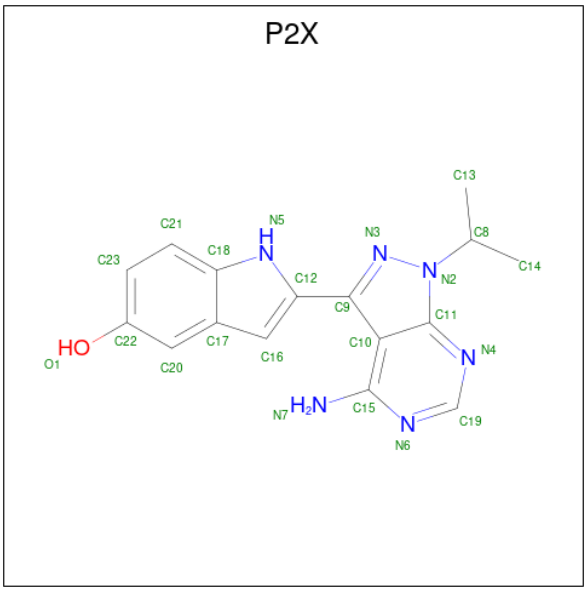
- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	317	2456	1526	436	476	18	0	0	0
2	C	317	2456	1526	436	476	18	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	324	VAL	-	expression tag	UNP Q9BVC4
D	325	LEU	-	expression tag	UNP Q9BVC4
D	326	GLY	-	expression tag	UNP Q9BVC4
C	324	VAL	-	expression tag	UNP Q9BVC4
C	325	LEU	-	expression tag	UNP Q9BVC4
C	326	GLY	-	expression tag	UNP Q9BVC4

- Molecule 3 is 2-[4-amino-1-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-3-yl]-1H-indol-5-ol (three-letter code: P2X) (formula: $C_{16}H_{16}N_6O$).



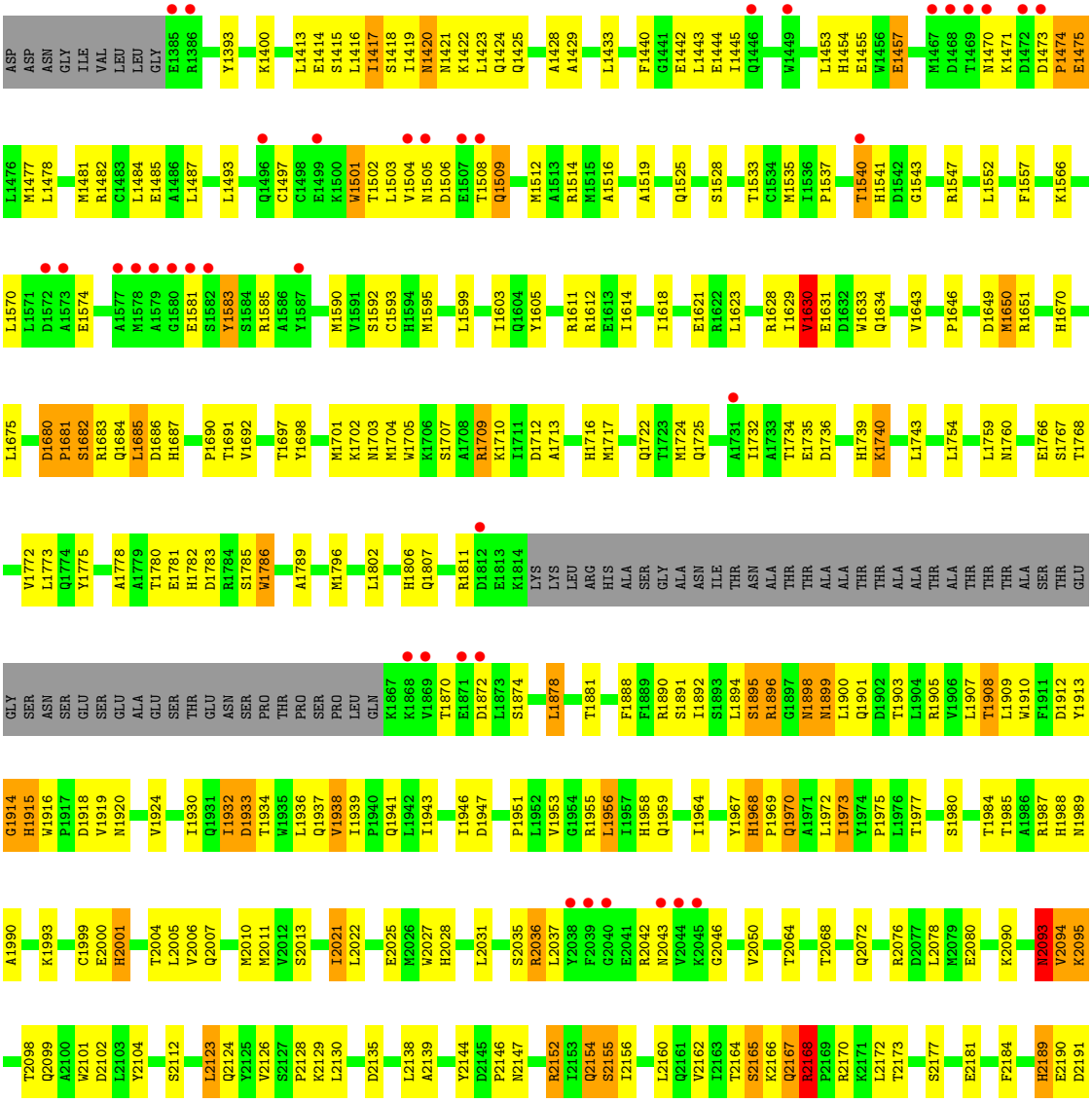
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	23	16	6	1	0	0
			Total	C	N	O		
3	A	1	23	16	6	1	0	0

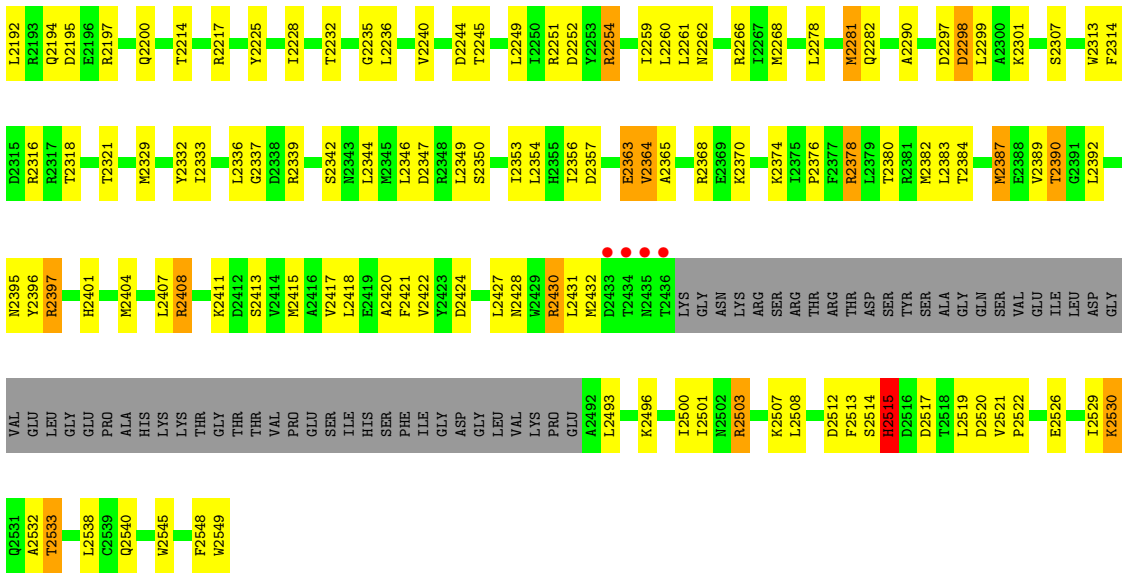
3 Residue-property plots (i)

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: Serine/threonine-protein kinase mTOR

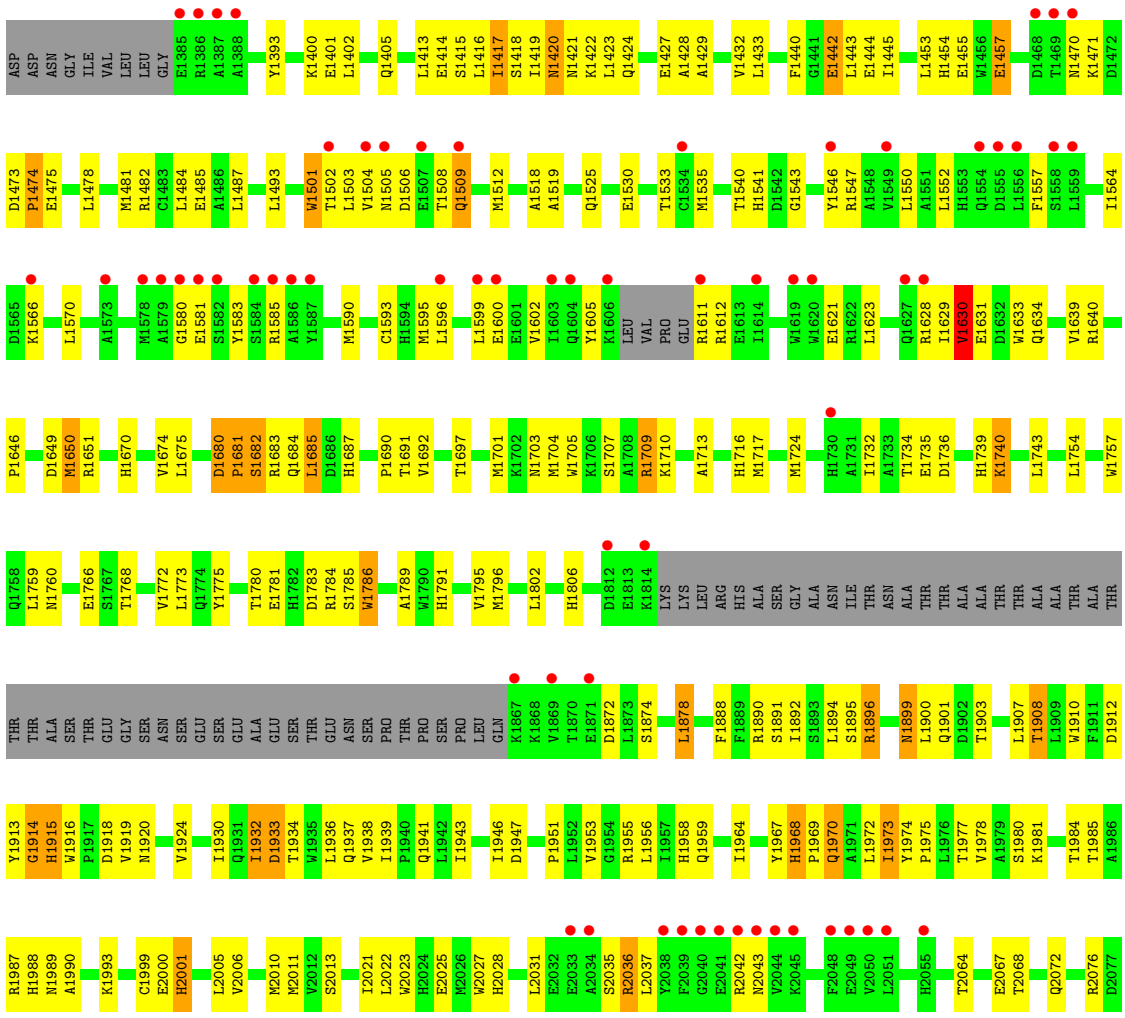
Chain B:

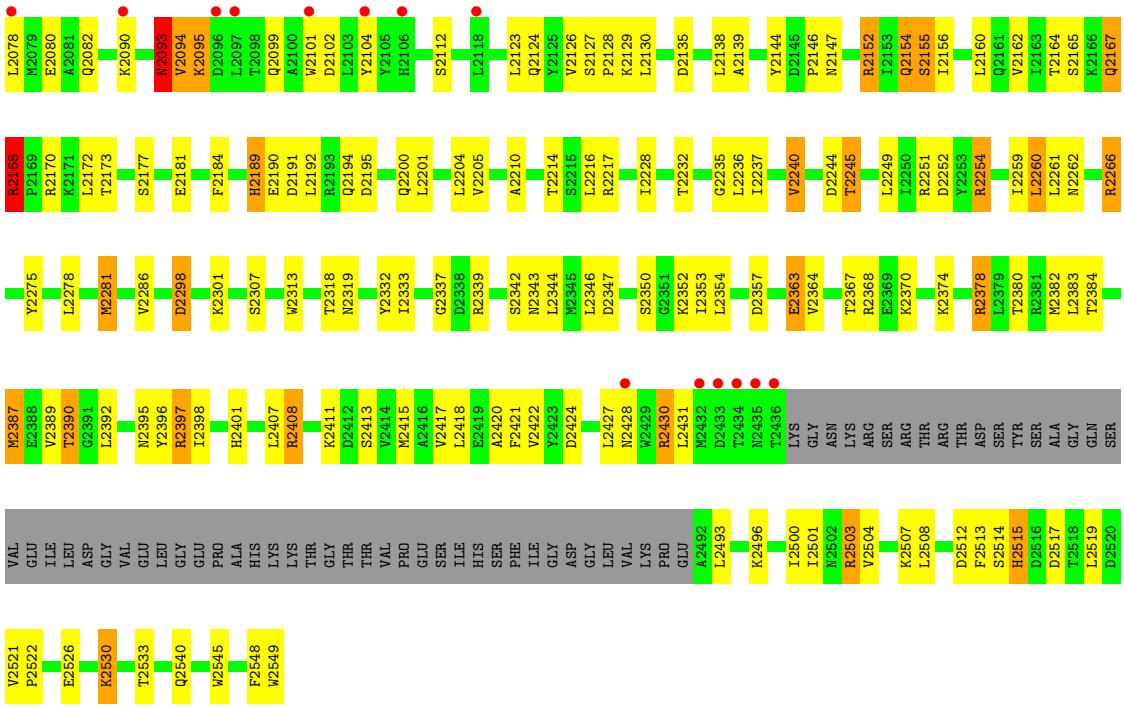




• Molecule 1: Serine/threonine-protein kinase mTOR

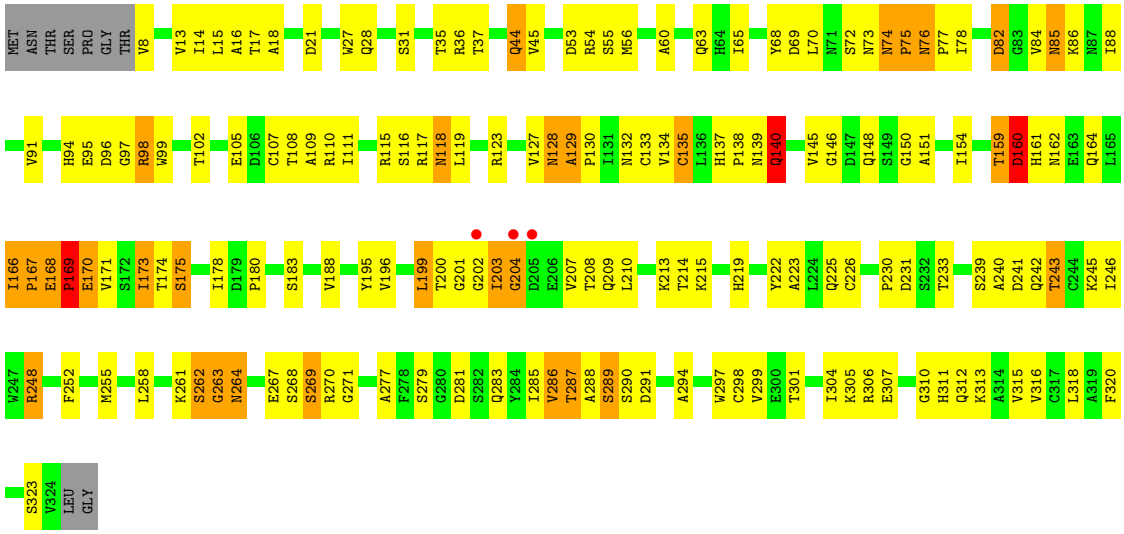
Chain A: 7% 56% 29% • 10%





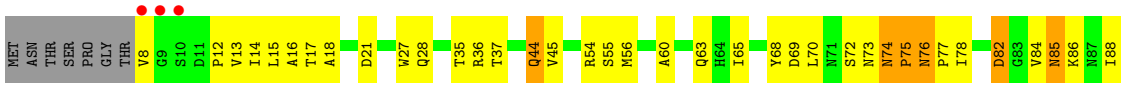
- Molecule 2: Target of rapamycin complex subunit LST8

