



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:35 PM UTC

PDB ID : 3HWS / pdb_00003hws
Title : Crystal structure of nucleotide-bound hexameric ClpX
Authors : Glynn, S.E.; Martin, A.; Baker, T.A.; Sauer, R.T.
Deposited on : 2009-06-18
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

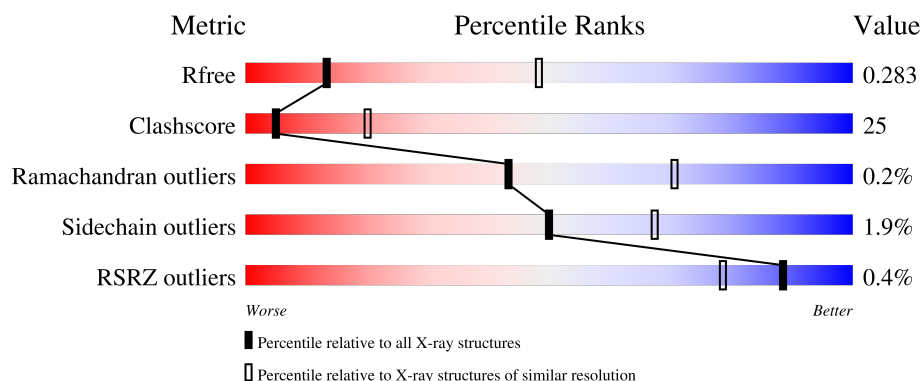
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	

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Mol	Chain	Length	Quality of chain
1	F	363	 49% 36% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	E	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14292 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 ATP-dependent Clp protease ATP-binding subunit clpX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2381	1514	396	465	6			
1	B	315	Total	C	N	O	S	0	0	0
			2388	1519	405	458	6			
1	C	307	Total	C	N	O	S	0	0	0
			2333	1485	392	450	6			
1	D	316	Total	C	N	O	S	0	0	0
			2333	1485	393	449	6			
1	E	313	Total	C	N	O	S	0	0	0
			2310	1468	384	452	6			
1	F	314	Total	C	N	O	S	0	0	0
			2367	1502	398	461	6			

There are 12 discrepancies between the modelled and reference sequences:

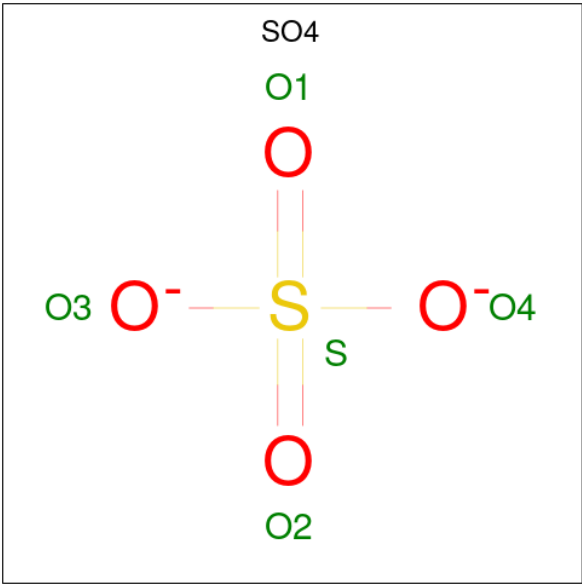
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLN	GLU	engineered mutation	UNP P0A6H1
A	408	GLU	LYS	engineered mutation	UNP P0A6H1
B	185	GLN	GLU	engineered mutation	UNP P0A6H1
B	408	GLU	LYS	engineered mutation	UNP P0A6H1
C	185	GLN	GLU	engineered mutation	UNP P0A6H1
C	408	GLU	LYS	engineered mutation	UNP P0A6H1
D	185	GLN	GLU	engineered mutation	UNP P0A6H1
D	408	GLU	LYS	engineered mutation	UNP P0A6H1
E	185	GLN	GLU	engineered mutation	UNP P0A6H1
E	408	GLU	LYS	engineered mutation	UNP P0A6H1
F	185	GLN	GLU	engineered mutation	UNP P0A6H1
F	408	GLU	LYS	engineered mutation	UNP P0A6H1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	1	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	2	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	3	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	1	0
			27	10	5	10	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

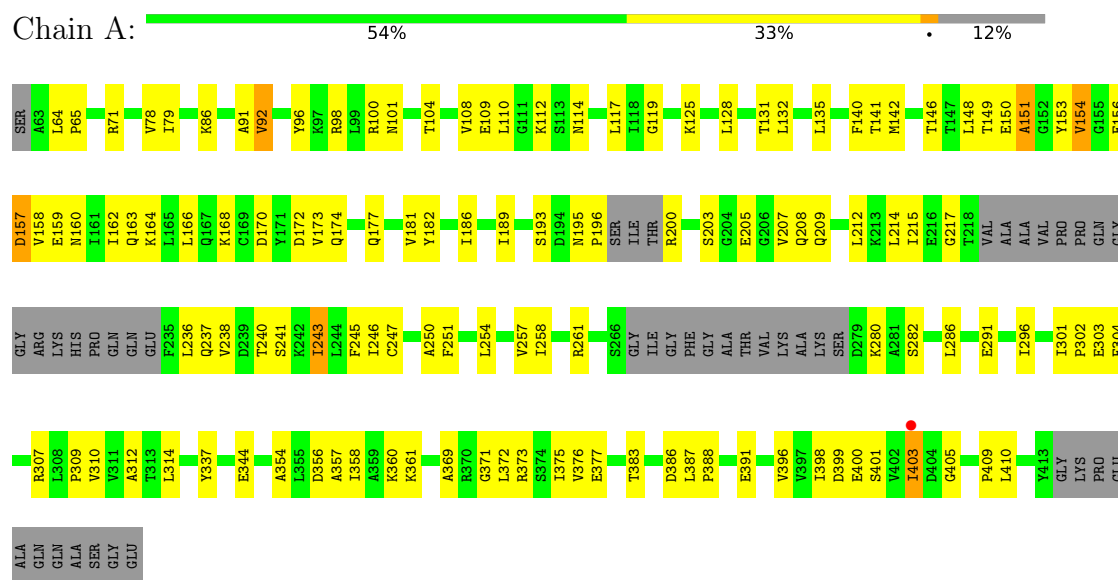
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0
5	C	3	Total O 3 3	0	0
5	E	1	Total O 1 1	0	0

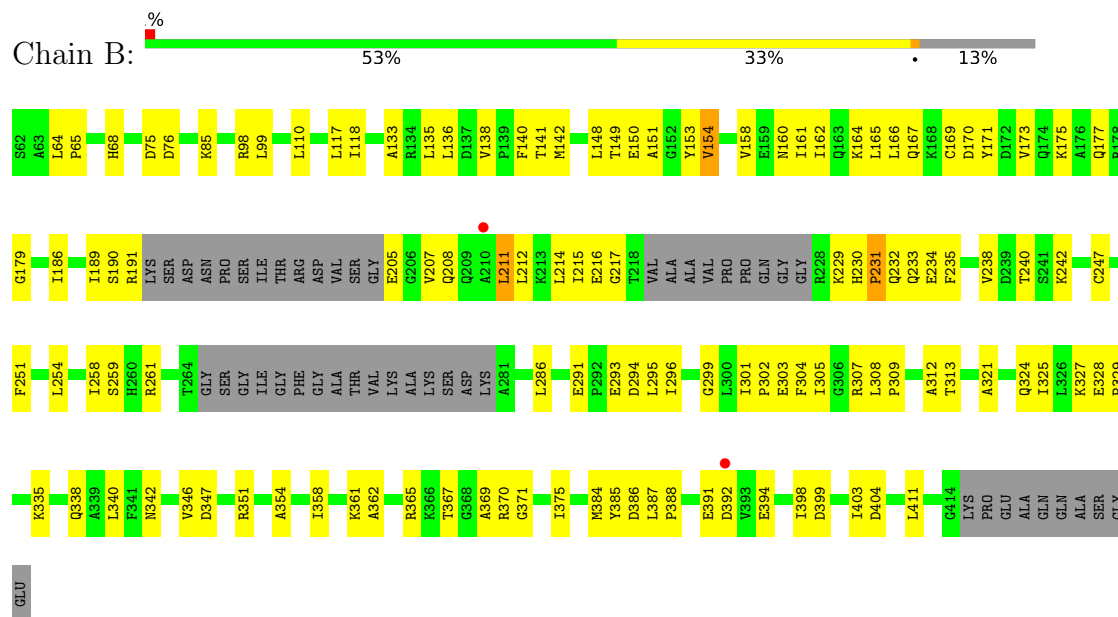
3 Residue-property plots

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

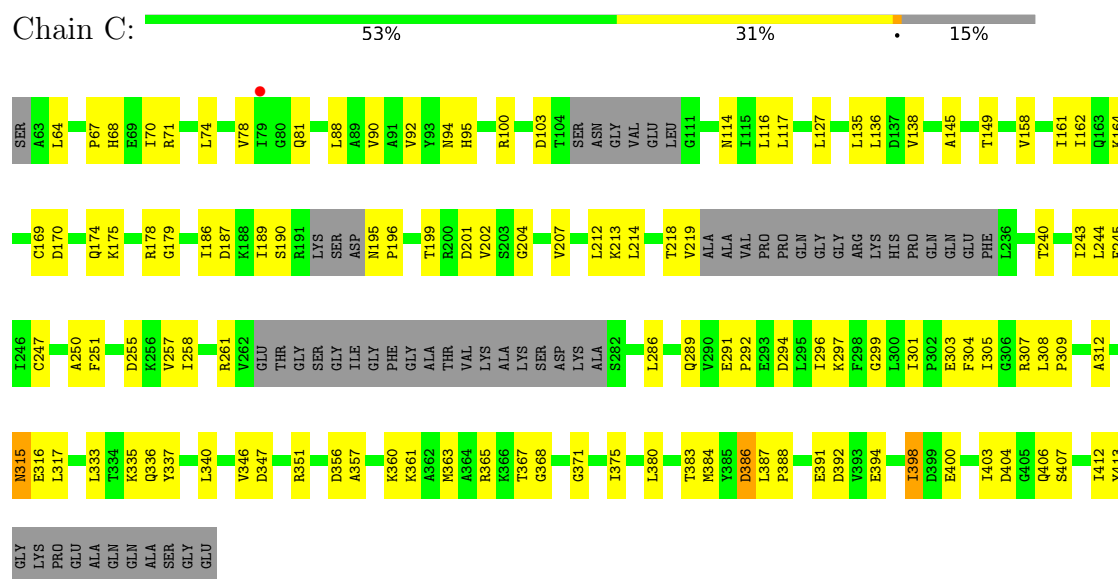
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



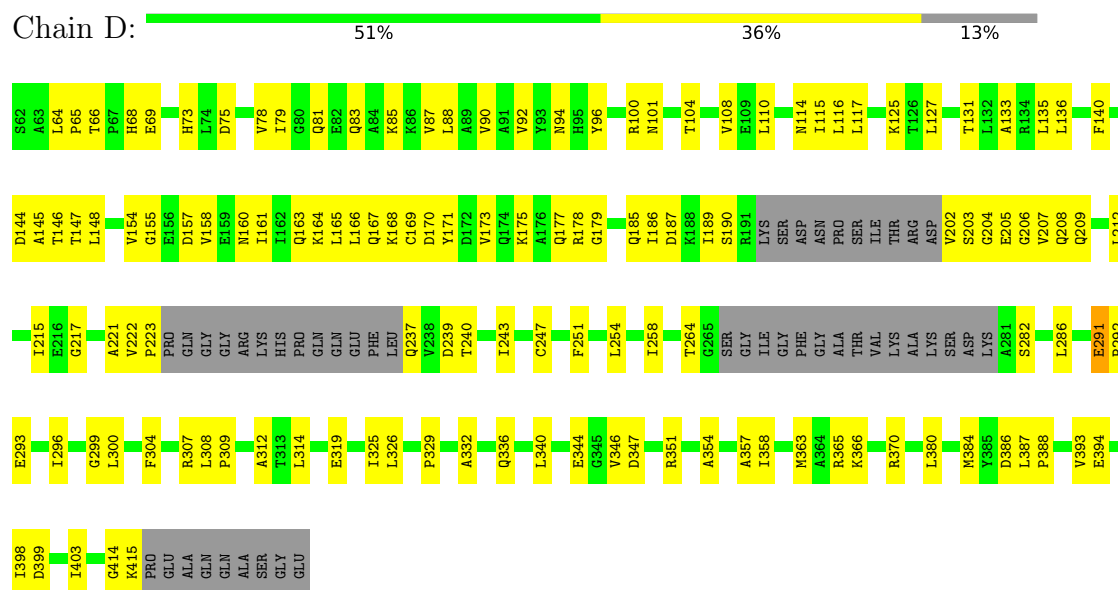
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