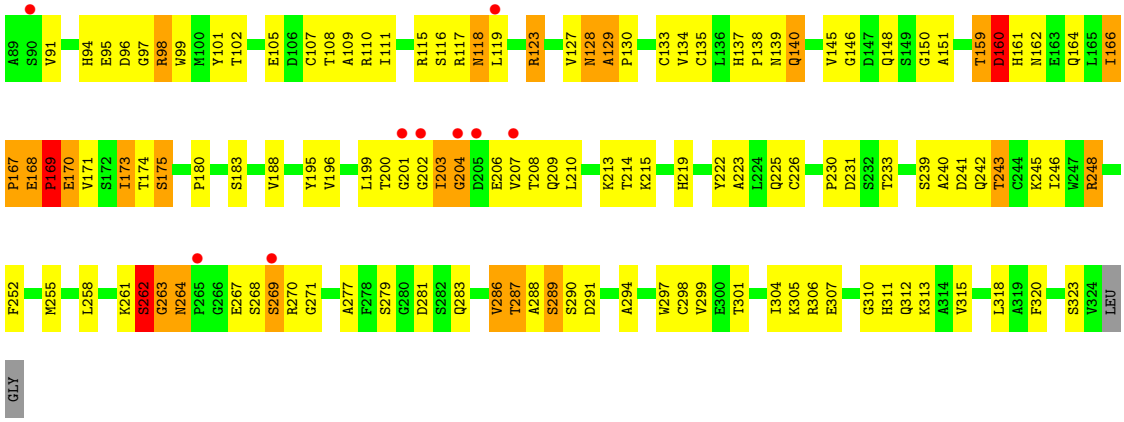
Chain D:



- Molecule 2: Target of rapamycin complex subunit LST8

Chain C:




A89 S90 V91 H94 E95 D96 G97 R98 W99 M100 Y101 T102 E105 D106 C107 T108 A109 R110 I111 R115 S116 R117 N118 L119 R123 V127 N128 A129 P130 C133 V134 C135 L136 H137 P138 N139 Q140 V145 G146 D147 Q148 S149 G150 A151 T159 D160 H161 N162 E163 Q164 L165 I166
P167 E168 P169 E170 V171 S172 I173 T174 S175 P180 S183 V188 Y195 V196 L199 T200 G201 G202 I203 G204 D205 E206 V207 T208 Q209 L210 K213 T214 K215 H219 Y222 A223 L224 Q225 C226 P230 D231 S232 T233 S239 A240 D241 Q242 T243 C244 K245 I246 W247 R248
F252 M255 L258 K261 S262 G263 N264 P265 G266 E267 S268 S269 R270 G271 A277 F278 S279 G280 D281 S282 Q283 V286 T287 A288 S289 S290 D291 A294 W297 C298 V299 E300 T301 I304 K305 R306 E307 G310 H311 Q312 K313 A314 V315 L318 A319 F320 S323 V324 LEU
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.40Å 163.20Å 207.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.67 – 3.45 39.64 – 3.43	Depositor EDS
% Data completeness (in resolution range)	85.8 (39.67-3.45) 85.2 (39.64-3.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.233 , 0.271 0.235 , 0.275	Depositor DCC
R_{free} test set	1869 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22143	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4826e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P2X

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	0.35	0/8772	0.60	1/11872 (0.0%)
1	B	0.35	0/8805	0.61	1/11920 (0.0%)
2	C	0.38	0/2514	0.67	0/3426
2	D	0.41	0/2514	0.69	0/3426
All	All	0.36	0/22605	0.62	2/30644 (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	A	0	2
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1915	HIS	N-CA-C	5.58	126.08	111.00
1	B	1915	HIS	N-CA-C	5.40	125.57	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1442	GLU	Peptide
1	A	1914	GLY	Peptide
1	B	1914	GLY	Peptide
2	C	169	PRO	Peptide
2	D	169	PRO	Peptide

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	8577	0	8559	262	0
1	B	8608	0	8593	263	0
2	C	2456	0	2341	131	0
2	D	2456	0	2341	137	0
3	A	23	0	16	3	0
3	B	23	0	16	4	0
All	All	22143	0	21866	784	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 18.