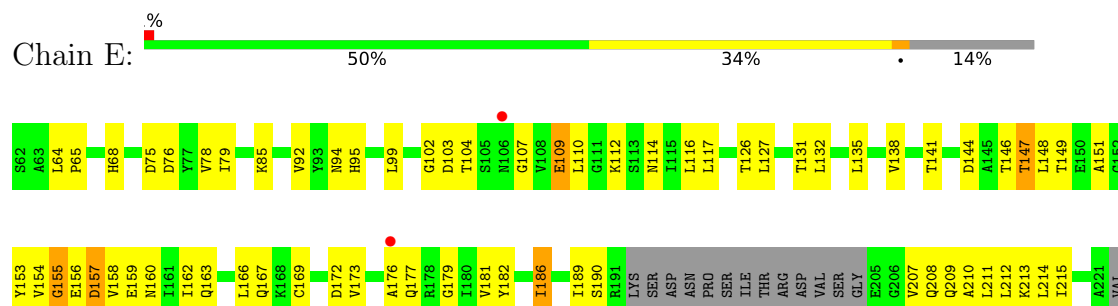
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX

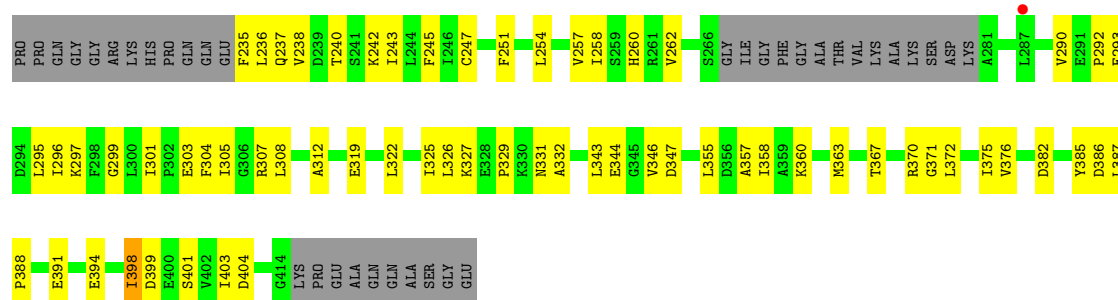


- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX



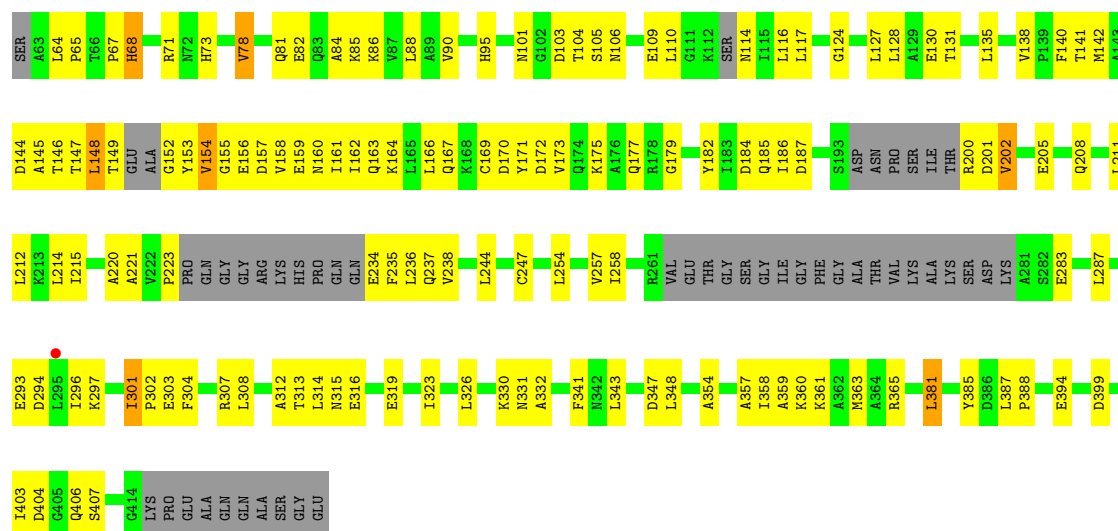
- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX





- Molecule 1: ATP-dependent Clp protease ATP-binding subunit clpX

Chain F: 49% 36% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.09Å 178.50Å 201.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.08 – 3.25 45.08 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (45.08-3.25) 99.5 (45.08-3.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.282 0.241 , 0.283	Depositor DCC
R_{free} test set	1573 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 113.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14292	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP, MG

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	0.31	0/2408	0.74	1/3265 (0.0%)
1	B	0.29	0/2416	0.72	0/3268
1	C	0.29	0/2359	0.71	0/3193
1	D	0.29	0/2360	0.73	2/3201 (0.1%)
1	E	0.35	0/2337	0.78	3/3172 (0.1%)
1	F	0.31	0/2393	0.70	0/3239
All	All	0.31	0/14273	0.73	6/19338 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	155	GLY	N-CA-C	-8.82	101.48	112.77
1	D	264	THR	CB-CA-C	-6.15	109.47	116.54
1	E	162	ILE	CB-CA-C	-5.92	102.67	112.26
1	A	151	ALA	N-CA-C	5.70	118.76	109.24
1	D	203	SER	N-CA-C	-5.42	105.77	112.38
1	E	147	THR	N-CA-C	-5.14	105.75	111.36

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	2381	0	2363	117	0
1	B	2388	0	2417	106	0
1	C	2333	0	2370	110	0
1	D	2333	0	2317	120	0
1	E	2310	0	2279	171	0
1	F	2367	0	2362	132	0
2	A	27	0	12	1	0
2	B	27	0	12	3	0
2	D	27	0	12	4	0
2	E	27	0	12	9	0
3	A	15	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	1	0
5	E	1	0	0	0	0
All	All	14292	0	14156	711	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 25.

All (711) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:THR:HG21	1:F:301:ILE:HG22	1.35	1.09
1:D:148:LEU:HD21	1:D:158:VAL:HG12	1.34	1.08
1:E:303:GLU:HG2	1:E:307:ARG:HH22	1.13	1.08
1:B:161:ILE:HA	1:B:164:LYS:HE2	1.35	1.07
1:A:150:GLU:HA	1:A:203:SER:CB	1.87	1.05
1:A:150:GLU:CA	1:A:203:SER:HB2	1.88	1.02
1:A:154:VAL:HA	1:A:157:ASP:HB3	1.41	1.01
1:A:151:ALA:HB3	1:A:154:VAL:HB	1.45	0.98
1:E:148:LEU:HA	1:E:154:VAL:HG21	1.41	0.98
1:E:177:GLN:HB3	1:E:238:VAL:HG21	1.45	0.98
1:F:152:GLY:O	1:F:154:VAL:HG23	1.64	0.97
1:A:150:GLU:HA	1:A:203:SER:HB2	0.99	0.96
1:B:186:ILE:HG13	1:B:247:CYS:HB3	1.49	0.92
1:D:186:ILE:HG13	1:D:247:CYS:HB3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LYS:HD2	1:B:233:GLN:HB3	1.52	0.91
1:F:158:VAL:HB	1:F:214:LEU:HD23	1.53	0.91
1:B:148:LEU:HB3	1:B:154:VAL:HG23	1.54	0.90
1:E:212:LEU:HD22	1:E:307:ARG:HH21	1.37	0.89
1:E:173:VAL:HG13	1:E:238:VAL:HB	1.54	0.89
1:E:151:ALA:O	1:E:154:VAL:HG12	1.73	0.88
1:D:144:ASP:O	1:D:147:THR:HG22	1.74	0.87
1:A:186:ILE:HG13	1:A:247:CYS:HB3	1.58	0.85
1:C:169:CYS:SG	1:C:175:LYS:HB2	2.17	0.85
1:A:148:LEU:O	1:A:154:VAL:HG11	1.77	0.85
1:E:154:VAL:O	1:E:158:VAL:HG23	1.76	0.83
1:A:357:ALA:HB1	1:A:403:ILE:HG23	1.58	0.83
1:D:155:GLY:O	1:D:158:VAL:HG22	1.78	0.83
1:E:148:LEU:CA	1:E:154:VAL:HG21	2.08	0.83
1:A:148:LEU:HA	1:A:154:VAL:HG21	1.61	0.83
1:A:280:LYS:CB	1:A:286:LEU:HD11	2.09	0.82
1:F:81:GLN:HE22	1:F:316:GLU:H	1.26	0.81
1:A:215:ILE:HG21	1:A:307:ARG:HB3	1.61	0.81
1:E:157:ASP:OD1	1:E:157:ASP:C	2.23	0.80
1:E:357:ALA:HB1	1:E:403:ILE:HG23	1.62	0.80
1:F:173:VAL:HG13	1:F:238:VAL:HG22	1.62	0.80
1:C:186:ILE:HG13	1:C:247:CYS:HB3	1.61	0.79
1:F:71:ARG:HG3	1:F:85:LYS:HB3	1.65	0.78
1:A:337:TYR:OH	1:A:377:GLU:HG2	1.82	0.78
1:E:144:ASP:O	1:E:148:LEU:HG	1.84	0.78
1:E:147:THR:CG2	1:F:301:ILE:HG22	2.14	0.77
1:A:114:ASN:ND2	1:A:215:ILE:HG23	2.01	0.76
1:E:157:ASP:O	1:E:160:ASN:HB3	1.85	0.76
1:C:315:ASN:HD22	1:C:315:ASN:H	1.31	0.75
1:E:127:LEU:HD22	2:E:603:ADP:H2'	1.67	0.75
1:A:149:THR:HA	1:A:207:VAL:HG21	1.68	0.75
1:A:157:ASP:O	1:A:160:ASN:HB3	1.86	0.75
1:E:303:GLU:HG2	1:E:307:ARG:NH2	1.98	0.75
1:B:233:GLN:CD	1:B:234:GLU:H	1.94	0.75
1:B:169:CYS:SG	1:B:175:LYS:HB2	2.26	0.75
1:A:214:LEU:HD22	1:A:240:THR:HG21	1.68	0.74
1:E:156:GLU:O	1:E:159:GLU:HG2	1.87	0.74
1:B:64:LEU:HD12	1:B:65:PRO:HD2	1.67	0.74
1:D:64:LEU:HD12	1:D:65:PRO:HD2	1.69	0.73
1:E:64:LEU:HD12	1:E:65:PRO:HD2	1.69	0.73
1:D:217:GLY:HA2	1:D:240:THR:OG1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ASP:O	1:A:403:ILE:HG12	1.89	0.73
1:B:229:LYS:HD2	1:B:233:GLN:CB	2.19	0.72
1:F:144:ASP:OD1	1:F:185:GLN:HG3	1.89	0.72
1:D:357:ALA:HB1	1:D:403:ILE:HG12	1.72	0.72
1:A:373:ARG:HD3	1:B:309:PRO:HB3	1.72	0.72
1:C:175:LYS:HD3	1:C:178:ARG:HH12	1.51	0.72
1:D:189:ILE:HD11	1:D:204:GLY:O	1.90	0.72
1:D:164:LYS:O	1:D:167:GLN:HG2	1.89	0.71
1:E:236:LEU:HD23	1:E:236:LEU:H	1.55	0.71
1:B:164:LYS:HG2	1:C:213:LYS:HD2	1.73	0.71
1:E:148:LEU:O	1:E:154:VAL:HG11	1.91	0.71
1:F:81:GLN:NE2	1:F:316:GLU:H	1.88	0.70
1:F:158:VAL:HB	1:F:214:LEU:CD2	2.21	0.70
1:F:211:LEU:O	1:F:214:LEU:HG	1.90	0.70
1:D:64:LEU:HB2	1:D:100:ARG:HH11	1.55	0.70
1:A:173:VAL:HG13	1:A:238:VAL:HG22	1.74	0.70
1:F:114:ASN:HB3	1:F:308:LEU:HD13	1.74	0.70
1:B:230:HIS:N	1:B:231:PRO:HD2	2.07	0.69
1:E:399:ASP:O	1:E:403:ILE:HG12	1.92	0.69
1:D:144:ASP:HB3	1:D:147:THR:HG22	1.73	0.69
1:F:162:ILE:O	1:F:166:LEU:HD12	1.92	0.69
1:B:212:LEU:CD1	1:B:304:PHE:HA	2.22	0.69
1:B:158:VAL:HG13	1:B:214:LEU:HD22	1.74	0.69
1:C:186:ILE:O	1:C:189:ILE:HG12	1.93	0.69
1:D:169:CYS:SG	1:D:175:LYS:HB2	2.32	0.69
1:B:205:GLU:HA	1:B:208:GLN:HG3	1.74	0.69
1:A:112:LYS:HE3	1:A:307:ARG:HE	1.56	0.68
1:B:160:ASN:O	1:B:164:LYS:HG3	1.93	0.68
1:B:150:GLU:O	1:C:196:PRO:HG3	1.92	0.68
1:A:151:ALA:HB2	1:A:153:TYR:CZ	2.29	0.68
1:A:212:LEU:CD1	1:A:307:ARG:HG3	2.22	0.68
1:B:211:LEU:O	1:B:215:ILE:HG12	1.93	0.68
1:A:149:THR:HA	1:A:207:VAL:CG2	2.24	0.68
1:D:66:THR:HG23	1:D:69:GLU:H	1.58	0.68
1:F:236:LEU:H	1:F:236:LEU:HD23	1.58	0.68
1:B:365:ARG:HG3	1:B:367:THR:HG23	1.76	0.68
1:B:212:LEU:HD11	1:B:303:GLU:O	1.93	0.67
1:C:158:VAL:HG11	1:C:214:LEU:HB2	1.75	0.67
1:C:400:GLU:HB2	1:C:406:GLN:HE21	1.59	0.67
1:B:138:VAL:HG13	1:B:179:GLY:HA2	1.77	0.67
1:A:217:GLY:HA2	1:A:240:THR:OG1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:THR:O	1:D:135:LEU:HG	1.94	0.67
1:B:149:THR:HA	1:B:207:VAL:HG21	1.76	0.67
1:D:116:LEU:HB2	1:D:308:LEU:HD23	1.75	0.67
1:A:243:ILE:HD11	1:A:245:PHE:CZ	2.29	0.67
1:A:212:LEU:HD11	1:A:307:ARG:HG3	1.77	0.67
1:E:388:PRO:HG2	1:F:67:PRO:HD2	1.77	0.67
1:C:161:ILE:HD11	1:C:214:LEU:HD22	1.76	0.66
1:A:282:SER:O	1:A:286:LEU:HD13	1.95	0.66
1:B:327:LYS:O	1:B:335:LYS:HE3	1.95	0.66
1:D:291:GLU:HG3	1:D:292:PRO:HD2	1.77	0.66
1:F:81:GLN:HE22	1:F:315:ASN:N	1.94	0.66
1:B:177:GLN:HG3	1:B:238:VAL:HG23	1.78	0.65
1:B:141:THR:HG22	1:B:165:LEU:HD13	1.78	0.65
1:F:357:ALA:HB1	1:F:403:ILE:HG23	1.79	0.65
1:F:399:ASP:O	1:F:403:ILE:HG12	1.96	0.65
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.79	0.65
1:D:64:LEU:HB2	1:D:100:ARG:NH1	2.11	0.65
1:C:81:GLN:HE22	1:C:316:GLU:H	1.44	0.65
1:D:319:GLU:CD	1:D:319:GLU:H	2.04	0.65
1:E:104:THR:HG21	1:E:109:GLU:N	2.11	0.65
1:C:158:VAL:O	1:C:161:ILE:HG12	1.97	0.65
1:E:104:THR:CG2	1:E:109:GLU:HB2	2.27	0.65
1:E:367:THR:HG21	1:E:371:GLY:HA3	1.79	0.65
1:E:370:ARG:HG2	2:E:603:ADP:H5'2	1.79	0.65
1:E:169:CYS:SG	1:E:176:ALA:HB2	2.37	0.65
1:A:117:LEU:HD23	1:A:312:ALA:HB3	1.78	0.64
1:E:149:THR:HA	1:E:207:VAL:HG11	1.78	0.64
1:B:291:GLU:HB2	1:B:293:GLU:HG2	1.79	0.64
1:E:301:ILE:HG13	1:E:304:PHE:H	1.61	0.64
1:E:147:THR:HG21	1:F:301:ILE:CG2	2.21	0.64
1:A:146:THR:O	1:A:149:THR:HG22	1.98	0.64
1:B:385:TYR:OH	1:C:71:ARG:HD3	1.98	0.64
1:A:151:ALA:O	1:A:154:VAL:HG12	1.97	0.63
1:C:367:THR:HB	1:D:291:GLU:HG2	1.78	0.63
1:F:211:LEU:O	1:F:215:ILE:HD12	1.98	0.63
1:C:392:ASP:HB2	1:C:412:ILE:O	1.98	0.63
1:C:335:LYS:HB3	1:D:108:VAL:HG11	1.79	0.63
1:C:138:VAL:HG12	1:C:179:GLY:HA2	1.81	0.63
1:E:212:LEU:HD22	1:E:307:ARG:NH2	2.11	0.63
1:E:212:LEU:HD21	1:E:304:PHE:HD1	1.63	0.63
1:E:92:VAL:HG21	1:E:132:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:CD2	1:E:307:ARG:HH21	2.11	0.63
1:C:357:ALA:O	1:C:361:LYS:HG2	1.99	0.62
1:E:258:ILE:HD11	1:E:290:VAL:HG23	1.81	0.62
1:E:303:GLU:CG	1:E:307:ARG:HH22	2.02	0.62
1:E:347:ASP:O	1:E:394:GLU:HG3	1.99	0.62
1:B:351:ARG:HD3	1:B:398:ILE:HG22	1.81	0.62
1:A:200:ARG:HD2	1:A:200:ARG:N	2.15	0.62
1:B:186:ILE:O	1:B:189:ILE:HG12	2.00	0.62
1:E:159:GLU:HB2	1:E:235:PHE:CZ	2.35	0.62
1:A:148:LEU:HA	1:A:154:VAL:CG2	2.30	0.62
1:B:148:LEU:HB3	1:B:154:VAL:CG2	2.28	0.62
1:B:214:LEU:HD12	1:B:240:THR:HG21	1.81	0.62
1:E:360:LYS:HA	1:E:363:MET:HE2	1.81	0.62
1:E:403:ILE:HG13	1:E:404:ASP:H	1.65	0.62
1:D:365:ARG:O	1:D:366:LYS:HG2	2.00	0.62
1:C:162:ILE:HD11	1:C:214:LEU:HD11	1.81	0.62
1:E:104:THR:HG22	1:E:109:GLU:HB2	1.82	0.62
1:B:362:ALA:O	1:B:365:ARG:HG2	1.99	0.61
1:A:157:ASP:C	1:A:157:ASP:OD1	2.43	0.61
1:E:186:ILE:HD12	1:E:247:CYS:HB3	1.80	0.61
1:E:370:ARG:HG2	2:E:603:ADP:C5'	2.31	0.61
1:B:138:VAL:CG1	1:B:179:GLY:HA2	2.30	0.61
1:D:144:ASP:HB3	1:D:147:THR:CG2	2.30	0.61
1:F:211:LEU:HD12	1:F:214:LEU:HD21	1.82	0.61
1:D:386:ASP:HB3	1:E:68:HIS:NE2	2.15	0.61
1:F:403:ILE:HG13	1:F:404:ASP:N	2.16	0.61
1:C:212:LEU:HD11	1:C:307:ARG:HG3	1.83	0.61
1:B:212:LEU:HD13	1:B:304:PHE:HA	1.82	0.61
1:A:114:ASN:HD21	1:A:215:ILE:HG23	1.66	0.60
1:E:331:ASN:CG	1:F:109:GLU:HG2	2.26	0.60
1:F:146:THR:C	1:F:148:LEU:HD23	2.26	0.60
1:F:147:THR:O	1:F:149:THR:HG23	2.01	0.60
1:B:340:LEU:HD21	1:C:94:ASN:ND2	2.16	0.60
1:F:301:ILE:HG12	1:F:304:PHE:HB2	1.83	0.60
1:C:258:ILE:HD13	1:C:286:LEU:O	2.02	0.60
1:E:166:LEU:HA	1:E:169:CYS:SG	2.41	0.60
1:D:158:VAL:O	1:D:161:ILE:HG12	2.02	0.59
1:C:258:ILE:HD11	1:C:289:GLN:C	2.27	0.59
1:C:161:ILE:HA	1:C:164:LYS:HE2	1.83	0.59
1:B:190:SER:HB2	1:B:299:GLY:HA3	1.85	0.59
1:D:399:ASP:O	1:D:403:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:LEU:N	1:F:65:PRO:HD3	2.17	0.59
1:E:296:ILE:CD1	1:E:305:ILE:HD12	2.32	0.59
1:F:173:VAL:O	1:F:177:GLN:HG3	2.03	0.59
1:D:81:GLN:O	1:D:85:LYS:HG3	2.02	0.59
1:A:156:GLU:O	1:A:159:GLU:HG2	2.02	0.59
1:B:384:MET:HE3	1:C:90:VAL:HG11	1.83	0.59
1:B:307:ARG:C	1:B:309:PRO:HD3	2.28	0.58
1:E:151:ALA:HB3	1:E:154:VAL:HB	1.86	0.58
1:B:76:ASP:O	1:B:329:PRO:HA	2.03	0.58
1:D:177:GLN:OE1	1:D:239:ASP:HB2	2.04	0.58
1:B:259:SER:OG	1:B:286:LEU:HD21	2.04	0.58
1:D:293:GLU:HA	1:D:296:ILE:HG22	1.85	0.58
1:A:200:ARG:HD3	1:B:191:ARG:NH1	2.18	0.58
1:B:117:LEU:HD23	1:B:312:ALA:HB3	1.85	0.58
1:B:217:GLY:HA2	1:B:240:THR:OG1	2.04	0.58
1:E:212:LEU:HD21	1:E:304:PHE:HA	1.85	0.58
1:E:211:LEU:O	1:E:215:ILE:HG13	2.03	0.58
1:E:292:PRO:O	1:E:296:ILE:HG12	2.03	0.58
1:E:212:LEU:HD13	1:E:307:ARG:NH2	2.19	0.58
1:A:154:VAL:O	1:A:158:VAL:HG23	2.03	0.58
1:C:175:LYS:HD3	1:C:178:ARG:NH1	2.18	0.58
1:F:73:HIS:CD2	1:F:135:LEU:HD13	2.38	0.58
1:E:213:LYS:HG2	1:E:214:LEU:N	2.19	0.57
1:F:186:ILE:HG21	1:F:247:CYS:HB3	1.85	0.57
1:E:79:ILE:H	2:E:603:ADP:HN62	1.52	0.57
1:A:71:ARG:HD3	1:F:385:TYR:OH	2.04	0.57
1:B:205:GLU:O	1:B:208:GLN:HB2	2.05	0.57
1:C:158:VAL:CG1	1:C:214:LEU:HB2	2.33	0.57
1:D:75:ASP:HA	1:D:85:LYS:NZ	2.20	0.57
1:C:365:ARG:HB2	1:C:367:THR:HG23	1.86	0.57
1:E:104:THR:HG21	1:E:110:LEU:N	2.19	0.57
1:F:138:VAL:HG13	1:F:179:GLY:HA2	1.86	0.57
1:A:356:ASP:O	1:A:360:LYS:HG3	2.05	0.57
1:C:212:LEU:HD21	1:C:303:GLU:HG2	1.86	0.57
1:E:398:ILE:HD12	1:E:401:SER:H	1.69	0.57
1:E:126:THR:HG22	1:E:182:TYR:CE2	2.39	0.56
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.87	0.56
1:D:370:ARG:CG	2:D:602:ADP:H5'1	2.35	0.56
1:E:153:TYR:HB3	1:F:202:VAL:HG11	1.85	0.56
1:C:292:PRO:O	1:C:296:ILE:HG13	2.06	0.56
1:E:210:ALA:HA	1:E:213:LYS:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD21	1:A:303:GLU:CG	2.35	0.56
1:D:114:ASN:HD21	1:D:215:ILE:HG23	1.69	0.56
1:E:186:ILE:O	1:E:189:ILE:HG12	2.05	0.56
1:E:209:GLN:HA	1:E:212:LEU:HD12	1.87	0.56
1:A:357:ALA:O	1:A:361:LYS:HG2	2.06	0.56
1:A:383:THR:OG1	1:A:409:PRO:HG3	2.06	0.56
1:E:367:THR:CG2	1:E:371:GLY:HA3	2.36	0.56
1:F:130:GLU:HG2	1:F:140:PHE:CE2	2.41	0.56
1:F:200:ARG:HG3	1:F:201:ASP:N	2.21	0.56
1:F:293:GLU:O	1:F:297:LYS:HG3	2.05	0.56
1:D:370:ARG:HG2	2:D:602:ADP:H5'1	1.88	0.55
1:D:319:GLU:HG3	1:D:363:MET:SD	2.47	0.55
1:E:177:GLN:HA	1:E:243:ILE:HG22	1.88	0.55
1:C:189:ILE:O	1:C:204:GLY:HA3	2.06	0.55
1:F:301:ILE:HG13	1:F:304:PHE:H	1.71	0.55
1:A:154:VAL:CA	1:A:157:ASP:HB3	2.25	0.55
1:E:189:ILE:HB	1:E:207:VAL:HG21	1.89	0.55
1:D:254:LEU:O	1:D:258:ILE:HG13	2.06	0.55
1:E:210:ALA:O	1:E:213:LYS:HG2	2.07	0.55
1:C:95:HIS:CD2	1:C:244:LEU:HD13	2.42	0.55
1:D:251:PHE:HB3	1:D:254:LEU:HB2	1.89	0.55
1:F:114:ASN:HD21	1:F:215:ILE:HG21	1.71	0.55
1:D:215:ILE:HG21	1:D:307:ARG:HB3	1.89	0.54
1:B:98:ARG:HG3	1:B:110:LEU:HD12	1.89	0.54
1:E:322:LEU:HD23	1:E:372:LEU:HD21	1.89	0.54
1:D:92:VAL:HG11	1:D:136:LEU:HD11	1.89	0.54
1:D:160:ASN:O	1:D:164:LYS:HG3	2.07	0.54
1:A:391:GLU:N	1:A:391:GLU:CD	2.66	0.54
1:A:307:ARG:O	1:A:309:PRO:HD3	2.07	0.54
1:B:392:ASP:OD2	1:B:411:LEU:HG	2.07	0.54
1:D:148:LEU:HD21	1:D:158:VAL:CG1	2.23	0.54
1:E:293:GLU:CD	1:E:293:GLU:H	2.16	0.54
1:F:149:THR:C	1:F:157:ASP:CB	2.81	0.54
1:F:387:LEU:HB3	1:F:388:PRO:HD3	1.89	0.54
1:A:151:ALA:HB1	1:A:153:TYR:CD1	2.42	0.54
1:B:386:ASP:HA	1:C:68:HIS:CD2	2.43	0.54
1:E:243:ILE:HD11	1:E:245:PHE:CZ	2.43	0.54
1:D:307:ARG:C	1:D:309:PRO:HD3	2.33	0.54
1:F:138:VAL:CG1	1:F:179:GLY:HA2	2.37	0.54
1:A:98:ARG:HD2	1:A:110:LEU:CB	2.38	0.53
1:A:344:GLU:HG3	1:A:387:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ARG:HG3	1:D:398:ILE:HG22	1.90	0.53
1:E:148:LEU:HA	1:E:154:VAL:CG2	2.28	0.53
1:E:254:LEU:O	1:E:258:ILE:HG12	2.08	0.53
1:E:235:PHE:CE1	1:E:236:LEU:HD22	2.44	0.53
1:B:208:GLN:OE1	1:B:301:ILE:HG23	2.09	0.53
1:F:169:CYS:SG	1:F:175:LYS:HB2	2.48	0.53
1:C:392:ASP:HB3	1:C:413:TYR:CD2	2.43	0.53
1:E:358:ILE:HD13	1:E:376:VAL:HG22	1.90	0.53
1:A:140:PHE:CE2	1:A:142:MET:HG3	2.44	0.53
1:E:104:THR:HG21	1:E:109:GLU:H	1.72	0.53
1:F:145:ALA:HB3	1:F:185:GLN:HB2	1.90	0.53
1:D:157:ASP:OD1	1:D:157:ASP:C	2.52	0.53
1:F:220:ALA:HA	1:F:237:GLN:OE1	2.09	0.53
1:A:104:THR:CB	1:A:108:VAL:HB	2.40	0.52
1:A:154:VAL:O	1:A:158:VAL:N	2.42	0.52
1:A:172:ASP:OD1	1:A:174:GLN:HG2	2.09	0.52
1:C:214:LEU:O	1:C:240:THR:OG1	2.26	0.52
1:D:144:ASP:OD2	1:D:146:THR:OG1	2.27	0.52
1:E:104:THR:HG21	1:E:109:GLU:CA	2.38	0.52
1:E:331:ASN:OD1	1:F:109:GLU:HG2	2.09	0.52
1:F:116:LEU:HD12	1:F:247:CYS:O	2.09	0.52
1:D:354:ALA:O	1:D:358:ILE:HG13	2.10	0.52
1:A:212:LEU:HD21	1:A:303:GLU:HG3	1.92	0.52
1:E:104:THR:HG21	1:E:110:LEU:H	1.74	0.52
1:E:208:GLN:O	1:E:212:LEU:HG	2.10	0.52
1:F:234:GLU:HG2	1:F:235:PHE:CD2	2.44	0.52
1:C:161:ILE:HD11	1:C:214:LEU:CD2	2.39	0.52
1:A:109:GLU:HG3	1:F:330:LYS:O	2.10	0.52
1:E:95:HIS:NE2	1:E:99:LEU:HD11	2.24	0.52
1:A:254:LEU:O	1:A:257:VAL:HG12	2.10	0.52
1:B:154:VAL:HG21	1:B:207:VAL:HG22	1.91	0.52
1:B:386:ASP:HB3	1:C:68:HIS:NE2	2.25	0.52
1:C:255:ASP:O	1:C:258:ILE:HG22	2.10	0.52
1:D:145:ALA:HB3	1:D:185:GLN:O	2.08	0.52
1:D:293:GLU:O	1:D:296:ILE:HG22	2.09	0.52
1:A:358:ILE:HD13	1:A:376:VAL:HG22	1.91	0.52
1:B:232:GLN:O	1:B:233:GLN:HG3	2.09	0.52
1:C:406:GLN:HG3	1:C:407:SER:N	2.25	0.52
1:D:96:TYR:CE1	1:D:136:LEU:HD13	2.45	0.52
1:C:404:ASP:HB3	1:C:406:GLN:HG2	1.91	0.52
1:D:127:LEU:HD22	2:D:602:ADP:H2'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:CA	1:A:207:VAL:HG21	2.39	0.52
1:E:102:GLY:O	1:E:103:ASP:C	2.52	0.52
1:E:138:VAL:CG1	1:E:179:GLY:HA2	2.39	0.52
1:E:148:LEU:HB3	1:E:154:VAL:HG21	1.92	0.52
1:F:110:LEU:HD12	1:F:110:LEU:N	2.25	0.52
1:D:282:SER:O	1:D:286:LEU:HG	2.10	0.52
1:E:138:VAL:HG13	1:E:179:GLY:HA2	1.92	0.52
1:F:177:GLN:HG2	1:F:238:VAL:HG13	1.90	0.51
1:F:214:LEU:C	1:F:214:LEU:HD12	2.35	0.51
1:F:319:GLU:O	1:F:323:ILE:HG13	2.10	0.51
1:B:167:GLN:NE2	1:C:218:THR:HG22	2.25	0.51
1:C:291:GLU:CG	1:C:292:PRO:HD2	2.39	0.51
1:C:351:ARG:HG3	1:C:398:ILE:HG22	1.92	0.51
1:D:387:LEU:HB3	1:D:388:PRO:HD3	1.91	0.51
1:B:135:LEU:HD12	1:B:136:LEU:HG	1.91	0.51
1:E:388:PRO:HG2	1:F:67:PRO:CD	2.39	0.51
1:A:193:SER:O	1:A:196:PRO:HD3	2.10	0.51
1:E:403:ILE:HG13	1:E:404:ASP:N	2.23	0.51
1:A:91:ALA:HB2	1:A:310:VAL:HG11	1.91	0.51
1:D:205:GLU:O	1:D:208:GLN:HB2	2.11	0.51
1:D:344:GLU:OE2	1:D:388:PRO:HG3	2.11	0.51
1:E:79:ILE:N	2:E:603:ADP:HN62	2.08	0.51
1:E:144:ASP:OD2	1:F:302:PRO:HD3	2.11	0.51
1:E:325:ILE:HG23	2:E:603:ADP:N3	2.26	0.51
1:A:78:VAL:HG21	1:A:128:LEU:HD23	1.93	0.51
1:C:240:THR:O	1:C:243:ILE:HG12	2.10	0.51
1:E:148:LEU:CB	1:E:154:VAL:HG21	2.40	0.51
1:B:399:ASP:O	1:B:403:ILE:HG22	2.11	0.51
1:E:212:LEU:HD11	1:E:301:ILE:HD11	1.93	0.51
1:E:251:PHE:HB3	1:E:254:LEU:HB3	1.92	0.51
1:C:398:ILE:HG13	1:C:400:GLU:HG2	1.92	0.51
1:D:104:THR:HG22	1:D:110:LEU:HB3	1.92	0.51
1:E:212:LEU:CD2	1:E:304:PHE:HD1	2.22	0.51
1:F:81:GLN:HE22	1:F:316:GLU:N	2.02	0.51
1:F:144:ASP:O	1:F:147:THR:HG22	2.10	0.51
1:B:387:LEU:HB3	1:B:388:PRO:HD3	1.91	0.50
1:A:101:ASN:HD22	1:F:343:LEU:HD22	1.76	0.50
1:A:209:GLN:O	1:A:212:LEU:HB3	2.11	0.50
1:B:177:GLN:HB3	1:B:242:LYS:HB2	1.92	0.50
1:C:336:GLN:O	1:C:340:LEU:HD13	2.11	0.50
1:E:189:ILE:HD12	1:E:207:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:LEU:HD23	1:F:313:THR:HB	1.94	0.50
1:E:160:ASN:OD1	1:E:160:ASN:O	2.30	0.50
1:A:108:VAL:HG12	1:A:109:GLU:N	2.26	0.50
1:E:79:ILE:H	2:E:603:ADP:N6	2.09	0.50
1:F:186:ILE:HG13	1:F:187:ASP:N	2.25	0.50
1:D:75:ASP:HA	1:D:85:LYS:HZ3	1.75	0.50
1:F:152:GLY:O	1:F:154:VAL:CG2	2.49	0.50
1:C:307:ARG:O	1:C:309:PRO:HD3	2.12	0.50
1:D:296:ILE:HD12	1:D:300:LEU:O	2.12	0.50
1:E:258:ILE:O	1:E:262:VAL:HG22	2.11	0.50
1:F:403:ILE:HG13	1:F:404:ASP:H	1.75	0.50
1:E:99:LEU:HD13	1:E:242:LYS:HE3	1.93	0.50
1:F:155:GLY:O	1:F:158:VAL:HG22	2.11	0.50
1:F:360:LYS:HA	1:F:363:MET:HE2	1.94	0.50
1:D:187:ASP:OD1	1:D:187:ASP:N	2.45	0.49
1:D:307:ARG:O	1:D:309:PRO:HD3	2.12	0.49
1:E:343:LEU:HD22	1:F:101:ASN:HD22	1.78	0.49
1:F:160:ASN:O	1:F:164:LYS:HG3	2.12	0.49
1:A:96:TYR:O	1:A:100:ARG:HG3	2.12	0.49
1:F:184:ASP:C	1:F:185:GLN:HG2	2.37	0.49
1:F:354:ALA:O	1:F:358:ILE:HG13	2.11	0.49