All (784) 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:C:76:ASN:HB3	2:C:77:PRO:HD2	1.35	1.09
1:A:1418:SER:HB2	1:A:1581:GLU:HG2	1.35	1.05
2:D:76:ASN:HB3	2:D:77:PRO:HD2	1.36	1.04
2:D:170:GLU:HA	2:D:170:GLU:OE2	1.61	0.98
2:C:170:GLU:OE2	2:C:170:GLU:HA	1.62	0.96
1:B:2380:THR:HG22	1:B:2383:LEU:HG	1.50	0.94
1:A:2380:THR:HG22	1:A:2383:LEU:HG	1.50	0.94
2:D:69:ASP:HB2	2:D:78:ILE:HD11	1.48	0.93
2:C:95:GLU:HB2	2:C:140:GLN:NE2	1.85	0.91
2:D:95:GLU:HB2	2:D:140:GLN:NE2	1.86	0.90
2:D:117:ARG:O	2:D:118:ASN:HB2	1.73	0.89
1:A:2387:MET:HE3	1:A:2396:TYR:HB2	1.56	0.87
2:C:231:ASP:HB3	2:C:233:THR:OG1	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:ASP:HB2	2:C:78:ILE:HD11	1.54	0.86
2:C:95:GLU:HB2	2:C:140:GLN:HE22	1.37	0.86
2:C:117:ARG:O	2:C:118:ASN:HB2	1.74	0.86
1:B:1623:LEU:HG	1:B:1633:TRP:CH2	2.11	0.85
2:C:76:ASN:HB3	2:C:77:PRO:CD	2.06	0.85
1:A:2064:THR:HG22	1:A:2128:PRO:HD3	1.58	0.84
1:A:1969:PRO:O	1:A:1970:GLN:HB2	1.77	0.83
2:D:231:ASP:HB3	2:D:233:THR:OG1	1.78	0.83
2:D:95:GLU:HB2	2:D:140:GLN:HE22	1.41	0.82
1:A:2192:LEU:HD12	1:A:2235:GLY:HA3	1.61	0.82
2:D:76:ASN:HB3	2:D:77:PRO:CD	2.08	0.82
2:D:146:GLY:HA3	2:D:173:ILE:HD11	1.61	0.82
1:A:2390:THR:HG23	1:A:2390:THR:O	1.80	0.81
1:B:2192:LEU:HD12	1:B:2235:GLY:HA3	1.61	0.80
2:C:146:GLY:HA3	2:C:173:ILE:HD11	1.61	0.80
2:C:63:GLN:HE21	2:C:86:LYS:H	1.27	0.80
1:B:1958:HIS:CE1	1:B:1990:ALA:HB1	2.17	0.80
1:A:1422:LYS:HD3	1:A:1580:GLY:HA3	1.61	0.80
1:B:1969:PRO:O	1:B:1970:GLN:HB2	1.82	0.79
3:B:2601:P2X:H15	3:B:2601:P2X:C16	1.96	0.79
1:A:1908:THR:O	1:A:1912:ASP:HB2	1.83	0.79
1:A:2397:ARG:NH2	1:A:2526:GLU:OE1	2.15	0.78
1:A:2387:MET:CE	1:A:2396:TYR:HB2	2.13	0.78
1:B:2387:MET:HE3	1:B:2396:TYR:HB2	1.66	0.78
1:B:2387:MET:CE	1:B:2396:TYR:HB2	2.14	0.78
2:D:63:GLN:HE21	2:D:86:LYS:H	1.29	0.77
1:B:2390:THR:HG23	1:B:2390:THR:O	1.84	0.76
1:A:1704:MET:HG2	1:A:1713:ALA:HB2	1.66	0.76
1:A:1943:ILE:HA	1:A:1946:ILE:HG13	1.67	0.76
1:A:2421:PHE:HA	1:A:2424:ASP:HB2	1.66	0.76
1:A:1968:HIS:HB3	1:A:2144:TYR:OH	1.87	0.75
2:D:8:VAL:HG21	2:D:36:ARG:HD3	1.67	0.75
2:C:8:VAL:HG21	2:C:36:ARG:HD3	1.66	0.74
1:B:2397:ARG:NH2	1:B:2526:GLU:OE1	2.19	0.74
1:B:1422:LYS:HE2	1:B:1581:GLU:HG3	1.68	0.74
2:C:150:GLY:HA3	2:C:169:PRO:HB3	1.70	0.74
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.68	0.74
3:B:2601:P2X:H15	3:B:2601:P2X:H5	1.52	0.73
1:A:1958:HIS:CE1	1:A:1990:ALA:HB1	2.23	0.73
2:D:167:PRO:HD2	2:D:169:PRO:HG2	1.71	0.73
2:D:150:GLY:HA3	2:D:169:PRO:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2064:THR:HG22	1:B:2128:PRO:HD3	1.70	0.72
1:A:2298:ASP:HB2	1:A:2382:MET:CE	2.19	0.72
1:B:1943:ILE:HA	1:B:1946:ILE:HG13	1.72	0.72
1:A:2022:LEU:HD21	1:A:2126:VAL:HG13	1.72	0.71
1:B:1958:HIS:HE1	1:B:1990:ALA:HB1	1.53	0.71
1:B:1908:THR:O	1:B:1912:ASP:HB2	1.91	0.70
1:B:1941:GLN:HE22	1:B:2200:GLN:HE22	1.37	0.70
1:B:1704:MET:HG2	1:B:1713:ALA:HB2	1.73	0.70
1:B:2298:ASP:HB2	1:B:2382:MET:CE	2.21	0.70
2:C:98:ARG:HD2	2:C:115:ARG:HB2	1.73	0.70
1:A:1670:HIS:HE1	1:A:1681:PRO:HB3	1.56	0.70
2:D:17:THR:HB	2:D:311:HIS:HE1	1.56	0.70
1:A:1493:LEU:HD23	1:A:1519:ALA:HB2	1.74	0.69
2:C:167:PRO:HD2	2:C:169:PRO:HG2	1.74	0.69
2:D:137:HIS:CD2	2:D:138:PRO:HD2	2.27	0.69
1:A:1415:SER:O	1:A:1419:ILE:HG22	1.93	0.69
2:D:98:ARG:HD2	2:D:115:ARG:HB2	1.74	0.69
2:D:123:ARG:NH2	2:D:160:ASP:OD1	2.26	0.69
1:A:1732:ILE:HD13	1:A:1740:LYS:HB2	1.76	0.68
2:D:241:ASP:OD2	2:D:243:THR:HB	1.94	0.68
1:B:1415:SER:O	1:B:1419:ILE:HG22	1.94	0.68
2:C:231:ASP:CB	2:C:233:THR:OG1	2.41	0.67
1:A:1920:ASN:O	1:A:1924:VAL:HG23	1.94	0.67
1:B:1901:GLN:HG3	1:B:2413:SER:HA	1.76	0.67
1:B:1913:TYR:O	1:B:1915:HIS:HA	1.93	0.67
1:A:1508:THR:O	1:A:1512:MET:HB2	1.94	0.67
1:B:1920:ASN:O	1:B:1924:VAL:HG23	1.93	0.67
1:B:2093:ASN:O	1:B:2094:VAL:HB	1.95	0.67
2:D:17:THR:HB	2:D:311:HIS:CE1	2.30	0.67
1:B:2249:LEU:HD13	1:B:2346:LEU:HD12	1.77	0.67
1:A:1701:MET:HE1	1:A:1716:HIS:C	2.14	0.67
1:B:1433:LEU:HD23	1:B:1453:LEU:HD23	1.76	0.67
1:B:1508:THR:O	1:B:1512:MET:HB2	1.93	0.67
1:A:2160:LEU:HD22	1:A:2172:LEU:HA	1.77	0.67
1:B:2278:LEU:HD23	2:D:44:GLN:HG2	1.75	0.66
1:B:1701:MET:HE1	1:B:1716:HIS:C	2.15	0.66
1:B:2022:LEU:HD21	1:B:2126:VAL:HG13	1.78	0.66
1:B:1680:ASP:O	1:B:1682:SER:N	2.28	0.66
1:B:2514:SER:OG	1:B:2517:ASP:HB2	1.96	0.66
1:B:2363:GLU:OE2	1:B:2503:ARG:HD2	1.95	0.66
2:D:306:ARG:HG2	2:D:307:GLU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:LEU:HG	1:A:1772:VAL:HG11	1.77	0.66
1:B:1393:TYR:CZ	1:B:1422:LYS:HD2	2.30	0.66
2:D:69:ASP:CB	2:D:78:ILE:HD11	2.24	0.66
1:A:2278:LEU:HD23	2:C:44:GLN:HG2	1.76	0.65
2:D:108:THR:OG1	2:D:110:ARG:NH1	2.30	0.65
1:A:1393:TYR:CZ	1:A:1422:LYS:HD2	2.32	0.65
1:A:2093:ASN:O	1:A:2094:VAL:HB	1.96	0.65
1:A:1874:SER:O	1:A:1878:LEU:HB2	1.96	0.65
1:A:1680:ASP:O	1:A:1682:SER:N	2.29	0.65
1:B:1968:HIS:HB3	1:B:2144:TYR:OH	1.97	0.64
2:D:231:ASP:CB	2:D:233:THR:OG1	2.45	0.64
1:A:1969:PRO:O	1:A:1970:GLN:CB	2.45	0.64
1:A:2249:LEU:HD13	1:A:2346:LEU:HD12	1.78	0.64
2:C:306:ARG:HG2	2:C:307:GLU:H	1.62	0.64
1:B:2389:VAL:O	1:B:2390:THR:HG22	1.97	0.64
1:B:1907:LEU:HD11	1:B:1938:VAL:CG1	2.28	0.64
2:D:55:SER:O	2:D:56:MET:HG2	1.97	0.64
1:A:1734:THR:O	1:A:1736:ASP:N	2.25	0.64
2:C:279:SER:HA	2:C:320:PHE:HE2	1.62	0.64
3:A:2601:P2X:H5	3:A:2601:P2X:H15	1.63	0.64
1:B:2167:GLN:HG2	1:B:2189:HIS:HD2	1.62	0.64
1:A:2130:LEU:HD22	1:A:2156:ILE:CD1	2.28	0.64
2:C:137:HIS:CD2	2:C:138:PRO:HD2	2.32	0.64
1:B:1422:LYS:HE2	1:B:1581:GLU:CG	2.28	0.63
2:C:17:THR:HB	2:C:311:HIS:HE1	1.63	0.63
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.31	0.63
1:A:1913:TYR:O	1:A:1915:HIS:HA	1.97	0.63
2:C:166:ILE:HG13	2:C:166:ILE:O	1.97	0.63
1:B:2298:ASP:HB2	1:B:2382:MET:HE2	1.81	0.63
2:C:94:HIS:CE1	2:C:96:ASP:HB2	2.34	0.63
1:B:1915:HIS:HE1	1:B:1919:VAL:HG11	1.63	0.63
2:D:279:SER:HA	2:D:320:PHE:HE2	1.63	0.63
1:A:1783:ASP:O	1:A:1785:SER:N	2.32	0.63
1:A:2363:GLU:OE2	1:A:2503:ARG:HD2	1.99	0.63
1:A:1958:HIS:HE1	1:A:1990:ALA:HB1	1.62	0.62
1:A:2194:GLN:HG2	1:A:2427:LEU:HD22	1.79	0.62
2:D:134:VAL:HG22	2:D:145:VAL:HG22	1.80	0.62
2:C:105:GLU:HA	2:C:130:PRO:HB3	1.81	0.62
1:B:2421:PHE:HD1	1:B:2430:ARG:NH2	1.97	0.62
1:B:1701:MET:HE1	1:B:1717:MET:N	2.15	0.62
1:B:1969:PRO:O	1:B:1970:GLN:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2298:ASP:HB2	1:A:2382:MET:HE2	1.81	0.62
1:A:2389:VAL:O	1:A:2390:THR:HG22	1.99	0.62
1:A:2503:ARG:HH11	1:A:2507:LYS:HE3	1.64	0.62
1:A:2167:GLN:HG2	1:A:2189:HIS:HD2	1.63	0.62
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.32	0.62
1:B:1646:PRO:HG3	1:B:1675:LEU:HD21	1.82	0.62
1:B:2418:LEU:HD23	1:B:2421:PHE:CZ	2.35	0.62
1:A:2390:THR:O	1:A:2390:THR:CG2	2.47	0.62
1:B:2160:LEU:HD22	1:B:2172:LEU:HA	1.82	0.62
2:C:17:THR:HB	2:C:311:HIS:CE1	2.35	0.62
1:B:2281:MET:HE1	2:D:222:TYR:CD2	2.35	0.61
2:C:108:THR:OG1	2:C:110:ARG:NH1	2.33	0.61
2:C:123:ARG:NH2	2:C:160:ASP:OD1	2.33	0.61
2:C:241:ASP:OD2	2:C:243:THR:HB	1.99	0.61
1:B:2167:GLN:HG2	1:B:2189:HIS:CD2	2.35	0.61
1:B:2515:HIS:N	1:B:2515:HIS:ND1	2.47	0.61
1:B:1878:LEU:HD21	1:B:1918:ASP:HB2	1.81	0.61
1:B:2278:LEU:CD2	2:D:44:GLN:HG2	2.29	0.61
1:B:2194:GLN:HG2	1:B:2427:LEU:HD22	1.82	0.61
2:C:134:VAL:HG22	2:C:145:VAL:HG22	1.81	0.61
2:D:94:HIS:CE1	2:D:96:ASP:HB2	2.36	0.61
1:A:2167:GLN:HG2	1:A:2189:HIS:CD2	2.35	0.61
1:A:2278:LEU:CD2	2:C:44:GLN:HG2	2.30	0.61
1:A:2421:PHE:HD1	1:A:2430:ARG:NH2	1.97	0.61
2:C:69:ASP:CB	2:C:78:ILE:HD11	2.28	0.61
1:B:1759:LEU:HG	1:B:1772:VAL:HG11	1.82	0.61
1:B:2251:ARG:NH1	1:B:2252:ASP:OD1	2.34	0.61
1:B:2392:LEU:O	1:B:2397:ARG:HB2	2.01	0.61
1:A:2392:LEU:O	1:A:2397:ARG:HB2	2.01	0.61
1:A:1428:ALA:HB2	1:A:2395:ASN:ND2	2.16	0.60
1:B:1874:SER:O	1:B:1878:LEU:HB2	2.01	0.60
1:A:1701:MET:HE1	1:A:1717:MET:N	2.17	0.60
1:A:2281:MET:HE1	2:C:222:TYR:CD2	2.36	0.60
1:B:2281:MET:HA	1:B:2281:MET:CE	2.31	0.60
1:B:1420:ASN:HB3	1:B:1429:ALA:HB2	1.83	0.60
1:B:1686:ASP:O	1:A:2266:ARG:HG3	2.02	0.60
2:C:248:ARG:HD2	2:C:255:MET:HB2	1.84	0.60
1:A:2337:GLY:O	1:A:2339:ARG:NH1	2.34	0.60
1:B:1783:ASP:O	1:B:1785:SER:N	2.35	0.59
1:A:2514:SER:OG	1:A:2517:ASP:HB2	2.02	0.59
2:D:128:ASN:H	2:D:128:ASN:ND2	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2344:LEU:HD13	1:A:2353:ILE:HD11	1.83	0.59
1:B:2380:THR:HG23	1:B:2549:TRP:O	2.02	0.59
1:A:2415:MET:CE	1:A:2501:ILE:HG23	2.31	0.59
2:D:21:ASP:HB3	2:D:313:LYS:H	1.67	0.59
1:A:1878:LEU:HD21	1:A:1918:ASP:HB2	1.84	0.59
1:B:1785:SER:O	1:B:1786:TRP:CB	2.48	0.59
2:D:133:CYS:SG	2:D:175:SER:HA	2.42	0.59
1:A:1915:HIS:HE1	1:A:1919:VAL:HG11	1.67	0.59
1:B:2167:GLN:O	1:B:2168:ARG:C	2.40	0.59
3:B:2601:P2X:H5	3:B:2601:P2X:N7	2.17	0.59
2:C:271:GLY:HA2	2:C:290:SER:HB2	1.84	0.59
1:A:1890:ARG:O	1:A:1894:LEU:HG	2.01	0.59
1:A:1703:ASN:O	1:A:1707:SER:HB2	2.03	0.59
1:A:2515:HIS:ND1	1:A:2515:HIS:N	2.49	0.59
1:B:1422:LYS:CE	1:B:1581:GLU:HG3	2.33	0.58
2:D:105:GLU:HA	2:D:130:PRO:HB3	1.85	0.58
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.85	0.58
1:A:1680:ASP:C	1:A:1682:SER:N	2.56	0.58
1:A:2254:ARG:HD3	1:A:2298:ASP:OD2	2.04	0.58
2:D:166:ILE:HG13	2:D:166:ILE:O	2.02	0.58
2:C:21:ASP:HB3	2:C:313:LYS:H	1.68	0.58
1:B:1907:LEU:HD11	1:B:1938:VAL:HG11	1.84	0.58
1:A:1583:TYR:C	1:A:1585:ARG:H	2.06	0.58
1:A:1785:SER:O	1:A:1786:TRP:CB	2.49	0.58
2:D:248:ARG:HD2	2:D:255:MET:HB2	1.86	0.58
1:A:1710:LYS:NZ	1:A:1760:ASN:HD21	2.01	0.58
1:A:2415:MET:HE2	1:A:2501:ILE:HG23	1.86	0.58
1:B:2154:GLN:HE21	1:B:2155:SER:HB3	1.68	0.58
2:C:55:SER:O	2:C:56:MET:HG2	2.03	0.58
1:B:2503:ARG:HH11	1:B:2507:LYS:HE3	1.69	0.58
2:C:199:LEU:HD22	2:C:210:LEU:HD22	1.85	0.58
1:A:1907:LEU:HD11	1:A:1938:VAL:CG1	2.34	0.57
1:B:1428:ALA:HB2	1:B:2395:ASN:ND2	2.19	0.57
1:A:2037:LEU:HD22	1:A:2043:ASN:HD22	1.69	0.57
2:C:133:CYS:SG	2:C:175:SER:HA	2.43	0.57
1:B:2390:THR:O	1:B:2390:THR:CG2	2.52	0.57
1:A:2240:VAL:HG23	3:A:2601:P2X:N6	2.20	0.57
1:A:2503:ARG:HH11	1:A:2507:LYS:CE	2.17	0.57
2:C:86:LYS:HE2	2:C:105:GLU:HB3	1.87	0.57
1:A:2521:VAL:HB	1:A:2522:PRO:HD3	1.86	0.57
1:B:1493:LEU:HD23	1:B:1519:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:LEU:HD22	2:D:210:LEU:HD22	1.86	0.57
2:C:128:ASN:ND2	2:C:128:ASN:H	2.01	0.57
3:A:2601:P2X:H15	3:A:2601:P2X:C16	2.17	0.57
1:B:1680:ASP:C	1:B:1682:SER:N	2.57	0.57
1:A:1475:GLU:HA	1:A:1478:LEU:HD12	1.86	0.57
1:A:2251:ARG:HA	1:A:2261:LEU:CD1	2.35	0.57
1:A:2408:ARG:HG2	1:A:2508:LEU:O	2.05	0.56
1:B:2130:LEU:HD22	1:B:2156:ILE:CD1	2.34	0.56
1:A:2428:ASN:HB3	1:A:2493:LEU:HD13	1.86	0.56
1:B:1888:PHE:O	1:B:1892:ILE:HG13	2.05	0.56
1:B:2254:ARG:HD3	1:B:2298:ASP:OD2	2.06	0.56
1:A:1414:GLU:O	1:A:1417:ILE:HG13	2.05	0.56
1:A:1646:PRO:HG3	1:A:1675:LEU:HD21	1.88	0.56
2:D:86:LYS:HE2	2:D:105:GLU:HB3	1.88	0.56
1:A:2154:GLN:HE21	1:A:2155:SER:HB3	1.70	0.56
2:C:96:ASP:O	2:C:98:ARG:N	2.37	0.56
2:D:60:ALA:HB1	2:D:88:ILE:HG22	1.86	0.56
1:A:1888:PHE:O	1:A:1892:ILE:HG13	2.05	0.56
1:B:2503:ARG:HH11	1:B:2507:LYS:CE	2.19	0.56
2:D:107:CYS:HB3	2:D:127:VAL:O	2.05	0.56
1:A:1457:GLU:HG2	1:A:1487:LEU:HD21	1.88	0.56
1:A:1595:MET:HG2	1:A:1639:VAL:HG21	1.87	0.56
1:A:2152:ARG:HG2	1:A:2177:SER:OG	2.06	0.56
2:C:279:SER:HA	2:C:320:PHE:CE2	2.41	0.56
1:B:1457:GLU:HG2	1:B:1487:LEU:HD21	1.88	0.56
1:B:1583:TYR:C	1:B:1585:ARG:H	2.08	0.56
2:D:188:VAL:HG13	2:D:223:ALA:HB3	1.87	0.56
1:B:1802:LEU:HD22	1:B:1806:HIS:NE2	2.20	0.56
1:A:2167:GLN:O	1:A:2168:ARG:C	2.43	0.56
1:A:1420:ASN:HB3	1:A:1429:ALA:HB2	1.88	0.55
1:B:2307:SER:CB	1:B:2313:TRP:HB2	2.36	0.55
1:A:1941:GLN:HE22	1:A:2200:GLN:HE22	1.53	0.55
1:B:2251:ARG:HA	1:B:2261:LEU:CD1	2.36	0.55
1:B:1703:ASN:O	1:B:1707:SER:HB2	2.05	0.55
2:D:268:SER:O	2:D:269:SER:HB3	2.07	0.55
1:A:1901:GLN:HG3	1:A:2413:SER:HA	1.89	0.55
1:B:2415:MET:CE	1:B:2501:ILE:HG23	2.36	0.55
2:C:36:ARG:NH2	2:C:69:ASP:O	2.39	0.55
1:B:1475:GLU:HA	1:B:1478:LEU:HD12	1.88	0.55
1:B:2387:MET:HE1	1:B:2396:TYR:HB2	1.87	0.55
2:C:15:LEU:HD11	2:C:286:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:VAL:HG11	2:C:252:PHE:CZ	2.42	0.55