1:B:232:GLN:C	1:B:233:GLN:HG3	2.37	0.49
1:B:258:ILE:O	1:B:261:ARG:HG2	2.12	0.49
1:E:257:VAL:HA	1:E:260:HIS:HD2	1.77	0.49
1:A:141:THR:CG2	1:A:181:VAL:HG22	2.43	0.49
1:A:148:LEU:O	1:A:154:VAL:HG21	2.13	0.49
1:E:370:ARG:HD3	2:E:603:ADP:H4'	1.95	0.49
1:B:170:ASP:O	1:B:171:TYR:HB2	2.12	0.49
1:C:199:THR:HG22	1:C:201:ASP:H	1.78	0.49
1:D:96:TYR:O	1:D:100:ARG:HG3	2.12	0.49
1:E:151:ALA:C	1:E:154:VAL:HG12	2.37	0.49
1:F:236:LEU:H	1:F:236:LEU:CD2	2.26	0.49
1:A:119:GLY:O	1:A:250:ALA:HA	2.12	0.49
1:E:296:ILE:HD13	1:E:305:ILE:HD12	1.93	0.49
1:F:81:GLN:HE22	1:F:315:ASN:H	1.60	0.49
1:C:386:ASP:HB3	1:D:68:HIS:NE2	2.27	0.49
1:E:99:LEU:HD22	1:E:242:LYS:HG3	1.94	0.49
1:F:301:ILE:HG12	1:F:304:PHE:CB	2.43	0.49
1:A:109:GLU:HG3	1:F:331:ASN:HA	1.94	0.48
1:C:315:ASN:HD22	1:C:315:ASN:N	2.03	0.48
1:D:64:LEU:CD1	1:D:65:PRO:HD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:GLN:OE1	1:E:301:ILE:HG12	2.12	0.48
1:F:301:ILE:CG1	1:F:304:PHE:HB2	2.42	0.48
1:D:222:VAL:N	1:D:223:PRO:CD	2.76	0.48
1:E:177:GLN:HB2	1:E:242:LYS:HD3	1.96	0.48
1:F:153:TYR:O	1:F:154:VAL:HB	2.12	0.48
1:F:221:ALA:O	1:F:223:PRO:HD3	2.13	0.48
1:E:95:HIS:O	1:E:99:LEU:HG	2.13	0.48
1:E:163:GLN:HA	1:E:166:LEU:HG	1.95	0.48
1:E:173:VAL:HG21	1:E:237:GLN:OE1	2.13	0.48
1:F:202:VAL:HA	1:F:205:GLU:HG3	1.95	0.48
1:C:243:ILE:HD11	1:C:245:PHE:CZ	2.47	0.48
1:D:212:LEU:C	1:D:212:LEU:HD23	2.38	0.48
1:C:117:LEU:HD23	1:C:312:ALA:HB3	1.95	0.48
1:D:169:CYS:O	1:D:170:ASP:HB2	2.14	0.48
1:E:212:LEU:HD13	1:E:307:ARG:HH21	1.79	0.48
1:D:164:LYS:NZ	1:E:209:GLN:HE22	2.10	0.48
1:D:251:PHE:HB3	1:D:254:LEU:CB	2.44	0.48
1:F:254:LEU:O	1:F:258:ILE:HG13	2.13	0.48
1:A:236:LEU:O	1:A:237:GLN:HG2	2.14	0.48
1:A:243:ILE:HD11	1:A:245:PHE:CE2	2.49	0.48
1:D:78:VAL:HG13	2:D:602:ADP:N6	2.29	0.48
1:C:400:GLU:HB2	1:C:406:GLN:NE2	2.28	0.48
1:A:307:ARG:C	1:A:309:PRO:HD3	2.38	0.48
1:B:361:LYS:NZ	1:B:403:ILE:HA	2.29	0.48
1:A:125:LYS:HG2	1:A:314:LEU:HD22	1.95	0.47
1:B:370:ARG:CG	2:B:601:ADP:H5'1	2.45	0.47
1:D:73:HIS:HB3	1:D:135:LEU:HD22	1.97	0.47
1:F:172:ASP:OD2	1:F:175:LYS:HG3	2.14	0.47
1:D:346:VAL:HG21	1:D:387:LEU:HD11	1.94	0.47
1:E:157:ASP:C	1:E:160:ASN:H	2.22	0.47
1:B:142:MET:SD	1:C:303:GLU:HB2	2.54	0.47
1:B:169:CYS:O	1:B:170:ASP:HB2	2.14	0.47
1:B:346:VAL:HG21	1:B:387:LEU:HD11	1.97	0.47
1:E:343:LEU:HD13	1:F:101:ASN:HD22	1.78	0.47
1:A:150:GLU:CB	1:B:191:ARG:HH22	2.27	0.47
1:D:202:VAL:C	1:D:204:GLY:N	2.71	0.47
1:F:163:GLN:O	1:F:167:GLN:HG2	2.14	0.47
1:F:212:LEU:HD21	1:F:303:GLU:HG2	1.97	0.47
1:F:220:ALA:HA	1:F:237:GLN:CD	2.39	0.47
1:C:296:ILE:HG12	1:C:305:ILE:HD12	1.97	0.47
1:D:169:CYS:SG	1:D:175:LYS:CB	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HD22	1:E:307:ARG:HE	1.80	0.47
1:E:214:LEU:O	1:E:240:THR:HB	2.15	0.47
1:F:78:VAL:HG23	1:F:127:LEU:HD23	1.96	0.47
1:B:347:ASP:O	1:B:394:GLU:HB2	2.15	0.47
1:C:149:THR:O	1:C:202:VAL:HB	2.15	0.47
1:C:190:SER:HB2	1:C:299:GLY:HA3	1.97	0.47
1:C:261:ARG:HD3	1:C:294:ASP:OD1	2.15	0.47
1:E:103:ASP:C	1:E:104:THR:HG23	2.40	0.47
1:A:387:LEU:HB3	1:A:388:PRO:HD3	1.96	0.47
1:E:116:LEU:HD13	1:E:308:LEU:HD23	1.97	0.47
1:A:151:ALA:HB3	1:A:154:VAL:CB	2.33	0.47
1:C:70:ILE:O	1:C:74:LEU:HG	2.15	0.47
1:D:144:ASP:O	1:D:147:THR:CG2	2.54	0.47
1:C:135:LEU:C	1:C:135:LEU:HD12	2.39	0.46
1:D:332:ALA:O	1:D:336:GLN:HG3	2.15	0.46
1:E:319:GLU:OE2	1:E:360:LYS:HE2	2.16	0.46
1:B:301:ILE:HG12	1:B:304:PHE:HB2	1.95	0.46
1:C:138:VAL:HG11	1:C:178:ARG:O	2.15	0.46
1:C:403:ILE:HG23	1:C:404:ASP:N	2.29	0.46
1:D:165:LEU:HD23	1:D:165:LEU:O	2.15	0.46
1:E:104:THR:CG2	1:E:110:LEU:N	2.79	0.46
1:F:161:ILE:HA	1:F:164:LYS:HE2	1.97	0.46
1:C:383:THR:O	1:C:387:LEU:HB2	2.14	0.46
1:E:190:SER:OG	1:E:299:GLY:HA3	2.15	0.46
1:F:86:LYS:O	1:F:90:VAL:HG23	2.14	0.46
1:A:160:ASN:HA	1:A:163:GLN:HG2	1.96	0.46
1:A:217:GLY:HA3	1:A:241:SER:OG	2.16	0.46
1:B:230:HIS:N	1:B:231:PRO:CD	2.77	0.46
1:C:317:LEU:HD21	1:C:368:GLY:HA2	1.98	0.46
1:D:90:VAL:HG12	1:D:94:ASN:ND2	2.29	0.46
1:D:114:ASN:H	1:D:309:PRO:HD2	1.79	0.46
1:D:148:LEU:CD2	1:D:158:VAL:HG12	2.25	0.46
1:D:166:LEU:HD22	1:D:171:TYR:HA	1.96	0.46
1:A:151:ALA:CB	1:A:153:TYR:CZ	2.97	0.46
1:C:403:ILE:CG2	1:C:404:ASP:N	2.78	0.46
1:E:163:GLN:O	1:E:167:GLN:HG3	2.16	0.46
1:E:370:ARG:HD3	1:E:370:ARG:HA	1.76	0.46
1:F:170:ASP:O	1:F:171:TYR:HB2	2.14	0.46
1:A:182:TYR:HA	1:A:246:ILE:O	2.16	0.46
1:B:162:ILE:HD11	1:B:240:THR:HG22	1.98	0.46
1:C:169:CYS:O	1:C:170:ASP:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:LEU:HD21	1:E:94:ASN:ND2	2.31	0.46
1:A:79:ILE:H	2:A:600:ADP:HN62	1.64	0.46
1:C:158:VAL:HG12	1:C:214:LEU:HD13	1.98	0.46
1:C:174:GLN:HE21	1:C:178:ARG:HH11	1.62	0.46
1:E:149:THR:HB	1:E:189:ILE:HG22	1.96	0.46
1:F:114:ASN:HD22	1:F:307:ARG:HG3	1.80	0.46
1:F:117:LEU:HD23	1:F:312:ALA:HB3	1.96	0.46
1:F:205:GLU:O	1:F:208:GLN:HG2	2.16	0.46
1:A:108:VAL:HG12	1:A:109:GLU:H	1.81	0.46
1:B:170:ASP:OD2	1:C:219:VAL:HG13	2.15	0.46
1:B:371:GLY:O	1:B:375:ILE:HG13	2.16	0.46
1:D:161:ILE:HA	1:D:164:LYS:HD2	1.98	0.46
1:E:177:GLN:O	1:E:242:LYS:HG2	2.16	0.46
1:E:212:LEU:CD2	1:E:304:PHE:HA	2.45	0.46
1:A:112:LYS:CE	1:A:307:ARG:HE	2.27	0.46
1:A:151:ALA:CB	1:A:153:TYR:CE1	2.99	0.46
1:A:166:LEU:HD11	1:A:238:VAL:HG21	1.98	0.45
1:A:401:SER:O	1:A:405:GLY:HA2	2.15	0.45
1:C:92:VAL:CG1	1:C:136:LEU:HD11	2.46	0.45
1:F:114:ASN:HB2	1:F:307:ARG:O	2.15	0.45
1:F:124:GLY:O	1:F:128:LEU:HG	2.16	0.45
1:F:258:ILE:HG12	1:F:294:ASP:OD2	2.16	0.45
1:B:151:ALA:O	1:B:154:VAL:HG12	2.16	0.45
1:E:157:ASP:OD1	1:E:157:ASP:O	2.33	0.45
1:F:359:ALA:O	1:F:363:MET:HG3	2.15	0.45
1:F:404:ASP:C	1:F:406:GLN:H	2.24	0.45
1:A:261:ARG:NH2	1:A:291:GLU:HG3	2.31	0.45
1:B:216:GLU:CD	1:B:307:ARG:HD2	2.41	0.45
1:C:257:VAL:HG13	1:C:297:LYS:HD3	1.99	0.45
1:C:307:ARG:C	1:C:309:PRO:HD3	2.41	0.45
1:D:73:HIS:HB3	1:D:135:LEU:CD2	2.47	0.45
1:B:338:GLN:O	1:B:342:ASN:HB2	2.17	0.45
1:C:149:THR:HA	1:C:207:VAL:HG21	1.98	0.45
1:F:73:HIS:HE1	1:F:131:THR:HG23	1.82	0.45
1:F:283:GLU:O	1:F:287:LEU:HD13	2.17	0.45
1:B:261:ARG:HD2	1:B:294:ASP:OD1	2.16	0.45
1:D:101:ASN:OD1	1:D:101:ASN:C	2.59	0.45
1:E:391:GLU:HG2	1:E:391:GLU:O	2.17	0.45
1:B:148:LEU:O	1:B:154:VAL:HB	2.16	0.45
1:B:205:GLU:HA	1:B:208:GLN:CG	2.42	0.45
1:C:78:VAL:HG22	1:C:127:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASN:HB2	1:C:307:ARG:O	2.16	0.45
1:C:404:ASP:C	1:C:406:GLN:N	2.74	0.45
1:E:371:GLY:O	1:E:375:ILE:HG13	2.17	0.45
1:D:190:SER:OG	1:D:299:GLY:C	2.60	0.45
1:E:114:ASN:ND2	1:E:215:ILE:HD13	2.31	0.45
1:E:212:LEU:HD21	1:E:304:PHE:CD1	2.46	0.45
1:F:156:GLU:HA	1:F:159:GLU:HG2	1.98	0.45
1:A:354:ALA:O	1:A:358:ILE:HG13	2.17	0.45
1:F:73:HIS:HB3	1:F:135:LEU:HD22	1.99	0.45
1:C:114:ASN:HB3	1:C:308:LEU:HD23	1.98	0.45
1:F:81:GLN:NE2	1:F:314:LEU:HB3	2.31	0.45
1:A:195:ASN:N	1:A:196:PRO:CD	2.80	0.45
1:B:354:ALA:O	1:B:358:ILE:HG13	2.17	0.45
1:D:66:THR:CG2	1:D:69:GLU:HB2	2.47	0.45
1:E:327:LYS:HD3	1:E:355:LEU:HD13	1.99	0.45
1:F:296:ILE:HD11	1:F:302:PRO:HA	1.97	0.45
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.82	0.44
1:B:347:ASP:HB3	1:B:394:GLU:HB2	1.98	0.44
1:C:145:ALA:HB1	1:C:189:ILE:CG2	2.47	0.44
1:C:317:LEU:HB2	1:C:363:MET:HG2	1.99	0.44
1:E:251:PHE:HB3	1:E:254:LEU:CB	2.47	0.44
1:F:152:GLY:O	1:F:153:TYR:C	2.60	0.44
1:B:135:LEU:HD12	1:B:135:LEU:C	2.42	0.44
1:B:173:VAL:HG13	1:B:238:VAL:HB	1.98	0.44
1:D:83:GLN:O	1:D:87:VAL:HG23	2.17	0.44
1:E:172:ASP:O	1:E:173:VAL:HB	2.17	0.44
1:B:133:ALA:CB	1:B:140:PHE:HB2	2.47	0.44
1:B:208:GLN:O	1:B:212:LEU:HB2	2.17	0.44
1:B:212:LEU:HD21	1:B:303:GLU:CG	2.48	0.44
1:E:104:THR:HG21	1:E:109:GLU:HB2	1.98	0.44
1:E:131:THR:O	1:E:135:LEU:HG	2.18	0.44
1:E:163:GLN:NE2	1:E:166:LEU:HD11	2.33	0.44
1:E:387:LEU:N	1:E:388:PRO:CD	2.80	0.44
1:F:71:ARG:NH2	1:F:82:GLU:OE1	2.50	0.44
1:F:254:LEU:HA	1:F:257:VAL:HG12	1.99	0.44
1:A:301:ILE:HG13	1:A:304:PHE:H	1.81	0.44
1:D:117:LEU:HD23	1:D:312:ALA:HB3	1.98	0.44
1:A:148:LEU:CA	1:A:154:VAL:HG21	2.39	0.44
1:A:151:ALA:HB1	1:A:153:TYR:CG	2.53	0.44
1:E:386:ASP:HB3	1:F:68:HIS:CE1	2.51	0.44
1:F:177:GLN:CG	1:F:238:VAL:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:SER:OG	1:D:299:GLY:HA3	2.17	0.44
1:E:114:ASN:HB2	1:E:307:ARG:O	2.17	0.44
1:D:79:ILE:HD12	1:D:325:ILE:HA	2.00	0.43
1:E:110:LEU:CB	1:E:112:LYS:HE2	2.48	0.43
1:E:391:GLU:CD	1:E:391:GLU:H	2.26	0.43
1:C:170:ASP:CG	1:C:170:ASP:O	2.60	0.43
1:C:317:LEU:CD2	1:C:368:GLY:HA2	2.49	0.43
1:C:356:ASP:O	1:C:360:LYS:HG3	2.17	0.43
1:B:365:ARG:HG3	1:B:367:THR:CG2	2.47	0.43
1:D:114:ASN:HB2	1:D:307:ARG:O	2.18	0.43
1:E:344:GLU:OE2	1:E:388:PRO:HG3	2.18	0.43
1:F:361:LYS:HD3	1:F:365:ARG:NH2	2.34	0.43
1:A:154:VAL:C	1:A:157:ASP:H	2.27	0.43
1:B:324:GLN:HG3	1:B:328:GLU:OE2	2.18	0.43
1:D:204:GLY:O	1:D:207:VAL:N	2.50	0.43
1:D:414:GLY:C	1:D:415:LYS:HG3	2.44	0.43
1:E:258:ILE:HD12	1:E:290:VAL:HA	2.00	0.43
1:A:254:LEU:O	1:A:258:ILE:HG13	2.19	0.43
1:B:296:ILE:HD12	1:B:302:PRO:HG3	2.01	0.43
1:C:64:LEU:HD22	1:C:100:ARG:HD2	2.00	0.43
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.83	0.43
1:C:136:LEU:HB3	1:C:138:VAL:HG23	2.00	0.43
1:D:222:VAL:CG1	1:D:223:PRO:HD3	2.49	0.43
1:D:357:ALA:HB1	1:D:403:ILE:CG1	2.42	0.43
1:D:393:VAL:CB	1:D:414:GLY:HA3	2.48	0.43
1:E:78:VAL:O	1:E:85:LYS:NZ	2.51	0.43
1:B:232:GLN:HB3	1:B:235:PHE:HB3	2.00	0.43
1:B:388:PRO:HG2	1:C:67:PRO:CD	2.49	0.43
1:C:195:ASN:HA	1:C:196:PRO:HD2	1.83	0.43
1:C:392:ASP:OD1	1:C:392:ASP:N	2.48	0.43
1:F:201:ASP:OD1	1:F:202:VAL:HG23	2.19	0.43
1:A:149:THR:N	1:A:207:VAL:HG21	2.33	0.43
1:D:88:LEU:HD23	1:D:115:ILE:HD13	2.01	0.43
1:D:175:LYS:HA	1:D:178:ARG:HD2	2.00	0.43
1:E:155:GLY:O	1:E:158:VAL:HB	2.19	0.43
1:E:295:LEU:HB2	1:E:305:ILE:HD13	2.00	0.43
1:F:404:ASP:C	1:F:406:GLN:N	2.76	0.43
1:A:86:LYS:HG3	1:F:385:TYR:CD1	2.54	0.43
1:D:326:LEU:O	1:D:332:ALA:HB1	2.18	0.43
1:D:386:ASP:HA	1:E:68:HIS:CD2	2.53	0.43
1:E:343:LEU:HD22	1:F:101:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:THR:HG23	1:F:185:GLN:HB3	2.01	0.43
1:A:186:ILE:O	1:A:189:ILE:HG12	2.19	0.43
1:C:367:THR:CB	1:D:291:GLU:HG2	2.47	0.43
1:D:167:GLN:CG	1:D:168:LYS:N	2.81	0.43
1:D:173:VAL:O	1:D:177:GLN:HG2	2.19	0.42
1:D:208:GLN:O	1:D:212:LEU:N	2.52	0.42
1:D:221:ALA:CB	1:D:223:PRO:HD2	2.49	0.42
1:F:156:GLU:O	1:F:159:GLU:HG2	2.19	0.42
1:F:95:HIS:NE2	1:F:244:LEU:HB2	2.34	0.42
1:F:142:MET:HG3	1:F:182:TYR:HD2	1.84	0.42
1:B:118:ILE:O	1:B:313:THR:HA	2.19	0.42
1:C:116:LEU:HD12	1:C:247:CYS:O	2.19	0.42
1:D:125:LYS:HG2	1:D:314:LEU:CD1	2.49	0.42
1:D:160:ASN:O	1:D:163:GLN:HB3	2.19	0.42
1:E:160:ASN:HA	1:E:163:GLN:HB3	2.01	0.42
1:F:184:ASP:OD1	1:F:185:GLN:N	2.52	0.42
1:F:406:GLN:HG3	1:F:407:SER:N	2.35	0.42
1:A:92:VAL:HG21	1:A:132:LEU:HD22	2.02	0.42
1:B:75:ASP:OD1	1:B:85:LYS:HE2	2.18	0.42
1:C:347:ASP:O	1:C:394:GLU:HB2	2.19	0.42
1:F:156:GLU:O	1:F:157:ASP:C	2.61	0.42
1:A:131:THR:O	1:A:135:LEU:HG	2.20	0.42
1:A:398:ILE:HG13	1:A:400:GLU:N	2.34	0.42
1:D:133:ALA:CB	1:D:140:PHE:HB2	2.49	0.42
1:E:154:VAL:O	1:E:154:VAL:HG22	2.20	0.42
1:E:154:VAL:O	1:E:158:VAL:N	2.52	0.42
1:F:186:ILE:HD13	1:F:247:CYS:HB3	2.02	0.42
1:A:163:GLN:HG3	1:A:164:LYS:N	2.35	0.42
1:B:235:PHE:O	1:B:238:VAL:HG12	2.18	0.42
1:A:86:LYS:HD2	1:F:381:LEU:CD1	2.50	0.42
1:B:99:LEU:HD22	1:B:242:LYS:HD2	2.01	0.42
1:B:361:LYS:HE3	1:B:361:LYS:HB2	1.89	0.42
1:C:391:GLU:N	1:C:391:GLU:CD	2.78	0.42
1:D:221:ALA:HB3	1:D:223:PRO:HD2	2.02	0.42
1:D:79:ILE:HD11	1:D:329:PRO:HD3	2.02	0.42
1:D:189:ILE:CD1	1:D:208:GLN:HG3	2.49	0.42
1:E:326:LEU:O	1:E:332:ALA:HB1	2.20	0.42
1:A:141:THR:HB	1:A:168:LYS:HE3	2.02	0.42
1:C:360:LYS:HA	1:C:363:MET:CE	2.50	0.42
1:D:179:GLY:O	1:D:243:ILE:HG23	2.20	0.42
1:E:151:ALA:O	1:E:154:VAL:CG1	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ILE:HG23	1:B:404:ASP:N	2.34	0.42
1:F:341:PHE:CD1	1:F:348:LEU:HD22	2.54	0.42
1:A:369:ALA:HA	1:A:372:LEU:HG	2.02	0.41
1:C:371:GLY:O	1:C:375:ILE:HG13	2.20	0.41
1:E:104:THR:OG1	1:E:107:GLY:N	2.53	0.41
1:E:114:ASN:HD21	1:E:215:ILE:HD13	1.84	0.41
1:F:154:VAL:HG12	1:F:154:VAL:O	2.20	0.41
1:A:162:ILE:O	1:A:166:LEU:HD13	2.20	0.41
1:C:135:LEU:HD12	1:C:136:LEU:N	2.34	0.41
1:D:66:THR:HG22	1:D:69:GLU:HB2	2.01	0.41
1:B:166:LEU:HD22	1:B:171:TYR:HA	2.01	0.41
1:C:360:LYS:HA	1:C:363:MET:HE3	2.02	0.41
1:D:189:ILE:HG12	1:D:208:GLN:HE21	1.86	0.41
1:A:205:GLU:C	1:A:205:GLU:CD	2.89	0.41
1:B:295:LEU:HB2	1:B:305:ILE:HD13	2.02	0.41
1:D:380:LEU:O	1:D:384:MET:HG3	2.20	0.41
1:F:105:SER:O	1:F:106:ASN:HB2	2.21	0.41
1:F:347:ASP:O	1:F:394:GLU:HB2	2.20	0.41
1:A:177:GLN:HA	1:A:243:ILE:HG22	2.02	0.41
1:A:391:GLU:O	1:A:391:GLU:HG2	2.20	0.41
1:C:199:THR:HG22	1:C:201:ASP:N	2.35	0.41
1:E:254:LEU:HA	1:E:257:VAL:HG12	2.02	0.41
1:A:208:GLN:O	1:A:212:LEU:HB2	2.20	0.41
1:C:346:VAL:HG21	1:C:387:LEU:HD11	2.03	0.41
1:D:173:VAL:HG13	1:D:237:GLN:O	2.21	0.41
1:A:371:GLY:O	1:A:375:ILE:HG13	2.21	0.41
1:D:300:LEU:HD22	1:D:304:PHE:HD2	1.85	0.41
1:E:76:ASP:O	1:E:329:PRO:HA	2.21	0.41
1:E:159:GLU:HB2	1:E:235:PHE:CE1	2.56	0.41
1:A:386:ASP:HB3	1:B:68:HIS:NE2	2.35	0.41
1:E:144:ASP:HB3	1:E:147:THR:HG23	2.02	0.41
1:E:173:VAL:HG21	1:E:237:GLN:HB3	2.03	0.41
1:E:382:ASP:O	1:E:385:TYR:HB3	2.21	0.41
1:F:146:THR:HG23	1:F:185:GLN:CB	2.51	0.41
1:A:151:ALA:HB2	1:A:153:TYR:CE1	2.56	0.41
1:A:251:PHE:HB3	1:A:254:LEU:CB	2.51	0.41
1:A:396:VAL:HB	1:A:410:LEU:HB3	2.03	0.41
1:B:207:VAL:HG12	1:B:211:LEU:HD22	2.03	0.41
1:B:212:LEU:HD21	1:B:303:GLU:HG3	2.03	0.41
1:B:301:ILE:HG13	1:B:304:PHE:H	1.84	0.41
1:B:369:ALA:HB3	2:B:601:ADP:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ARG:HG3	2:B:601:ADP:H5'1	2.02	0.41
1:C:380:LEU:O	1:C:384:MET:HG3	2.21	0.41
1:D:202:VAL:HG12	1:D:202:VAL:O	2.21	0.41
1:E:346:VAL:HG21	1:E:387:LEU:HD11	2.03	0.41
1:F:114:ASN:HB3	1:F:308:LEU:CD1	2.48	0.41
1:A:296:ILE:HD11	1:A:302:PRO:HA	2.03	0.41
1:C:250:ALA:O	5:C:803:HOH:O	2.22	0.41
1:C:391:GLU:O	1:C:391:GLU:HG2	2.21	0.41
1:E:75:ASP:HA	1:E:85:LYS:HZ3	1.86	0.41
1:E:146:THR:O	1:E:149:THR:HG22	2.21	0.41
1:E:173:VAL:CG1	1:E:238:VAL:HB	2.38	0.41
1:B:151:ALA:HB1	1:B:153:TYR:CE1	2.57	0.40
1:C:333:LEU:HD22	1:C:337:TYR:HE1	1.86	0.40
1:E:104:THR:OG1	1:E:107:GLY:CA	2.69	0.40
1:E:141:THR:CG2	1:E:181:VAL:HG22	2.51	0.40
1:F:153:TYR:O	1:F:154:VAL:CB	2.68	0.40
1:C:367:THR:CG2	1:D:291:GLU:HG2	2.51	0.40
1:D:116:LEU:HD12	1:D:247:CYS:O	2.21	0.40
1:D:254:LEU:HG	1:D:258:ILE:HD11	2.02	0.40
1:E:329:PRO:CG	2:E:603:ADP:H2	2.34	0.40
1:F:104:THR:O	1:F:105:SER:HB2	2.21	0.40
1:A:261:ARG:HH21	1:F:365:ARG:HB3	1.86	0.40
1:B:251:PHE:HB3	1:B:254:LEU:HB2	2.03	0.40
1:B:321:ALA:O	1:B:325:ILE:HG13	2.21	0.40
1:C:81:GLN:NE2	1:C:316:GLU:H	2.15	0.40
1:D:206:GLY:O	1:D:209:GLN:HB3	2.20	0.40
1:E:117:LEU:HD23	1:E:312:ALA:HB3	2.02	0.40
1:F:84:ALA:O	1:F:88:LEU:HD13	2.22	0.40
1:F:147:THR:C	1:F:148:LEU:HD23	2.46	0.40
1:F:326:LEU:O	1:F:332:ALA:HB1	2.22	0.40
1:A:149:THR:O	1:A:150:GLU:CB	2.70	0.40
1:C:187:ASP:HB3	1:C:251:PHE:CD2	2.56	0.40
1:E:322:LEU:HA	1:E:325:ILE:HD12	2.04	0.40
1:B:388:PRO:HG2	1:C:67:PRO:HD2	2.04	0.40
1:C:301:ILE:HG13	1:C:304:PHE:H	1.86	0.40
1:C:317:LEU:HD11	1:C:368:GLY:HA2	2.02	0.40
1:D:347:ASP:O	1:D:394:GLU:HB2	2.20	0.40
1:E:158:VAL:HG12	1:E:214:LEU:HD13	2.03	0.40
1:E:257:VAL:HG21	1:E:297:LYS:HB2	2.02	0.40
1:F:147:THR:O	1:F:148:LEU:C	2.64	0.40
1:F:187:ASP:N	1:F:187:ASP:OD1	2.54	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	312/363 (86%)	298 (96%)	14 (4%)	0	100	100
1	B	307/363 (85%)	298 (97%)	8 (3%)	1 (0%)	36	66
1	C	297/363 (82%)	290 (98%)	6 (2%)	1 (0%)	36	66
1	D	308/363 (85%)	301 (98%)	6 (2%)	1 (0%)	36	66
1	E	305/363 (84%)	297 (97%)	8 (3%)	0	100	100
1	F	302/363 (83%)	292 (97%)	9 (3%)	1 (0%)	36	66
All	All	1831/2178 (84%)	1776 (97%)	51 (3%)	4 (0%)	43	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	154	VAL
1	D	154	VAL
1	C	103	ASP
1	B	231	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/299 (82%)	238 (98%)	6 (2%)	42	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	250/299 (84%)	246 (98%)	4 (2%)	55	70
1	C	248/299 (83%)	244 (98%)	4 (2%)	55	70
1	D	235/299 (79%)	234 (100%)	1 (0%)	84	84
1	E	235/299 (79%)	231 (98%)	4 (2%)	53	69
1	F	246/299 (82%)	238 (97%)	8 (3%)	33	57
All	All	1458/1794 (81%)	1431 (98%)	27 (2%)	50	67