2:C:268:SER:O	2:C:269:SER:HB3	2.07	0.55
1:A:1951:PRO:HB2	1:A:1955:ARG:HH21	1.72	0.55
2:C:286:VAL:HB	2:C:318:LEU:HD13	1.89	0.55
1:B:1970:GLN:NE2	1:B:2139:ALA:H	2.05	0.54
2:D:196:VAL:HG11	2:D:252:PHE:CZ	2.42	0.54
1:B:2281:MET:HE1	2:D:222:TYR:CG	2.42	0.54
2:D:279:SER:HA	2:D:320:PHE:CE2	2.43	0.54
1:B:2344:LEU:HD13	1:B:2353:ILE:HD11	1.89	0.54
1:A:1552:LEU:HD22	1:A:1602:VAL:HG12	1.89	0.54
2:C:65:ILE:HD11	2:C:88:ILE:HD13	1.89	0.54
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.89	0.54
1:B:1890:ARG:O	1:B:1894:LEU:HG	2.07	0.54
2:D:96:ASP:O	2:D:98:ARG:N	2.35	0.54
1:A:2298:ASP:HB2	1:A:2382:MET:HE1	1.89	0.54
2:D:65:ILE:HD11	2:D:88:ILE:HD13	1.89	0.54
2:C:246:ILE:HD13	2:C:299:VAL:HG13	1.88	0.54
1:B:1781:GLU:OE1	1:B:1781:GLU:HA	2.07	0.53
2:D:246:ILE:HD13	2:D:299:VAL:HG13	1.90	0.53
1:A:2380:THR:HG23	1:A:2549:TRP:O	2.07	0.53
1:B:1414:GLU:O	1:B:1417:ILE:HG13	2.07	0.53
1:B:1766:GLU:OE1	1:B:1766:GLU:N	2.42	0.53
1:B:1773:LEU:HG	1:B:1796:MET:HG3	1.91	0.53
1:B:2428:ASN:HB3	1:B:2493:LEU:HD13	1.89	0.53
1:A:1422:LYS:C	1:A:1424:GLN:H	2.12	0.53
1:A:2251:ARG:NH1	1:A:2252:ASP:OD1	2.42	0.53
2:D:128:ASN:O	2:D:129:ALA:HB3	2.08	0.53
1:A:2418:LEU:O	1:A:2422:VAL:HG23	2.09	0.53
2:C:168:GLU:N	2:C:169:PRO:HD2	2.24	0.53
1:A:2307:SER:CB	1:A:2313:TRP:HB2	2.38	0.53
2:C:94:HIS:HB3	2:C:99:TRP:HB2	1.89	0.53
2:C:288:ALA:HB2	2:C:318:LEU:HG	1.91	0.53
1:B:2095:LYS:O	1:B:2099:GLN:HG2	2.09	0.53
1:A:1401:GLU:HG2	1:A:2389:VAL:HG22	1.90	0.53
2:D:267:GLU:O	2:D:267:GLU:HG3	2.09	0.53
2:D:271:GLY:HA2	2:D:290:SER:HB2	1.91	0.53
2:D:289:SER:HB2	2:D:291:ASP:OD1	2.09	0.53
1:A:1913:TYR:HB2	1:A:1915:HIS:CE1	2.44	0.52
1:A:2095:LYS:O	1:A:2099:GLN:HG2	2.09	0.52
1:B:1433:LEU:HD23	1:B:1453:LEU:CD2	2.38	0.52
2:D:286:VAL:HB	2:D:318:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1732:ILE:CD1	1:A:1740:LYS:HB2	2.37	0.52
2:C:202:GLY:O	2:C:203:ILE:O	2.28	0.52
1:B:2037:LEU:HD22	1:B:2043:ASN:HD22	1.74	0.52
1:A:2192:LEU:HD12	1:A:2235:GLY:CA	2.37	0.52
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.43	0.52
2:C:128:ASN:O	2:C:129:ALA:HB3	2.09	0.52
1:B:1422:LYS:C	1:B:1424:GLN:H	2.13	0.52
1:B:1915:HIS:HD2	1:B:1953:VAL:HG22	1.74	0.52
1:B:2521:VAL:HB	1:B:2522:PRO:HD3	1.91	0.52
1:B:1552:LEU:HD11	1:B:1603:ILE:HG13	1.90	0.52
1:B:2417:VAL:O	1:B:2420:ALA:HB3	2.09	0.52
2:D:111:ILE:HD12	2:D:123:ARG:HD3	1.92	0.52
2:C:267:GLU:HG3	2:C:267:GLU:O	2.10	0.52
1:B:2337:GLY:O	1:B:2339:ARG:NH1	2.43	0.52
2:C:60:ALA:HB1	2:C:88:ILE:HG22	1.91	0.52
2:C:137:HIS:CD2	2:C:139:ASN:H	2.28	0.52
1:B:1631:GLU:CD	1:B:1631:GLU:H	2.13	0.52
1:A:1999:CYS:C	1:A:2001:HIS:H	2.12	0.52
2:C:74:ASN:H	2:C:75:PRO:HD3	1.75	0.52
1:B:2197:ARG:NH1	1:B:2424:ASP:OD2	2.26	0.52
2:D:288:ALA:HB2	2:D:318:LEU:HG	1.92	0.52
2:D:36:ARG:NH2	2:D:69:ASP:O	2.43	0.51
1:A:1649:ASP:O	1:A:1651:ARG:N	2.44	0.51
1:B:1684:GLN:HB3	1:B:1687:HIS:CD2	2.45	0.51
1:B:2028:HIS:HE1	1:B:2112:SER:OG	1.93	0.51
1:A:2281:MET:HA	1:A:2281:MET:CE	2.40	0.51
2:C:188:VAL:HG13	2:C:223:ALA:HB3	1.92	0.51
2:C:200:THR:O	2:C:208:THR:HA	2.11	0.51
1:A:1754:LEU:HD13	1:A:1775:TYR:CE2	2.45	0.51
1:B:1478:LEU:O	1:B:1482:ARG:HG3	2.11	0.51
2:D:137:HIS:CD2	2:D:139:ASN:H	2.28	0.51
1:A:1631:GLU:CD	1:A:1631:GLU:H	2.14	0.51
1:A:2152:ARG:HG2	1:A:2177:SER:CB	2.41	0.51
2:C:202:GLY:HA3	2:C:208:THR:H	1.76	0.51
1:B:2281:MET:HA	1:B:2281:MET:HE2	1.93	0.51
1:A:1422:LYS:HE2	1:A:1581:GLU:HG3	1.92	0.51
1:A:1802:LEU:HD22	1:A:1806:HIS:NE2	2.25	0.51
1:A:2418:LEU:HD23	1:A:2421:PHE:CZ	2.46	0.51
2:C:95:GLU:CB	2:C:140:GLN:HE22	2.15	0.51
2:D:54:ARG:HD2	2:D:323:SER:HB2	1.93	0.51
2:C:128:ASN:O	2:C:129:ALA:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1501:TRP:HA	1:B:1503:LEU:HG	1.92	0.51
1:B:2408:ARG:HG2	1:B:2508:LEU:O	2.10	0.51
2:D:82:ASP:H	2:D:119:LEU:HD22	1.76	0.51
1:A:2417:VAL:O	1:A:2420:ALA:HB3	2.11	0.51
2:C:54:ARG:HD2	2:C:323:SER:HB2	1.93	0.51
1:B:1972:LEU:O	1:B:1975:PRO:HG2	2.11	0.51
2:D:15:LEU:HD11	2:D:286:VAL:HG11	1.93	0.51
2:D:137:HIS:CD2	2:D:138:PRO:CD	2.94	0.51
2:D:168:GLU:N	2:D:169:PRO:HD2	2.26	0.51
2:D:202:GLY:O	2:D:203:ILE:O	2.29	0.51
1:A:1530:GLU:HA	1:A:1550:LEU:HD11	1.91	0.51
1:A:1999:CYS:C	1:A:2001:HIS:N	2.64	0.51
2:C:262:SER:OG	2:C:267:GLU:HG2	2.11	0.51
1:B:1951:PRO:HB2	1:B:1955:ARG:HH21	1.76	0.50
2:C:14:ILE:HD13	2:C:70:LEU:HD13	1.92	0.50
1:B:1440:PHE:HB3	1:B:1442:GLU:HB2	1.93	0.50
1:A:1907:LEU:HD11	1:A:1938:VAL:HG11	1.93	0.50
1:B:1428:ALA:HB2	1:B:2395:ASN:HD21	1.75	0.50
1:B:1977:THR:HG21	1:B:2013:SER:OG	2.12	0.50
1:A:1564:ILE:HG23	1:A:1596:LEU:HD22	1.94	0.50
2:C:130:PRO:HD2	2:C:148:GLN:HB2	1.92	0.50
1:A:1501:TRP:HA	1:A:1503:LEU:HG	1.92	0.50
2:C:107:CYS:HB3	2:C:127:VAL:O	2.11	0.50
1:A:1781:GLU:OE1	1:A:1781:GLU:HA	2.11	0.50
1:A:1936:LEU:HA	1:A:1939:ILE:HG13	1.92	0.50
1:A:1977:THR:HG22	1:A:1981:LYS:HE2	1.94	0.50
2:C:72:SER:O	2:C:74:ASN:N	2.45	0.50
2:C:207:VAL:HG12	2:C:209:GLN:HG2	1.94	0.50
1:B:1936:LEU:HA	1:B:1939:ILE:HG13	1.93	0.50
2:D:94:HIS:HD2	2:D:140:GLN:HB3	1.76	0.50
2:D:207:VAL:HG12	2:D:209:GLN:HG2	1.94	0.50
1:A:1670:HIS:HE1	1:A:1681:PRO:CB	2.22	0.50
1:B:2027:TRP:O	1:B:2031:LEU:HG	2.11	0.50
1:B:2512:ASP:OD1	1:B:2512:ASP:N	2.41	0.50
2:D:137:HIS:HD2	2:D:138:PRO:N	2.10	0.50
1:A:1564:ILE:HD13	1:A:1600:GLU:HG3	1.93	0.50
1:A:1766:GLU:OE1	1:A:1766:GLU:N	2.45	0.50
1:B:1605:TYR:CZ	1:B:1612:ARG:HG2	2.46	0.49
2:C:63:GLN:NE2	2:C:86:LYS:H	2.04	0.49
1:B:1623:LEU:HG	1:B:1633:TRP:CZ3	2.46	0.49
2:D:200:THR:O	2:D:208:THR:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:VAL:HG22	1:A:2390:THR:HG21	1.92	0.49
2:D:277:ALA:O	2:D:286:VAL:HG23	2.12	0.49
1:B:1649:ASP:O	1:B:1651:ARG:N	2.45	0.49
2:D:74:ASN:H	2:D:75:PRO:HD3	1.78	0.49
1:B:2298:ASP:HB2	1:B:2382:MET:HE1	1.92	0.49
2:C:277:ALA:O	2:C:286:VAL:HG23	2.12	0.49
2:D:202:GLY:HA3	2:D:208:THR:H	1.78	0.49
1:A:2006:VAL:O	1:A:2010:MET:HB2	2.12	0.49
2:D:63:GLN:NE2	2:D:86:LYS:H	2.05	0.49
1:A:1628:ARG:HB2	1:A:1633:TRP:CD1	2.48	0.49
1:A:1684:GLN:HB3	1:A:1687:HIS:CD2	2.47	0.49
1:B:1754:LEU:HD13	1:B:1775:TYR:CE2	2.47	0.49
1:A:1402:LEU:O	1:A:1405:GLN:HB2	2.13	0.49
1:A:1605:TYR:CZ	1:A:1612:ARG:HG2	2.47	0.49
2:C:180:PRO:HG2	2:C:230:PRO:HA	1.95	0.49
2:C:248:ARG:O	2:C:252:PHE:N	2.44	0.49
1:B:2162:VAL:HG22	1:B:2170:ARG:HG3	1.94	0.49
1:B:2415:MET:HE2	1:B:2501:ILE:HG23	1.95	0.49
1:A:1428:ALA:HB2	1:A:2395:ASN:HD21	1.78	0.49
1:A:1970:GLN:NE2	1:A:2139:ALA:H	2.10	0.49
1:A:1977:THR:HG21	1:A:2013:SER:OG	2.13	0.49
1:A:2281:MET:CE	2:C:222:TYR:CD2	2.96	0.49
2:D:72:SER:O	2:D:74:ASN:N	2.46	0.48
1:A:1786:TRP:CE3	1:A:1789:ALA:HB2	2.48	0.48
1:B:1913:TYR:HB2	1:B:1915:HIS:CE1	2.48	0.48
1:B:2374:LYS:HE3	1:B:2540:GLN:OE1	2.13	0.48
2:D:128:ASN:O	2:D:129:ALA:CB	2.62	0.48
1:A:1478:LEU:O	1:A:1482:ARG:HG3	2.13	0.48
1:B:1543:GLY:O	1:B:1547:ARG:HD2	2.13	0.48
2:D:258:LEU:HD22	2:D:297:TRP:CE3	2.48	0.48
1:A:1623:LEU:HD13	1:A:1640:ARG:NH1	2.28	0.48
1:A:1892:ILE:HG21	1:A:1930:ILE:HD11	1.95	0.48
1:A:2162:VAL:HG22	1:A:2170:ARG:HG3	1.94	0.48
2:C:82:ASP:H	2:C:119:LEU:HD22	1.79	0.48
1:B:1999:CYS:C	1:B:2001:HIS:H	2.16	0.48
2:D:94:HIS:CD2	2:D:140:GLN:HB3	2.48	0.48
2:C:287:THR:O	2:C:294:ALA:HA	2.14	0.48
1:B:1999:CYS:C	1:B:2001:HIS:N	2.67	0.48
1:A:1681:PRO:O	1:A:1682:SER:C	2.52	0.48
1:B:2411:LYS:O	1:B:2415:MET:HG3	2.14	0.48
1:B:1958:HIS:HE1	1:B:1990:ALA:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2336:LEU:HG	1:B:2339:ARG:HH11	1.79	0.48
1:B:2520:ASP:OD2	1:B:2522:PRO:HD2	2.13	0.48
1:A:1972:LEU:O	1:A:1975:PRO:HG2	2.14	0.48
1:B:2152:ARG:HG2	1:B:2177:SER:OG	2.14	0.48
1:A:1543:GLY:O	1:A:1547:ARG:HD2	2.13	0.48
1:B:1417:ILE:O	1:B:1421:ASN:ND2	2.47	0.47
1:B:1418:SER:HB2	1:B:1581:GLU:HG2	1.96	0.47
1:B:1907:LEU:HD11	1:B:1938:VAL:HG13	1.95	0.47
1:B:2154:GLN:NE2	1:B:2155:SER:HB3	2.28	0.47
2:D:130:PRO:HD2	2:D:148:GLN:HB2	1.95	0.47
1:A:2281:MET:HA	1:A:2281:MET:HE2	1.95	0.47
1:B:2281:MET:CE	2:D:222:TYR:CD2	2.97	0.47
1:B:2382:MET:SD	1:B:2549:TRP:HA	2.54	0.47
2:C:159:THR:C	2:C:161:HIS:H	2.16	0.47
2:D:168:GLU:HB3	2:D:195:TYR:OH	2.15	0.47
1:A:1440:PHE:HB3	1:A:1442:GLU:HB2	1.96	0.47
1:A:1773:LEU:HG	1:A:1796:MET:HG3	1.96	0.47
1:A:1791:HIS:O	1:A:1795:VAL:HG23	2.15	0.47
2:C:68:TYR:HE2	2:C:77:PRO:HD3	1.79	0.47
2:C:69:ASP:HB3	2:C:72:SER:OG	2.14	0.47
1:B:1973:ILE:H	1:B:1973:ILE:HG13	1.47	0.47
1:B:1416:LEU:O	1:B:1420:ASN:HB2	2.14	0.47
1:B:1670:HIS:HE1	1:B:1681:PRO:HB3	1.79	0.47
1:A:1502:THR:HG22	1:A:1504:VAL:HG23	1.97	0.47
1:A:2146:PRO:O	1:A:2147:ASN:HB2	2.14	0.47
2:C:288:ALA:HB1	2:C:315:VAL:HG12	1.96	0.47
1:B:2282:GLN:HE21	2:D:316:VAL:HG11	1.79	0.47
2:D:68:TYR:HE2	2:D:77:PRO:HD3	1.79	0.47
2:D:94:HIS:HE1	2:D:96:ASP:HB2	1.78	0.47
1:A:2154:GLN:NE2	1:A:2155:SER:HB3	2.29	0.47
1:A:2281:MET:HE1	2:C:222:TYR:CG	2.49	0.47
1:B:1690:PRO:HB2	1:B:1692:VAL:HG22	1.97	0.47
1:B:1915:HIS:HE1	1:B:1919:VAL:CG1	2.28	0.47
2:D:180:PRO:HG2	2:D:230:PRO:HA	1.97	0.47
1:A:1691:THR:HG22	1:A:1691:THR:O	2.15	0.47
1:A:1980:SER:O	1:A:1988:HIS:HB2	2.15	0.47
1:B:2347:ASP:OD1	1:B:2350:SER:OG	2.27	0.47
1:A:2411:LYS:O	1:A:2415:MET:HG3	2.15	0.47
2:C:258:LEU:HD22	2:C:297:TRP:CE3	2.49	0.47
1:B:1932:ILE:HD12	1:B:1933:ASP:H	1.78	0.47
2:C:139:ASN:HD22	2:C:203:ILE:HG12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:PRO:HB2	1:A:1692:VAL:HG22	1.97	0.46
2:C:111:ILE:HD12	2:C:123:ARG:HD3	1.97	0.46
1:B:1566:LYS:O	1:B:1570:LEU:HG	2.14	0.46
1:B:1574:GLU:HG2	1:B:1585:ARG:NH2	2.30	0.46
1:B:1605:TYR:CG	1:B:1643:VAL:HG11	2.50	0.46
2:D:94:HIS:HB3	2:D:99:TRP:HB2	1.96	0.46
2:D:139:ASN:HD22	2:D:203:ILE:HG12	1.79	0.46
2:D:154:ILE:HD11	2:D:210:LEU:HD11	1.97	0.46
2:D:159:THR:C	2:D:161:HIS:H	2.17	0.46
1:A:2245:THR:O	1:A:2249:LEU:HD12	2.15	0.46
1:B:1691:THR:O	1:B:1691:THR:HG22	2.15	0.46
2:C:168:GLU:HG2	2:C:169:PRO:N	2.30	0.46
1:B:1786:TRP:CE3	1:B:1789:ALA:HB2	2.50	0.46
2:D:167:PRO:HD2	2:D:169:PRO:CG	2.43	0.46
1:A:1401:GLU:HG2	1:A:2389:VAL:CG2	2.46	0.46
1:A:2382:MET:SD	1:A:2549:TRP:HA	2.56	0.46
2:C:225:GLN:HG2	2:C:226:CYS:N	2.30	0.46
1:B:1477:MET:HE2	1:B:1477:MET:HB3	1.89	0.46
1:B:1734:THR:O	1:B:1736:ASP:N	2.40	0.46
2:D:270:ARG:HD2	2:D:270:ARG:HA	1.77	0.46
2:D:288:ALA:HB1	2:D:315:VAL:HG12	1.97	0.46
1:A:1482:ARG:HA	1:A:1485:GLU:HG2	1.97	0.46
1:A:1947:ASP:CG	1:A:1987:ARG:HG2	2.36	0.46
1:A:2028:HIS:HE1	1:A:2112:SER:OG	1.98	0.46
1:A:1915:HIS:HD2	1:A:1953:VAL:HG22	1.81	0.46
1:B:1537:PRO:O	1:B:1543:GLY:HA3	2.15	0.46
1:B:2006:VAL:O	1:B:2010:MET:HB2	2.15	0.46
1:B:1497:CYS:SG	1:B:1516:ALA:HB2	2.56	0.46
1:B:1502:THR:HG22	1:B:1504:VAL:HG23	1.98	0.46
1:B:1680:ASP:HB3	1:B:1683:ARG:H	1.79	0.46
1:A:2214:THR:O	1:A:2217:ARG:HB3	2.16	0.46
1:A:2333:ILE:CD1	1:A:2407:LEU:HD13	2.46	0.46
1:A:1595:MET:O	1:A:1599:LEU:HB2	2.16	0.46
1:A:1907:LEU:HD11	1:A:1938:VAL:HG13	1.97	0.46
2:C:255:MET:HE1	2:C:299:VAL:HG12	1.96	0.46
2:D:225:GLN:HG2	2:D:226:CYS:N	2.30	0.46
1:A:2201:LEU:O	1:A:2205:VAL:HG23	2.15	0.46
2:C:94:HIS:HE1	2:C:96:ASP:HB2	1.81	0.46
2:C:159:THR:HB	2:C:161:HIS:HB2	1.97	0.46
1:B:1482:ARG:HA	1:B:1485:GLU:HG2	1.97	0.45
1:B:1913:TYR:O	1:B:1915:HIS:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2152:ARG:HG2	1:B:2177:SER:CB	2.46	0.45
1:B:2152:ARG:HE	1:B:2152:ARG:HB3	1.61	0.45
2:D:95:GLU:CB	2:D:140:GLN:HE22	2.18	0.45
2:D:262:SER:OG	2:D:267:GLU:HG2	2.16	0.45
1:A:1433:LEU:HD23	1:A:1453:LEU:HD23	1.99	0.45
1:A:2184:PHE:HB3	1:A:2236:LEU:HD22	1.98	0.45
1:A:2378:ARG:NH1	1:A:2380:THR:HG21	2.31	0.45
1:B:1915:HIS:CE1	1:B:1919:VAL:CG1	2.99	0.45
2:D:17:THR:HG1	2:D:27:TRP:HE1	1.63	0.45
1:A:1697:THR:O	1:A:1701:MET:HG3	2.16	0.45
2:C:270:ARG:HD2	2:C:270:ARG:HA	1.79	0.45
1:B:2214:THR:O	1:B:2217:ARG:HB3	2.16	0.45
2:D:115:ARG:O	2:D:116:SER:HB3	2.17	0.45
1:A:1964:ILE:O	1:A:1967:TYR:O	2.35	0.45
1:A:2333:ILE:HD12	1:A:2407:LEU:HD13	1.98	0.45
2:C:137:HIS:CD2	2:C:138:PRO:CD	2.99	0.45
2:D:132:ASN:HD21	2:D:148:GLN:HG2	1.81	0.45
1:A:1910:TRP:CD1	1:A:1910:TRP:C	2.90	0.45
1:A:1913:TYR:O	1:A:1915:HIS:CG	2.70	0.45
2:C:63:GLN:HE21	2:C:86:LYS:N	2.05	0.45