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	154	VAL
1	A	157	ASP
1	A	170	ASP
1	A	243	ILE
1	A	403	ILE
1	B	154	VAL
1	B	211	LEU
1	B	308	LEU
1	B	391	GLU
1	C	88	LEU
1	C	315	ASN
1	C	386	ASP
1	C	398	ILE
1	D	291	GLU
1	E	109	GLU
1	E	157	ASP
1	E	186	ILE
1	E	398	ILE
1	F	68	HIS
1	F	78	VAL
1	F	103	ASP
1	F	141	THR
1	F	148	LEU
1	F	202	VAL
1	F	301	ILE
1	F	381	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	101	ASN
1	A	114	ASN
1	B	95	HIS
1	B	209	GLN
1	C	101	ASN
1	C	174	GLN
1	C	315	ASN
1	C	406	GLN
1	D	73	HIS
1	D	94	ASN
1	D	185	GLN
1	D	209	GLN
1	D	336	GLN
1	E	160	ASN
1	E	209	GLN
1	E	260	HIS
1	F	73	HIS
1	F	81	GLN
1	F	101	ASN
1	F	114	ASN
1	F	260	HIS
1	F	324	GLN
1	F	406	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
3	SO4	C	704	-	4,4,4	0.24	0	6,6,6	0.08	0
2	ADP	B	601	-	28,29,29	1.58	5 (17%)	43,45,45	1.95	10 (23%)
3	SO4	A	701	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	705	-	4,4,4	0.25	0	6,6,6	0.09	0
2	ADP	A	600	-	28,29,29	1.60	5 (17%)	43,45,45	1.94	10 (23%)
3	SO4	A	700	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	B	708	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	B	709	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	C	703	-	4,4,4	0.23	0	6,6,6	0.08	0
2	ADP	E	603	-	28,29,29	1.58	5 (17%)	43,45,45	1.96	9 (20%)
3	SO4	F	500	-	4,4,4	0.23	0	6,6,6	0.14	0
3	SO4	B	702	-	4,4,4	0.25	0	6,6,6	0.06	0
2	ADP	D	602	-	28,29,29	1.57	5 (17%)	43,45,45	1.95	9 (20%)
3	SO4	C	500	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	706	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	710	-	4,4,4	1.05	0	6,6,6	1.39	1 (16%)
3	SO4	B	707	-	4,4,4	0.24	0	6,6,6	0.10	0

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
2	ADP	E	603	-	-	3/16/32/32	0/3/3/3
2	ADP	A	600	-	-	3/16/32/32	0/3/3/3
2	ADP	B	601	-	-	0/16/32/32	0/3/3/3
2	ADP	D	602	-	-	3/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	ADP	C5-C4	5.09	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	603	ADP	C5-C4	5.05	1.48	1.39
2	B	601	ADP	C5-C4	5.01	1.48	1.39
2	A	600	ADP	C5-C4	4.91	1.47	1.39
2	A	600	ADP	PA-O3A	3.23	1.63	1.59
2	B	601	ADP	C5-C6	2.98	1.49	1.41
2	B	601	ADP	C8-N7	2.98	1.37	1.31
2	E	603	ADP	C8-N7	2.97	1.37	1.31
2	D	602	ADP	C8-N7	2.91	1.37	1.31
2	A	600	ADP	C5-C6	2.91	1.49	1.41
2	D	602	ADP	C5-C6	2.91	1.49	1.41
2	E	603	ADP	C5-C6	2.91	1.49	1.41
2	A	600	ADP	C8-N7	2.83	1.37	1.31
2	B	601	ADP	PA-O3A	2.77	1.62	1.59
2	E	603	ADP	PA-O3A	2.76	1.62	1.59
2	D	602	ADP	PA-O3A	2.58	1.62	1.59
2	D	602	ADP	C5-N7	-2.54	1.34	1.39
2	E	603	ADP	C5-N7	-2.52	1.34	1.39
2	B	601	ADP	C5-N7	-2.51	1.34	1.39
2	A	600	ADP	C5-N7	-2.50	1.34	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5-C4-N3	-6.82	117.33	126.72
2	E	603	ADP	C5-C4-N3	-6.77	117.39	126.72
2	D	602	ADP	C5-C4-N3	-6.67	117.54	126.72
2	A	600	ADP	C5-C4-N3	-6.48	117.79	126.72
2	B	601	ADP	N3-C4-N9	4.95	135.59	127.17
2	E	603	ADP	N3-C4-N9	4.95	135.59	127.17
2	D	602	ADP	N3-C4-N9	4.92	135.54	127.17
2	A	600	ADP	N3-C4-N9	4.84	135.41	127.17
2	B	601	ADP	C2-N3-C4	4.04	121.69	111.83
2	D	602	ADP	C2-N3-C4	4.03	121.67	111.83
2	E	603	ADP	C2-N3-C4	3.98	121.55	111.83
2	A	600	ADP	C2-N3-C4	3.97	121.54	111.83
2	B	601	ADP	C4-C5-N7	-3.83	106.20	110.58
2	E	603	ADP	C4-C5-N7	-3.77	106.27	110.58
2	A	600	ADP	C4-C5-N7	-3.69	106.37	110.58
2	D	602	ADP	C4-C5-N7	-3.68	106.37	110.58
2	D	602	ADP	N3-C2-N1	-3.21	123.72	128.58
2	A	600	ADP	N3-C2-N1	-3.11	123.87	128.58
2	B	601	ADP	N3-C2-N1	-3.07	123.94	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	710	SO4	O4-S-O3	3.06	125.40	108.54
2	E	603	ADP	N3-C2-N1	-2.98	124.07	128.58
2	B	601	ADP	C5-N7-C8	2.91	108.02	103.45
2	A	600	ADP	C5-N7-C8	2.87	107.97	103.45
2	E	603	ADP	C5-N7-C8	2.82	107.88	103.45
2	D	602	ADP	C5-N7-C8	2.78	107.82	103.45
2	A	600	ADP	C2'-C3'-C4'	2.42	107.29	102.61
2	B	601	ADP	C2'-C3'-C4'	2.22	106.91	102.61
2	A	600	ADP	C4-N9-C8	2.20	108.05	105.74
2	A	600	ADP	N9-C8-N7	-2.20	110.81	113.94
2	D	602	ADP	C3'-C2'-C1'	2.20	105.62	101.46
2	B	601	ADP	C3'-C2'-C1'	2.18	105.58	101.46
2	E	603	ADP	C3'-C2'-C1'	2.18	105.58	101.46
2	D	602	ADP	C2'-C3'-C4'	2.15	106.76	102.61
2	A	600	ADP	C6-C5-N7	2.13	136.19	132.09
2	E	603	ADP	C2'-C3'-C4'	2.12	106.70	102.61
2	D	602	ADP	C6-C5-N7	2.07	136.08	132.09
2	B	601	ADP	N9-C8-N7	-2.05	111.03	113.94
2	B	601	ADP	C6-C5-N7	2.03	136.00	132.09
2	E	603	ADP	C6-C5-N7	2.03	136.00	132.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	ADP	C5'-O5'-PA-O1A
2	A	600	ADP	C5'-O5'-PA-O2A
2	A	600	ADP	C5'-O5'-PA-O3A
2	D	602	ADP	C5'-O5'-PA-O1A
2	D	602	ADP	C5'-O5'-PA-O2A
2	D	602	ADP	C5'-O5'-PA-O3A
2	E	603	ADP	C5'-O5'-PA-O1A
2	E	603	ADP	C5'-O5'-PA-O2A
2	E	603	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