1:A:1413:LEU:O	1:A:1417:ILE:HG12	2.16	0.45
1:B:1932:ILE:O	1:B:1933:ASP:C	2.55	0.45
1:B:2378:ARG:NH1	1:B:2380:THR:HG21	2.32	0.45
1:B:2418:LEU:O	1:B:2422:VAL:HG23	2.17	0.45
2:D:248:ARG:O	2:D:252:PHE:HA	2.17	0.45
1:A:2027:TRP:O	1:A:2031:LEU:HG	2.16	0.45
2:D:306:ARG:HG2	2:D:307:GLU:N	2.29	0.45
2:C:168:GLU:HB3	2:C:195:TYR:OH	2.17	0.45
1:B:1947:ASP:CG	1:B:1987:ARG:HG2	2.37	0.45
2:D:287:THR:O	2:D:294:ALA:HA	2.17	0.45
1:A:1989:ASN:O	1:A:1993:LYS:HD2	2.17	0.45
2:D:16:ALA:O	2:D:318:LEU:HA	2.17	0.45
1:A:1913:TYR:CB	1:A:1915:HIS:CE1	3.00	0.45
2:C:16:ALA:O	2:C:318:LEU:HA	2.17	0.45
1:B:1629:ILE:O	1:B:1630:VAL:C	2.56	0.45
1:B:1697:THR:O	1:B:1701:MET:HG3	2.17	0.45
2:D:188:VAL:HG13	2:D:223:ALA:CB	2.47	0.45
2:C:159:THR:C	2:C:161:HIS:N	2.70	0.45
1:B:1506:ASP:HA	1:B:1509:GLN:HB2	1.99	0.44
1:B:1698:TYR:O	1:B:1702:LYS:HG2	2.17	0.44
2:D:231:ASP:HB2	2:D:233:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1631:GLU:HA	1:A:1634:GLN:HE21	1.81	0.44
1:A:1785:SER:O	1:A:1786:TRP:HB3	2.17	0.44
1:A:2210:ALA:O	1:A:2216:LEU:HD22	2.17	0.44
2:C:137:HIS:HD2	2:C:138:PRO:N	2.16	0.44
1:B:2316:ARG:NH2	1:B:2349:LEU:HD23	2.32	0.44
2:D:69:ASP:HB3	2:D:72:SER:OG	2.17	0.44
1:A:2513:PHE:HB2	1:A:2519:LEU:HD11	1.99	0.44
1:B:1605:TYR:CE2	1:B:1612:ARG:HG2	2.53	0.44
1:B:1881:THR:HG23	1:B:1909:LEU:HD22	2.00	0.44
2:D:239:SER:OG	2:D:240:ALA:N	2.50	0.44
1:A:1674:VAL:HG11	1:A:1681:PRO:HD3	1.99	0.44
1:A:2192:LEU:HD21	1:A:2237:ILE:HD11	1.99	0.44
1:A:2260:LEU:HD12	1:A:2261:LEU:N	2.32	0.44
1:B:2281:MET:HE2	1:B:2281:MET:CA	2.48	0.44
1:B:2339:ARG:NH2	1:B:2356:ILE:O	2.50	0.44
2:D:21:ASP:HB3	2:D:313:LYS:HB2	1.99	0.44
2:D:82:ASP:HB2	2:D:119:LEU:HD13	1.99	0.44
2:D:135:CYS:SG	2:D:178:ILE:HG22	2.57	0.44
1:A:1629:ILE:O	1:A:1630:VAL:C	2.55	0.44
1:A:2363:GLU:HA	1:A:2363:GLU:OE1	2.18	0.44
2:C:28:GLN:O	2:C:28:GLN:HG3	2.17	0.44
1:B:1621:GLU:C	1:B:1623:LEU:H	2.20	0.44
1:B:1628:ARG:HB2	1:B:1633:TRP:CD1	2.53	0.44
1:B:1681:PRO:O	1:B:1682:SER:C	2.56	0.44
1:A:1393:TYR:CE2	1:A:1422:LYS:HD2	2.52	0.44
1:A:1506:ASP:HA	1:A:1509:GLN:HB2	1.99	0.44
1:A:1970:GLN:HA	1:A:1973:ILE:HD11	2.00	0.44
1:A:2261:LEU:HD23	1:A:2262:ASN:ND2	2.32	0.44
1:A:2401:HIS:CD2	1:A:2522:PRO:HA	2.52	0.44
2:C:169:PRO:HA	2:C:171:VAL:HG22	1.98	0.44
1:B:1712:ASP:OD1	1:A:2266:ARG:NH2	2.50	0.44
2:D:159:THR:HB	2:D:161:HIS:HB2	1.99	0.44
1:A:1427:GLU:HB2	1:A:2398:ILE:HD13	1.98	0.44
1:A:2021:ILE:HG22	1:A:2025:GLU:HB2	1.99	0.44
1:B:1964:ILE:O	1:B:1967:TYR:O	2.35	0.44
2:D:69:ASP:HB2	2:D:78:ILE:CD1	2.34	0.44
2:D:102:THR:O	2:D:109:ALA:HA	2.17	0.44
2:D:255:MET:HE1	2:D:299:VAL:HG12	1.99	0.44
1:A:1621:GLU:C	1:A:1623:LEU:H	2.20	0.44
1:B:1481:MET:HA	1:B:1484:LEU:HD12	1.99	0.44
1:B:2316:ARG:HH21	1:B:2349:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:THR:C	2:D:161:HIS:N	2.71	0.44
1:B:1413:LEU:O	1:B:1417:ILE:HG12	2.17	0.43
2:D:14:ILE:HD13	2:D:70:LEU:HD13	1.99	0.43
1:A:1739:HIS:O	1:A:1743:LEU:HB2	2.18	0.43
1:A:2281:MET:HE2	1:A:2281:MET:CA	2.48	0.43
2:C:263:GLY:O	2:C:264:ASN:HB3	2.18	0.43
2:D:219:HIS:CE1	2:D:245:LYS:HD2	2.53	0.43
1:A:1505:ASN:CB	1:A:1508:THR:HB	2.49	0.43
1:A:2319:ASN:HB3	1:A:2352:LYS:HG2	1.99	0.43
1:A:2496:LYS:HE3	1:A:2500:ILE:HD11	1.99	0.43
1:A:1680:ASP:HB3	1:A:1683:ARG:H	1.82	0.43
1:B:1453:LEU:O	1:B:1455:GLU:N	2.52	0.43
1:B:1605:TYR:HD2	1:B:1605:TYR:O	2.01	0.43
1:B:1899:ASN:O	1:B:1900:LEU:C	2.55	0.43
1:A:1416:LEU:O	1:A:1420:ASN:HB2	2.18	0.43
1:B:1691:THR:HG23	1:B:1724:MET:HE1	2.00	0.43
1:A:2332:TYR:O	1:A:2507:LYS:NZ	2.36	0.43
1:B:1705:TRP:CZ2	1:B:1710:LYS:HD2	2.54	0.43
1:A:1682:SER:O	1:A:1685:LEU:HD12	2.19	0.43
2:C:115:ARG:O	2:C:116:SER:HB3	2.19	0.43
1:A:2042:ARG:HA	1:A:2042:ARG:HD3	1.87	0.43
2:C:231:ASP:HB2	2:C:233:THR:H	1.84	0.43
1:B:1732:ILE:HD13	1:B:1740:LYS:HB2	2.01	0.43
1:B:1739:HIS:O	1:B:1743:LEU:HB2	2.18	0.43
1:B:1878:LEU:HD21	1:B:1918:ASP:CB	2.47	0.43
1:B:2036:ARG:HA	1:B:2036:ARG:HD3	1.62	0.43
1:B:2401:HIS:CD2	1:B:2522:PRO:HA	2.53	0.43
2:C:151:ALA:HA	2:C:166:ILE:HG22	2.01	0.43
1:B:1470:ASN:HB3	1:B:1471:LYS:H	1.60	0.43
1:B:1682:SER:O	1:B:1685:LEU:HD12	2.19	0.43
1:B:2387:MET:HE1	1:B:2396:TYR:CB	2.49	0.43
1:A:1415:SER:O	1:A:1419:ILE:CG2	2.65	0.43
1:A:1470:ASN:HB3	1:A:1471:LYS:H	1.60	0.43
1:A:1705:TRP:CZ3	1:A:1757:TRP:HB3	2.54	0.43
1:A:1759:LEU:HD11	1:A:1796:MET:HE3	1.99	0.43
1:A:2374:LYS:HE3	1:A:2540:GLN:OE1	2.19	0.43
2:C:94:HIS:HD2	2:C:140:GLN:HB3	1.83	0.43
2:C:94:HIS:CD2	2:C:140:GLN:HB3	2.53	0.43
2:C:262:SER:HB2	2:C:263:GLY:H	1.65	0.43
1:B:2424:ASP:O	1:B:2428:ASN:ND2	2.52	0.42
1:A:2387:MET:HE1	1:A:2396:TYR:HB2	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:THR:O	2:C:109:ALA:HA	2.18	0.42
1:B:1505:ASN:CB	1:B:1508:THR:HB	2.50	0.42
1:B:1892:ILE:HG21	1:B:1930:ILE:HD11	2.01	0.42
1:B:1910:TRP:CZ2	1:B:1956:LEU:HB3	2.54	0.42
1:B:2021:ILE:HG22	1:B:2025:GLU:HB2	2.01	0.42
1:B:2184:PHE:HB3	1:B:2236:LEU:HD22	2.01	0.42
1:A:1900:LEU:HD23	1:A:2204:LEU:HD22	2.00	0.42
1:A:2036:ARG:HA	1:A:2036:ARG:HD3	1.61	0.42
1:A:2064:THR:CG2	1:A:2128:PRO:HD3	2.40	0.42
2:C:17:THR:HG1	2:C:27:TRP:HE1	1.63	0.42
1:B:1473:ASP:HA	1:B:1474:PRO:HD2	1.83	0.42
2:D:169:PRO:HA	2:D:171:VAL:HG22	2.00	0.42
2:D:213:LYS:HD3	2:D:252:PHE:HE1	1.84	0.42
2:C:306:ARG:HG2	2:C:307:GLU:N	2.31	0.42
1:B:1631:GLU:HA	1:B:1634:GLN:HE21	1.84	0.42
1:B:1710:LYS:NZ	1:B:1760:ASN:HD21	2.17	0.42
1:B:1778:ALA:O	1:B:1782:HIS:HD2	2.01	0.42
2:D:248:ARG:O	2:D:252:PHE:N	2.50	0.42
1:A:1453:LEU:O	1:A:1455:GLU:N	2.53	0.42
2:C:150:GLY:HA3	2:C:169:PRO:CB	2.44	0.42
2:C:248:ARG:O	2:C:252:PHE:HA	2.20	0.42
1:B:2042:ARG:HA	1:B:2042:ARG:HD3	1.87	0.42
1:B:2165:SER:OG	1:B:2166:LYS:N	2.52	0.42
2:D:150:GLY:HA3	2:D:169:PRO:CB	2.43	0.42
1:A:1691:THR:HG23	1:A:1724:MET:HE1	2.01	0.42
1:A:1910:TRP:HD1	1:A:1910:TRP:O	2.03	0.42
1:A:2037:LEU:HD22	1:A:2043:ASN:ND2	2.33	0.42
1:A:2503:ARG:NH1	1:A:2507:LYS:CE	2.82	0.42
2:C:203:ILE:HG22	2:C:204:GLY:N	2.34	0.42
2:C:219:HIS:CE1	2:C:245:LYS:HD2	2.55	0.42
2:C:298:CYS:HB2	2:C:305:LYS:HE3	2.02	0.42
2:D:297:TRP:CZ3	2:D:304:ILE:HG12	2.54	0.42
1:A:1915:HIS:HE1	1:A:1919:VAL:CG1	2.33	0.42
1:A:2530:LYS:HE2	1:A:2530:LYS:HA	2.00	0.42
2:C:21:ASP:HB3	2:C:313:LYS:HB2	2.02	0.42
1:B:1595:MET:O	1:B:1599:LEU:HB2	2.20	0.42
1:B:2123:LEU:HD12	1:B:2123:LEU:HA	1.97	0.42
1:B:2368:ARG:HD2	1:B:2370:LYS:O	2.20	0.42
2:D:28:GLN:HG2	2:D:31:SER:OG	2.20	0.42
1:B:1614:ILE:O	1:B:1618:ILE:HG13	2.19	0.42
1:B:1910:TRP:CD1	1:B:1910:TRP:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2321:THR:HG23	1:B:2387:MET:HE3	2.02	0.42
1:B:2333:ILE:HD12	1:B:2407:LEU:HD13	2.01	0.42
1:B:2513:PHE:HB2	1:B:2519:LEU:HD11	2.01	0.42
1:A:1936:LEU:C	1:A:1938:VAL:H	2.23	0.42
1:A:2101:TRP:HA	1:A:2104:TYR:HB2	2.01	0.42
1:B:2022:LEU:HD23	1:B:2022:LEU:HA	1.91	0.42
1:B:2329:MET:SD	1:B:2404:MET:HE2	2.60	0.42
2:D:63:GLN:HE21	2:D:86:LYS:N	2.07	0.42
1:A:1974:TYR:O	1:A:1978:VAL:HG23	2.20	0.42
1:A:2421:PHE:HD1	1:A:2430:ARG:HH22	1.65	0.42
1:B:2364:VAL:HG12	1:B:2365:ALA:N	2.33	0.42
2:D:53:ASP:C	2:D:55:SER:H	2.23	0.42
2:D:75:PRO:HB2	2:D:76:ASN:H	1.48	0.42
2:D:203:ILE:HG22	2:D:204:GLY:N	2.35	0.42
1:A:2281:MET:CE	2:C:222:TYR:CE2	3.03	0.42
1:A:2424:ASP:O	1:A:2428:ASN:ND2	2.53	0.42
1:B:1400:LYS:HG3	1:B:1416:LEU:HD13	2.01	0.41
1:B:1533:THR:C	1:B:1535:MET:H	2.22	0.41
1:B:1903:THR:HG22	1:B:1938:VAL:HG21	2.02	0.41
1:B:2376:PRO:HG2	1:B:2532:ALA:HB2	2.02	0.41
1:A:1493:LEU:CD2	1:A:1519:ALA:HB2	2.46	0.41
1:A:1623:LEU:HD13	1:A:1640:ARG:HH12	1.84	0.41
1:A:1932:ILE:O	1:A:1933:ASP:C	2.58	0.41
1:A:2128:PRO:HD2	1:A:2129:LYS:H	1.85	0.41
1:A:2184:PHE:CB	1:A:2236:LEU:HD22	2.50	0.41
2:C:213:LYS:HD3	2:C:252:PHE:HE1	1.85	0.41
2:C:281:ASP:OD1	2:C:283:GLN:HG3	2.20	0.41
2:C:289:SER:HB2	2:C:291:ASP:OD1	2.20	0.41
1:B:1415:SER:O	1:B:1419:ILE:CG2	2.66	0.41
1:B:1970:GLN:C	1:B:1972:LEU:N	2.73	0.41
1:B:2004:THR:HA	1:B:2007:GLN:HB2	2.01	0.41
1:B:2146:PRO:O	1:B:2147:ASN:HB2	2.20	0.41
1:B:2261:LEU:HD23	1:B:2262:ASN:ND2	2.35	0.41
1:A:1481:MET:HA	1:A:1484:LEU:HD12	2.01	0.41
1:A:2418:LEU:HD13	1:A:2504:VAL:HG11	2.01	0.41
1:B:1497:CYS:SG	1:B:1516:ALA:CB	3.08	0.41
1:A:1566:LYS:O	1:A:1570:LEU:HG	2.19	0.41
1:A:1605:TYR:HD2	1:A:1605:TYR:O	2.03	0.41
1:A:1915:HIS:CE1	1:A:1919:VAL:CG1	3.03	0.41
1:A:2082:GLN:HE21	1:A:2082:GLN:HB3	1.64	0.41
1:B:2529:ILE:O	1:B:2533:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:HIS:CD2	2:D:138:PRO:N	2.87	0.41
1:A:1473:ASP:HA	1:A:1474:PRO:HD2	1.83	0.41
1:A:2382:MET:HG3	1:A:2549:TRP:O	2.19	0.41
2:C:127:VAL:HG12	2:C:128:ASN:N	2.34	0.41
2:C:203:ILE:HA	2:C:206:GLU:HG2	2.02	0.41
1:B:1701:MET:HE2	1:B:1701:MET:HB3	1.84	0.41
2:D:298:CYS:HB2	2:D:305:LYS:HE3	2.03	0.41
1:A:2500:ILE:O	1:A:2504:VAL:HG23	2.20	0.41
2:C:137:HIS:HD2	2:C:139:ASN:H	1.67	0.41
1:B:1629:ILE:HG22	1:B:1630:VAL:HG23	2.03	0.41
1:B:1895:SER:HB3	1:B:1898:ASN:O	2.20	0.41
1:B:2225:TYR:CD1	3:B:2601:P2X:H2	2.55	0.41
2:D:28:GLN:O	2:D:28:GLN:HG3	2.20	0.41
2:D:281:ASP:OD1	2:D:283:GLN:HG3	2.20	0.41
1:A:1899:ASN:O	1:A:1900:LEU:C	2.58	0.41
1:A:2339:ARG:NH2	1:A:2343:ASN:HB3	2.36	0.41
1:A:2347:ASP:OD1	1:A:2350:SER:OG	2.25	0.41
2:C:18:ALA:HB1	2:C:45:VAL:HG21	2.03	0.41
1:B:2496:LYS:HE3	1:B:2500:ILE:HD11	2.02	0.41
1:A:2127:SER:HA	1:A:2128:PRO:HD3	1.93	0.41
2:C:297:TRP:CZ3	2:C:304:ILE:HG12	2.55	0.41
1:B:1425:GLN:HG2	1:B:2314:PHE:HZ	1.84	0.41
1:B:1989:ASN:O	1:B:1993:LYS:HD2	2.21	0.41
1:A:1518:ALA:HB2	1:A:1546:TYR:OH	2.20	0.41
1:A:2023:TRP:CD2	1:A:2067:GLU:HG2	2.56	0.41
2:C:85:ASN:H	2:C:85:ASN:ND2	2.18	0.41
1:B:1514:ARG:HH21	1:B:1540:THR:HG21	1.86	0.41
1:B:1807:GLN:NE2	1:B:1811:ARG:HH21	2.19	0.41
1:B:1910:TRP:HZ2	1:B:1956:LEU:HB3	1.85	0.41
1:B:1936:LEU:C	1:B:1938:VAL:H	2.24	0.41
1:B:2046:GLY:O	1:B:2050:VAL:HG23	2.20	0.41
1:B:2128:PRO:HD2	1:B:2129:LYS:H	1.86	0.41
1:B:2268:MET:HG3	1:B:2290:ALA:HB2	2.03	0.41
1:B:2278:LEU:HB3	1:B:2282:GLN:HB2	2.03	0.41
2:D:150:GLY:HA2	2:D:173:ILE:HG23	2.03	0.41
2:D:151:ALA:HA	2:D:166:ILE:HG22	2.03	0.41
2:D:248:ARG:CZ	2:D:248:ARG:HB3	2.51	0.41
1:A:2275:TYR:HE1	1:A:2286:VAL:HB	1.85	0.41
2:C:82:ASP:HB2	2:C:119:LEU:HD13	2.02	0.41
2:D:263:GLY:O	2:D:264:ASN:HB3	2.21	0.41
1:A:1533:THR:C	1:A:1535:MET:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1913:TYR:CB	1:B:1915:HIS:CE1	3.05	0.40
1:B:2189:HIS:CD2	1:B:2189:HIS:N	2.89	0.40
1:B:2530:LYS:HE2	1:B:2530:LYS:HA	2.02	0.40
2:D:127:VAL:HG12	2:D:128:ASN:N	2.35	0.40
1:A:1400:LYS:HG3	1:A:1416:LEU:HD13	2.02	0.40
1:A:1417:ILE:O	1:A:1421:ASN:ND2	2.54	0.40
1:A:1605:TYR:CE2	1:A:1612:ARG:HG2	2.57	0.40
1:A:1681:PRO:HG2	1:A:1683:ARG:HG3	2.03	0.40
1:B:2101:TRP:HA	1:B:2104:TYR:HB2	2.03	0.40
2:D:258:LEU:HD11	2:D:285:ILE:HG21	2.02	0.40
1:A:1903:THR:HG22	1:A:1938:VAL:HG21	2.02	0.40
1:B:1722:GLN:HA	1:B:1725:GLN:HE21	1.86	0.40
1:B:2297:ASP:O	1:B:2299:LEU:N	2.54	0.40
1:B:2421:PHE:HD1	1:B:2430:ARG:HH22	1.68	0.40
2:D:68:TYR:CE2	2:D:77:PRO:HD3	2.57	0.40
1:A:1670:HIS:CE1	1:A:1681:PRO:HB3	2.47	0.40
2:C:168:GLU:N	2:C:169:PRO:CD	2.84	0.40
2:C:200:THR:HB	2:C:209:GLN:HB2	2.02	0.40
2:C:239:SER:OG	2:C:240:ALA:N	2.54	0.40
1:B:1618:ILE:HG13	1:B:1618:ILE:H	1.71	0.40
1:B:1905:ARG:HD3	1:B:1905:ARG:HA	1.80	0.40
1:B:1980:SER:O	1:B:1988:HIS:HB2	2.22	0.40
2:D:85:ASN:ND2	2:D:85:ASN:H	2.19	0.40
1:A:2368:ARG:HD2	1:A:2370:LYS:O	2.21	0.40
1:A:2378:ARG:HH11	1:A:2380:THR:HG21	1.86	0.40
2:C:12:PRO:O	2:C:54:ARG:NH2	2.54	0.40
2:C:68:TYR:CE2	2:C:77:PRO:HD3	2.57	0.40
1:B:2332:TYR:O	1:B:2507:LYS:NZ	2.38	0.40
2:D:18:ALA:HB1	2:D:45:VAL:HG21	2.04	0.40
2:D:313:LYS:HA	2:D:313:LYS:HD3	1.86	0.40
1:A:1401:GLU:CG	1:A:2389:VAL:HG22	2.51	0.40
1:A:2332:TYR:CE1	1:A:2507:LYS:HE2	2.56	0.40
2:C:101:TYR:HA	2:C:110:ARG:O	2.20	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	1046/1174 (89%)	904 (86%)	111 (11%)	31 (3%)	4 29
1	B	1052/1174 (90%)	913 (87%)	108 (10%)	31 (3%)	4 30
2	C	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	1 14
2	D	315/326 (97%)	266 (84%)	30 (10%)	19 (6%)	1 14
All	All	2728/3000 (91%)	2349 (86%)	279 (10%)	100 (4%)	3 25

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1525	GLN
1	B	1630	VAL
1	B	1650	MET
1	B	1680	ASP
1	B	1970	GLN
1	B	2094	VAL
1	B	2298	ASP
1	B	2364	VAL
2	D	74	ASN
2	D	97	GLY
2	D	203	ILE
2	D	269	SER
1	A	1454	HIS
1	A	1525	GLN
1	A	1630	VAL
1	A	1650	MET
1	A	1680	ASP
1	A	1970	GLN
1	A	2094	VAL
1	A	2298	ASP
1	A	2364	VAL
2	C	35	THR

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Mol	Chain	Res	Type
2	C	73	ASN
2	C	74	ASN
2	C	97	GLY
2	C	203	ILE
2	C	269	SER
1	B	1444	GLU
1	B	1454	HIS
1	B	1682	SER
1	B	1709	ARG
1	B	1735	GLU
1	B	1786	TRP
1	B	1914	GLY
1	B	1937	GLN
1	B	2000	GLU
2	D	35	THR
2	D	73	ASN
2	D	75	PRO
2	D	118	ASN
2	D	160	ASP
2	D	167	PRO
2	D	204	GLY
1	A	1444	GLU
1	A	1445	ILE
1	A	1682	SER
1	A	1709	ARG
1	A	1735	GLU
1	A	1786	TRP
1	A	1914	GLY
1	A	1937	GLN
1	A	2000	GLU
2	C	75	PRO
2	C	118	ASN
2	C	160	ASP
2	C	167	PRO
2	C	204	GLY
1	B	1445	ILE
1	B	1896	ARG
1	B	1933	ASP
1	B	2001	HIS
1	B	2093	ASN
1	B	2135	ASP
2	D	169	PRO