4 monomers are involved in 17 short contacts:

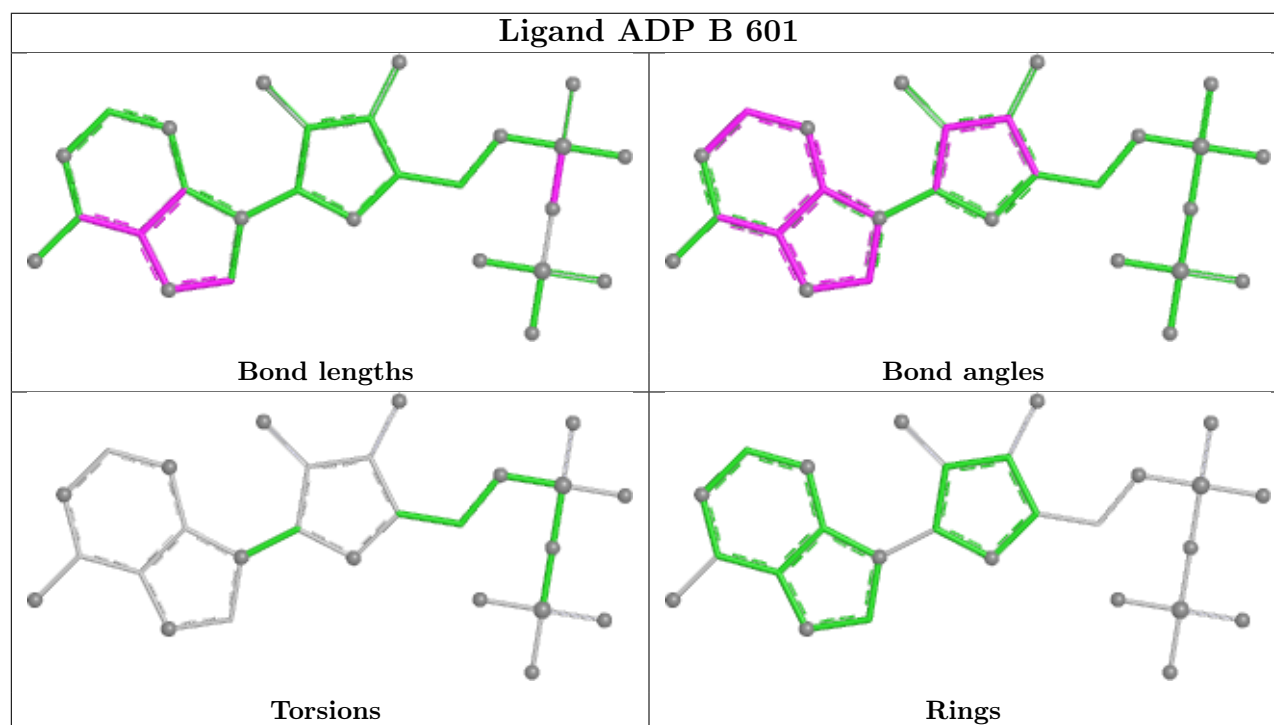
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	3	0
2	A	600	ADP	1	0