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Mol	Chain	Res	Type
2	D	264	ASN
1	A	1896	ARG
1	A	1933	ASP
1	A	2093	ASN
2	C	129	ALA
2	C	169	PRO
2	C	264	ASN
1	B	2357	ASP
1	B	2387	MET
2	D	129	ALA
1	A	2001	HIS
1	A	2135	ASP
1	A	2357	ASP
2	C	263	GLY
1	B	1583	TYR
1	B	1681	PRO
1	B	2515	HIS
2	D	140	GLN
2	D	263	GLY
1	A	1681	PRO
1	A	1784	ARG
1	A	2191	ASP
1	A	2515	HIS
2	C	262	SER
1	B	1474	PRO
1	B	2191	ASP
1	A	1474	PRO
1	A	2168	ARG
1	A	2387	MET
1	B	2168	ARG
2	D	201	GLY
2	C	76	ASN
2	C	201	GLY
2	C	310	GLY
2	D	76	ASN
2	D	310	GLY

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	927/1024 (90%)	837 (90%)	90 (10%)	8	32
1	B	931/1024 (91%)	830 (89%)	101 (11%)	6	27
2	C	269/276 (98%)	233 (87%)	36 (13%)	4	19
2	D	269/276 (98%)	233 (87%)	36 (13%)	4	19
All	All	2396/2600 (92%)	2133 (89%)	263 (11%)	6	27

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1417	ILE
1	B	1420	ASN
1	B	1423	LEU
1	B	1443	LEU
1	B	1457	GLU
1	B	1475	GLU
1	B	1501	TRP
1	B	1509	GLN
1	B	1528	SER
1	B	1540	THR
1	B	1541	HIS
1	B	1557	PHE
1	B	1590	MET
1	B	1592	SER
1	B	1593	CYS
1	B	1611	ARG
1	B	1630	VAL
1	B	1650	MET
1	B	1685	LEU
1	B	1709	ARG
1	B	1740	LYS
1	B	1767	SER
1	B	1768	THR
1	B	1780	THR
1	B	1870	THR
1	B	1872	ASP
1	B	1878	LEU
1	B	1891	SER
1	B	1895	SER
1	B	1896	ARG

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Mol	Chain	Res	Type
1	B	1898	ASN
1	B	1899	ASN
1	B	1908	THR
1	B	1916	TRP
1	B	1932	ILE
1	B	1938	VAL
1	B	1956	LEU
1	B	1959	GLN
1	B	1968	HIS
1	B	1973	ILE
1	B	1984	THR
1	B	1985	THR
1	B	2005	LEU
1	B	2011	MET
1	B	2021	ILE
1	B	2035	SER
1	B	2036	ARG
1	B	2068	THR
1	B	2072	GLN
1	B	2076	ARG
1	B	2078	LEU
1	B	2080	GLU
1	B	2090	LYS
1	B	2093	ASN
1	B	2095	LYS
1	B	2098	THR
1	B	2102	ASP
1	B	2123	LEU
1	B	2124	GLN
1	B	2138	LEU
1	B	2152	ARG
1	B	2154	GLN
1	B	2155	SER
1	B	2164	THR
1	B	2165	SER
1	B	2167	GLN
1	B	2168	ARG
1	B	2173	THR
1	B	2181	GLU
1	B	2189	HIS
1	B	2190	GLU
1	B	2195	ASP

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Mol	Chain	Res	Type
1	B	2228	ILE
1	B	2232	THR
1	B	2240	VAL
1	B	2244	ASP
1	B	2245	THR
1	B	2254	ARG
1	B	2259	ILE
1	B	2260	LEU
1	B	2266	ARG
1	B	2281	MET
1	B	2301	LYS
1	B	2318	THR
1	B	2342	SER
1	B	2354	LEU
1	B	2363	GLU
1	B	2378	ARG
1	B	2384	THR
1	B	2390	THR
1	B	2397	ARG
1	B	2408	ARG
1	B	2430	ARG
1	B	2431	LEU
1	B	2432	MET
1	B	2503	ARG
1	B	2515	HIS
1	B	2530	LYS
1	B	2533	THR
1	B	2538	LEU
1	B	2548	PHE
2	D	13	VAL
2	D	37	THR
2	D	44	GLN
2	D	82	ASP
2	D	84	VAL
2	D	85	ASN
2	D	91	VAL
2	D	98	ARG
2	D	128	ASN
2	D	135	CYS
2	D	140	GLN
2	D	159	THR
2	D	160	ASP

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Mol	Chain	Res	Type
2	D	162	ASN
2	D	164	GLN
2	D	166	ILE
2	D	168	GLU
2	D	169	PRO
2	D	170	GLU
2	D	173	ILE
2	D	174	THR
2	D	175	SER
2	D	183	SER
2	D	199	LEU
2	D	214	THR
2	D	215	LYS
2	D	242	GLN
2	D	243	THR
2	D	248	ARG
2	D	261	LYS
2	D	262	SER
2	D	286	VAL
2	D	287	THR
2	D	289	SER
2	D	301	THR
2	D	312	GLN
1	A	1417	ILE
1	A	1420	ASN
1	A	1423	LEU
1	A	1443	LEU
1	A	1457	GLU
1	A	1501	TRP
1	A	1509	GLN
1	A	1540	THR
1	A	1541	HIS
1	A	1557	PHE
1	A	1590	MET
1	A	1593	CYS
1	A	1611	ARG
1	A	1630	VAL
1	A	1650	MET
1	A	1685	LEU
1	A	1709	ARG
1	A	1740	LYS
1	A	1768	THR

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Mol	Chain	Res	Type
1	A	1780	THR
1	A	1872	ASP
1	A	1878	LEU
1	A	1891	SER
1	A	1895	SER
1	A	1896	ARG
1	A	1899	ASN
1	A	1908	THR
1	A	1916	TRP
1	A	1932	ILE
1	A	1956	LEU
1	A	1959	GLN
1	A	1968	HIS
1	A	1973	ILE
1	A	1984	THR
1	A	1985	THR
1	A	2005	LEU
1	A	2011	MET
1	A	2035	SER
1	A	2036	ARG
1	A	2068	THR
1	A	2072	GLN
1	A	2076	ARG
1	A	2078	LEU
1	A	2080	GLU
1	A	2090	LYS
1	A	2093	ASN
1	A	2095	LYS
1	A	2102	ASP
1	A	2123	LEU
1	A	2124	GLN
1	A	2138	LEU
1	A	2152	ARG
1	A	2154	GLN
1	A	2155	SER
1	A	2164	THR
1	A	2165	SER
1	A	2167	GLN
1	A	2168	ARG
1	A	2173	THR
1	A	2181	GLU
1	A	2189	HIS

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Mol	Chain	Res	Type
1	A	2190	GLU
1	A	2195	ASP
1	A	2228	ILE
1	A	2232	THR
1	A	2240	VAL
1	A	2244	ASP
1	A	2245	THR
1	A	2254	ARG
1	A	2259	ILE
1	A	2260	LEU
1	A	2266	ARG
1	A	2281	MET
1	A	2301	LYS
1	A	2318	THR
1	A	2342	SER
1	A	2354	LEU
1	A	2363	GLU
1	A	2367	THR
1	A	2378	ARG
1	A	2384	THR
1	A	2390	THR
1	A	2397	ARG
1	A	2408	ARG
1	A	2430	ARG
1	A	2431	LEU
1	A	2503	ARG
1	A	2530	LYS
1	A	2533	THR
1	A	2548	PHE
2	C	13	VAL
2	C	37	THR
2	C	44	GLN
2	C	82	ASP
2	C	84	VAL
2	C	85	ASN
2	C	91	VAL
2	C	98	ARG
2	C	123	ARG
2	C	128	ASN
2	C	135	CYS
2	C	140	GLN
2	C	159	THR

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Mol	Chain	Res	Type
2	C	160	ASP
2	C	162	ASN
2	C	164	GLN
2	C	166	ILE
2	C	168	GLU
2	C	169	PRO
2	C	170	GLU
2	C	173	ILE
2	C	174	THR
2	C	175	SER
2	C	183	SER
2	C	214	THR
2	C	215	LYS
2	C	242	GLN
2	C	243	THR
2	C	248	ARG
2	C	261	LYS
2	C	262	SER
2	C	286	VAL
2	C	287	THR
2	C	289	SER
2	C	301	THR
2	C	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1398	HIS
1	B	1496	GLN
1	B	1509	GLN
1	B	1594	HIS
1	B	1687	HIS
1	B	1760	ASN
1	B	1782	HIS
1	B	1807	GLN
1	B	1898	ASN
1	B	1941	GLN
1	B	1958	HIS
1	B	1970	GLN
1	B	2028	HIS
1	B	2082	GLN
1	B	2093	ASN

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Mol	Chain	Res	Type
1	B	2154	GLN
1	B	2161	GLN
1	B	2167	GLN
1	B	2189	HIS
1	B	2233	ASN
1	B	2262	ASN
1	B	2277	HIS
1	B	2385	ASN
1	B	2395	ASN
1	B	2401	HIS
1	B	2428	ASN
1	B	2502	ASN
2	D	22	HIS
2	D	30	HIS
2	D	39	GLN
2	D	40	HIS
2	D	41	GLN
2	D	63	GLN
2	D	74	ASN
2	D	85	ASN
2	D	94	HIS
2	D	118	ASN
2	D	128	ASN
2	D	132	ASN
2	D	137	HIS
2	D	140	GLN
2	D	153	HIS
2	D	161	HIS
2	D	311	HIS
2	D	312	GLN
1	A	1398	HIS
1	A	1496	GLN
1	A	1594	HIS
1	A	1627	GLN
1	A	1670	HIS
1	A	1687	HIS
1	A	1744	HIS
1	A	1760	ASN
1	A	1898	ASN
1	A	1941	GLN
1	A	1958	HIS
1	A	1970	GLN

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Mol	Chain	Res	Type
1	A	2028	HIS
1	A	2082	GLN
1	A	2093	ASN
1	A	2154	GLN
1	A	2161	GLN
1	A	2167	GLN
1	A	2189	HIS
1	A	2262	ASN
1	A	2292	ASN
1	A	2385	ASN
1	A	2395	ASN
1	A	2401	HIS
1	A	2428	ASN
1	A	2502	ASN
2	C	30	HIS
2	C	39	GLN
2	C	40	HIS
2	C	41	GLN
2	C	63	GLN
2	C	74	ASN
2	C	85	ASN
2	C	94	HIS
2	C	118	ASN
2	C	128	ASN
2	C	137	HIS
2	C	140	GLN
2	C	153	HIS
2	C	161	HIS
2	C	311	HIS
2	C	312	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)

2 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	$\#\|Z\| > 2$
3	P2X	B	2601	-	23,26,26	1.15	2 (8%)	22,39,39	2.74	10 (45%)
3	P2X	A	2601	-	23,26,26	1.13	2 (8%)	22,39,39	2.72	11 (50%)

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
3	P2X	B	2601	-	-	1/4/8/8	0/4/4/4
3	P2X	A	2601	-	-	2/4/8/8	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2601	P2X	N3-N2	2.72	1.40	1.37
3	A	2601	P2X	N3-N2	2.62	1.40	1.37
3	B	2601	P2X	C21-C23	2.59	1.42	1.36
3	A	2601	P2X	C21-C23	2.36	1.41	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2601	P2X	C16-C12-C9	-6.76	119.47	129.32
3	A	2601	P2X	C16-C12-C9	-6.06	120.48	129.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2601	P2X	C9-N3-N2	5.71	109.73	105.17
3	B	2601	P2X	C9-N3-N2	5.61	109.65	105.17
3	B	2601	P2X	N4-C19-N6	-5.22	120.52	128.68
3	A	2601	P2X	N4-C19-N6	-4.68	121.36	128.68
3	A	2601	P2X	C16-C17-C18	4.36	110.08	106.27
3	B	2601	P2X	C16-C17-C18	3.41	109.25	106.27
3	B	2601	P2X	C21-C23-C22	2.91	123.49	120.15
3	A	2601	P2X	C21-C23-C22	2.75	123.31	120.15
3	A	2601	P2X	C12-N5-C18	2.75	110.18	104.45
3	A	2601	P2X	C12-C16-C17	-2.60	103.31	106.55
3	A	2601	P2X	C22-C20-C17	-2.51	117.74	120.45
3	A	2601	P2X	C23-C21-C18	-2.49	117.70	120.84
3	A	2601	P2X	C16-C17-C20	-2.42	127.83	136.53
3	B	2601	P2X	C12-N5-C18	2.34	109.33	104.45
3	B	2601	P2X	C16-C17-C20	-2.32	128.18	136.53
3	B	2601	P2X	C23-C21-C18	-2.24	118.02	120.84
3	B	2601	P2X	C22-C20-C17	-2.19	118.08	120.45
3	B	2601	P2X	C21-C18-N5	2.06	136.75	130.78
3	A	2601	P2X	C21-C18-N5	2.05	136.72	130.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2601	P2X	C13-C8-N2-N3
3	A	2601	P2X	C13-C8-N2-C11
3	A	2601	P2X	C13-C8-N2-N3

There are no ring outliers.

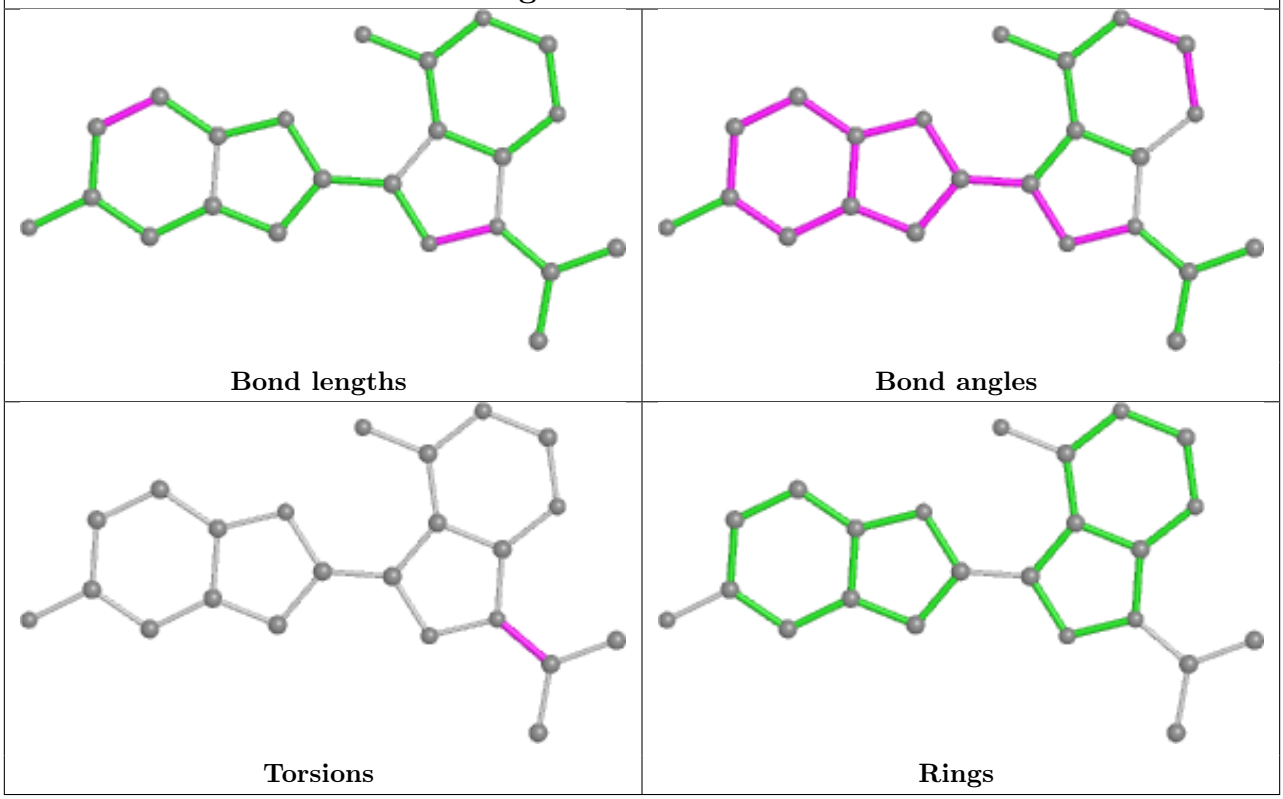
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2601	P2X	4	0
3	A	2601	P2X	3	0

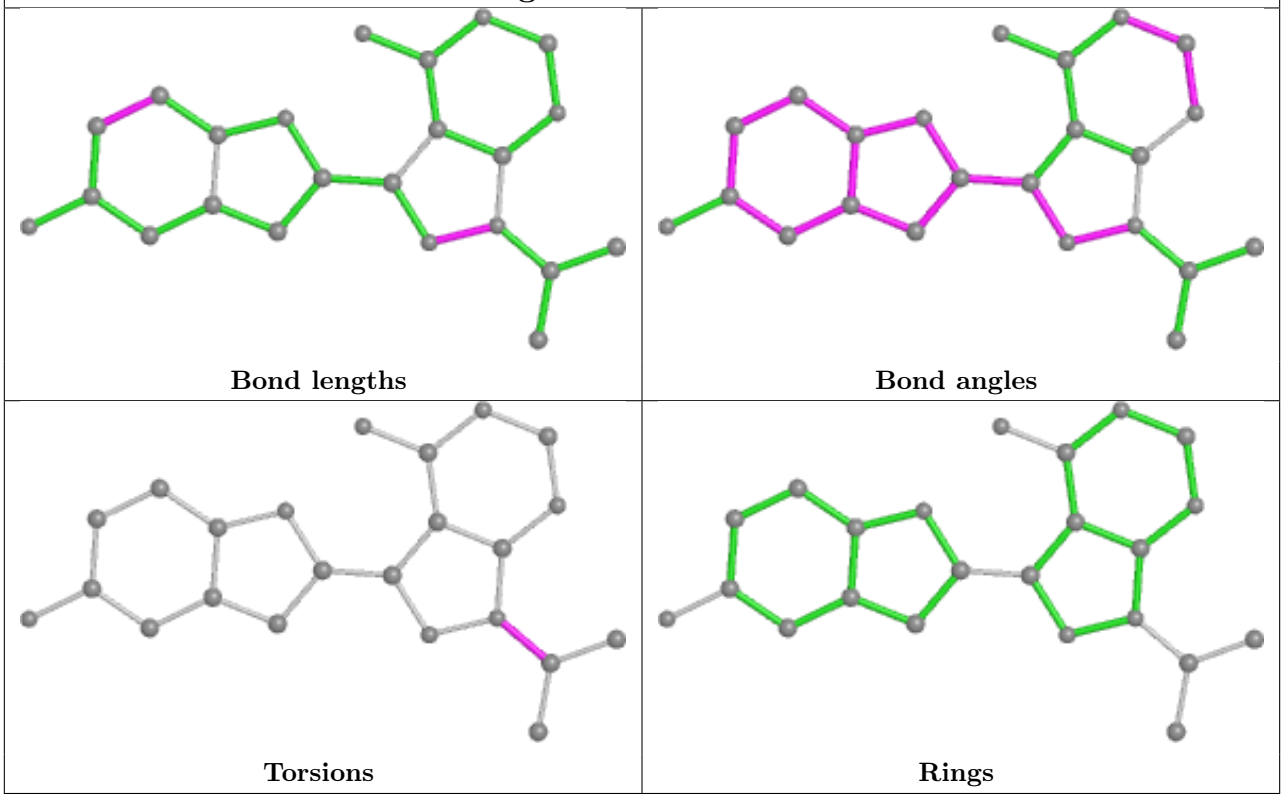
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand P2X B 2601



Ligand P2X A 2601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1054/1174 (89%)	0.30	78 (7%)	14	17	26, 62, 152, 178	0
1	B	1058/1174 (90%)	0.12	42 (3%)	38	36	23, 53, 128, 168	0
2	C	317/326 (97%)	0.20	12 (3%)	40	39	29, 61, 115, 156	0
2	D	317/326 (97%)	-0.05	3 (0%)	84	81	23, 40, 91, 142	0
All	All	2746/3000 (91%)	0.18	135 (4%)	29	29	23, 56, 140, 178	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2434	THR	6.0
1	A	2434	THR	5.8
1	B	1469	THR	5.5
1	A	2435	ASN	5.1
1	A	2044	VAL	4.9
1	A	1580	GLY	4.8
1	A	1619	TRP	4.8
2	C	205	ASP	4.8
1	B	1581	GLU	4.7
1	A	1582	SER	4.7
1	A	2436	THR	4.4
1	A	2048	PHE	4.4
1	A	1600	GLU	4.4
1	B	2435	ASN	4.3
1	B	1504	VAL	4.2
1	A	2038	TYR	4.2
1	A	2049	GLU	4.1
1	B	1499	GLU	4.0
1	A	1469	THR	4.0
1	B	1540	THR	4.0
1	A	1599	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	1587	TYR	3.9
1	A	1581	GLU	3.9
1	B	1580	GLY	3.8
1	A	1558	SER	3.8
1	B	2044	VAL	3.7
1	B	1577	ALA	3.7
1	A	1587	TYR	3.7
2	C	119	LEU	3.6
1	B	1446	GLN	3.6
1	A	1468	ASP	3.6
1	A	1554	GLN	3.6
1	A	2045	LYS	3.5
1	B	1582	SER	3.5
1	A	2055	HIS	3.4
2	C	202	GLY	3.4
1	B	2436	THR	3.4
1	B	1505	ASN	3.3
2	C	90	SER	3.3
1	A	1386	ARG	3.3
1	A	2101	TRP	3.2
1	B	1386	ARG	3.2
2	C	201	GLY	3.2
1	A	1584	SER	3.2
1	A	1603	ILE	3.2
1	A	1546	TYR	3.1
1	A	1606	LYS	3.1
1	A	2090	LYS	3.1
1	A	1388	ALA	3.1
1	B	1869	VAL	3.1
1	A	2433	ASP	3.1
1	B	1573	ALA	3.1
2	D	202	GLY	3.1
2	C	8	VAL	3.1
1	B	1872	ASP	3.0
2	C	10	SER	3.0
1	A	2042	ARG	3.0
1	A	1387	ALA	3.0
1	A	1628	ARG	3.0
1	A	1504	VAL	2.9
1	B	2433	ASP	2.9
1	A	1730	HIS	2.9
1	A	1867	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1578	MET	2.9
1	B	2040	GLY	2.9
1	A	1579	ALA	2.9
1	B	1385	GLU	2.9
1	B	2043	ASN	2.9
2	D	205	ASP	2.9
1	B	2045	LYS	2.8
1	B	2039	PHE	2.8
1	A	2104	TYR	2.8
1	B	1579	ALA	2.7
1	A	2097	LEU	2.7
2	C	204	GLY	2.7
1	B	1508	THR	2.6
1	A	1559	LEU	2.6
1	A	2432	MET	2.6
1	A	1604	GLN	2.6
1	A	1470	ASN	2.6
1	A	1578	MET	2.6
1	B	1572	ASP	2.6
1	B	1470	ASN	2.6
1	A	1556	LEU	2.6
1	A	1566	LYS	2.5
1	B	1468	ASP	2.5
1	A	1502	THR	2.5
1	B	1472	ASP	2.5
1	A	1555	ASP	2.4
1	B	1731	ALA	2.4
1	A	1627	GLN	2.4
1	A	2428	ASN	2.4
1	B	1496	GLN	2.4
2	C	207	VAL	2.4
1	A	2096	ASP	2.4
1	B	1868	LYS	2.4
1	B	1449	TRP	2.4
1	A	2040	GLY	2.4
1	B	2038	TYR	2.4
1	B	1871	GLU	2.4
1	A	2106	HIS	2.3
1	A	1385	GLU	2.3
1	A	2043	ASN	2.3
1	A	2118	LEU	2.3
2	C	9	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1505	ASN	2.3
1	A	1611	ARG	2.3
2	D	204	GLY	2.3
1	A	1573	ALA	2.3
1	A	1869	VAL	2.2
1	A	1534	CYS	2.2
1	A	2039	PHE	2.2
1	A	2034	ALA	2.2
2	C	265	PRO	2.2
1	A	1812	ASP	2.2
2	C	269	SER	2.2
1	A	1507	GLU	2.2
1	B	1507	GLU	2.2
1	A	2033	GLU	2.2
1	A	2041	GLU	2.2
1	A	1596	LEU	2.1
1	A	1549	VAL	2.1
1	A	1620	TRP	2.1
1	A	2051	LEU	2.1
1	A	2078	LEU	2.1
1	B	1473	ASP	2.1
1	B	1812	ASP	2.1
1	B	1467	MET	2.1
1	A	1586	ALA	2.1
1	A	1509	GLN	2.0
1	A	2050	VAL	2.0
1	A	1614	ILE	2.0
1	A	1871	GLU	2.0
1	A	1814	LYS	2.0
1	A	1585	ARG	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)

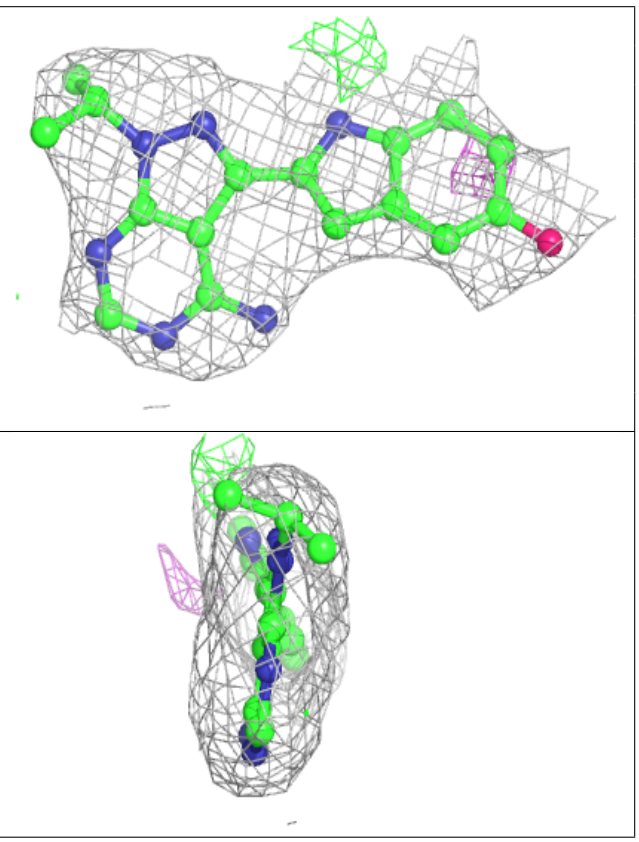
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P2X	B	2601	23/23	0.94	0.24	33,34,35,35	0
3	P2X	A	2601	23/23	0.95	0.21	37,37,38,38	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

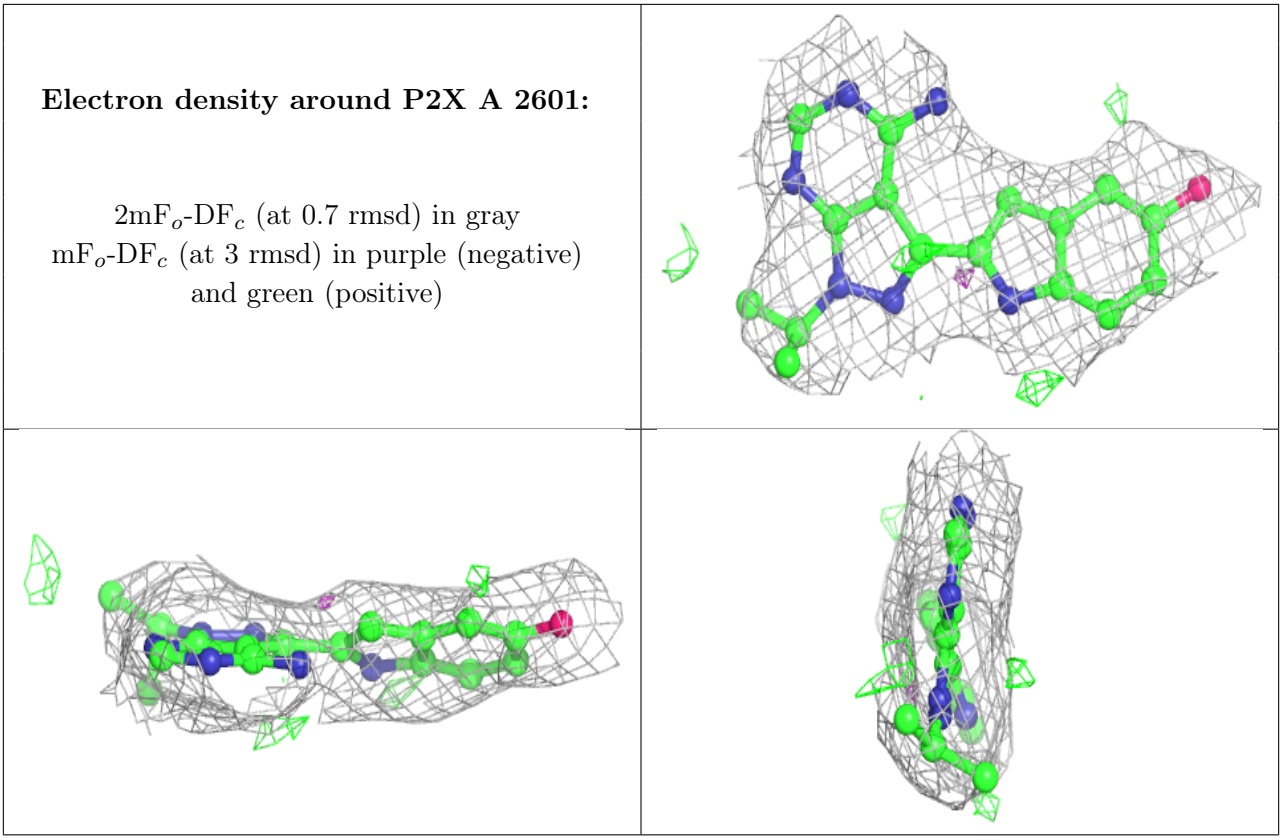
Electron density around P2X B 2601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P2X A 2601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.