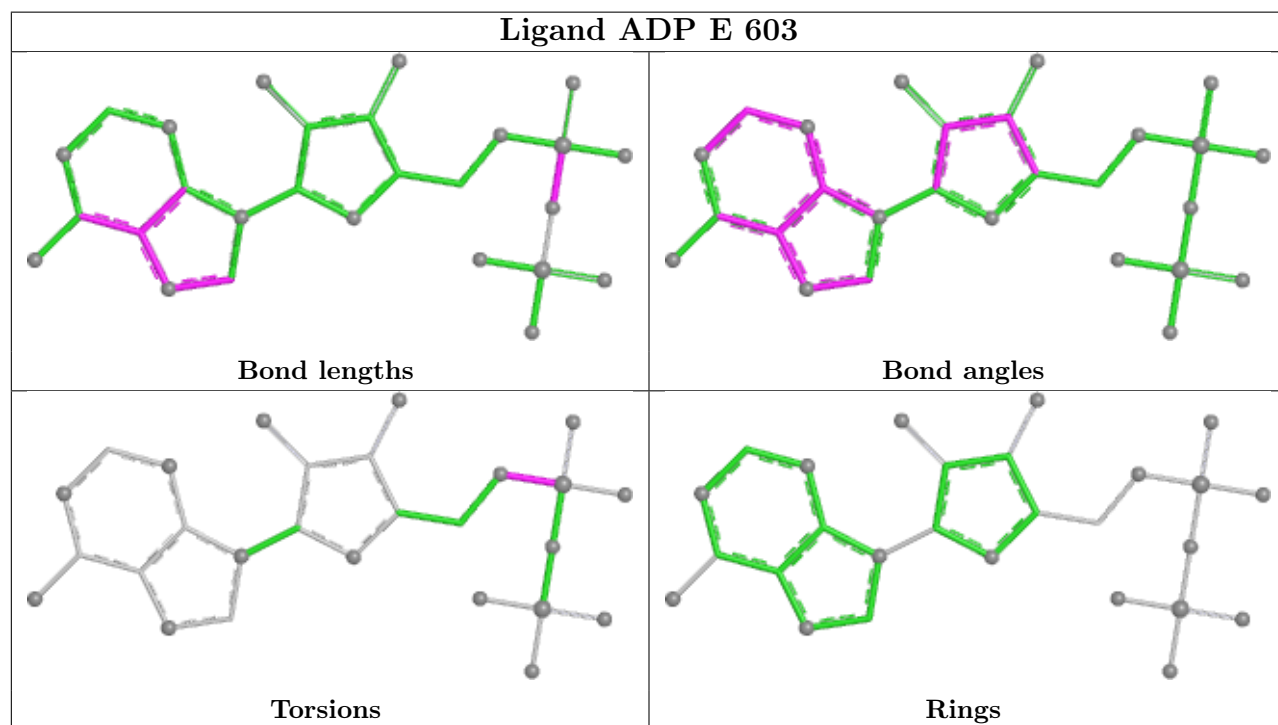
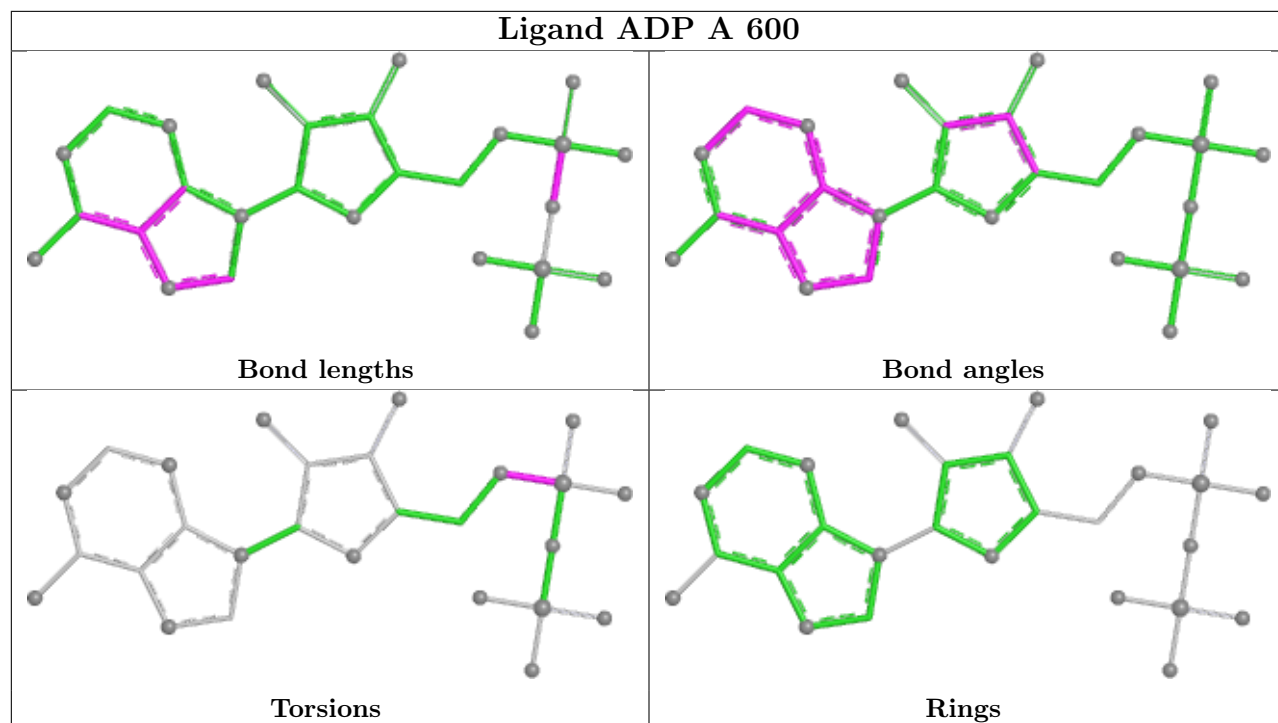
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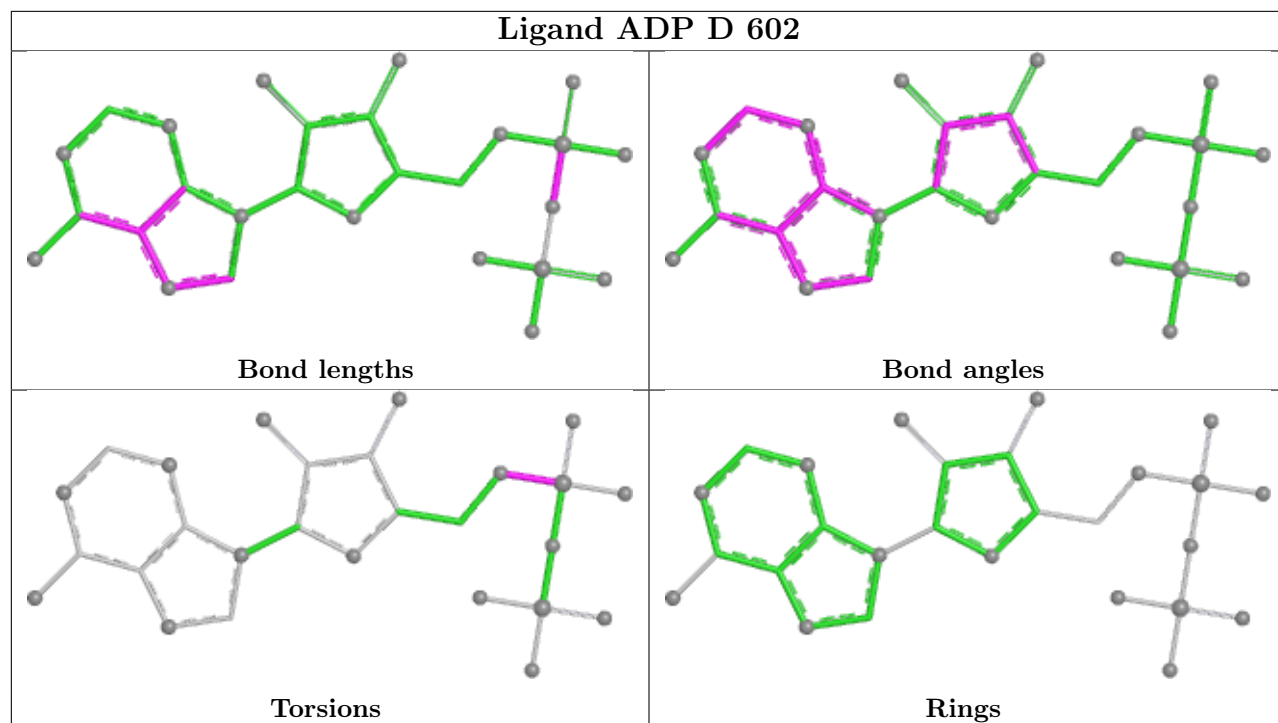
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	603	ADP	9	0
2	D	602	ADP	4	0

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 than 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.







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	320/363 (88%)	-0.35	1 (0%) 90 82	62, 109, 241, 416	0
1	B	315/363 (86%)	-0.22	2 (0%) 85 73	63, 120, 210, 373	0
1	C	307/363 (84%)	-0.28	1 (0%) 90 82	67, 123, 226, 412	0
1	D	316/363 (87%)	-0.29	0 100 100	72, 139, 235, 357	0
1	E	313/363 (86%)	-0.20	3 (0%) 79 62	74, 146, 301, 440	0
1	F	314/363 (86%)	-0.19	1 (0%) 90 82	65, 140, 272, 354	0
All	All	1885/2178 (86%)	-0.25	8 (0%) 88 78	62, 130, 249, 440	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	176	ALA	3.0
1	F	295	LEU	2.8
1	E	106	ASN	2.4
1	B	392	ASP	2.4
1	E	287	LEU	2.1
1	B	210	ALA	2.1
1	A	403	ILE	2.0
1	C	79	ILE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

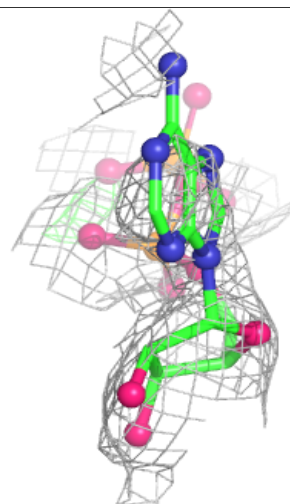
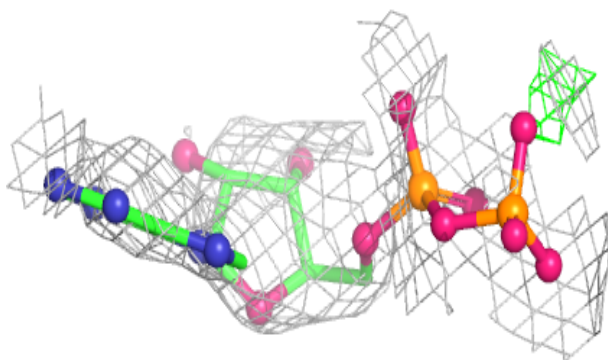
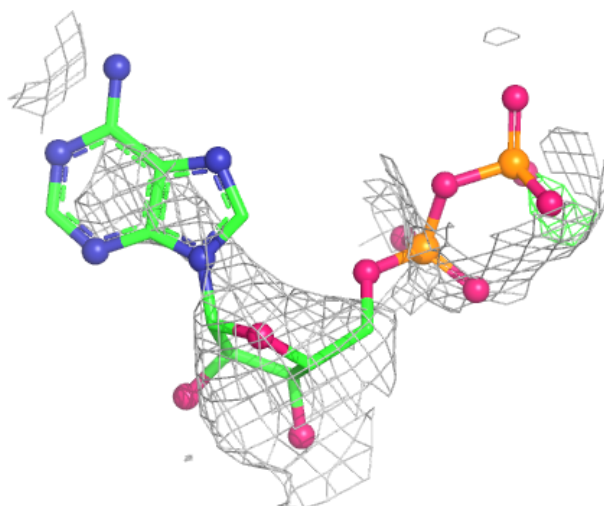
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	SO4	A	705	5/5	0.44	0.09	173,173,173,173	0
3	SO4	C	706	5/5	0.47	0.07	232,232,232,232	0
3	SO4	B	702	5/5	0.58	0.09	191,191,191,191	0
3	SO4	B	708	5/5	0.59	0.10	231,231,231,231	0
3	SO4	A	700	5/5	0.62	0.18	147,147,147,147	0
3	SO4	C	704	5/5	0.66	0.06	233,233,233,233	0
3	SO4	A	701	5/5	0.68	0.07	168,168,168,168	0
3	SO4	B	709	5/5	0.68	0.09	178,178,178,178	0
3	SO4	B	707	5/5	0.69	0.06	179,179,179,179	0
3	SO4	D	710	5/5	0.72	0.08	190,190,190,190	0
4	MG	B	901	1/1	0.74	0.19	115,115,115,115	0
3	SO4	C	703	5/5	0.78	0.07	169,169,169,169	0
4	MG	D	900	1/1	0.86	0.11	107,107,107,107	0
2	ADP	E	603	27/27	0.93	0.08	135,151,159,166	14
2	ADP	B	601	27/27	0.94	0.09	95,119,137,139	10
2	ADP	D	602	27/27	0.94	0.10	132,153,162,170	16
3	SO4	C	500	5/5	0.94	0.06	100,100,100,100	0
2	ADP	A	600	27/27	0.95	0.08	78,93,113,120	9
3	SO4	F	500	5/5	0.95	0.07	96,96,96,96	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.

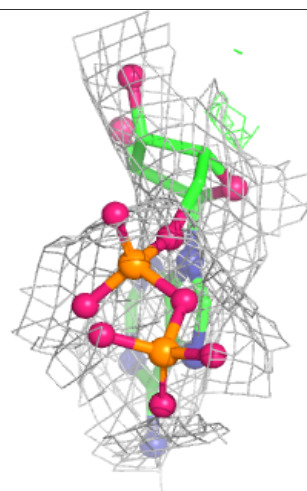
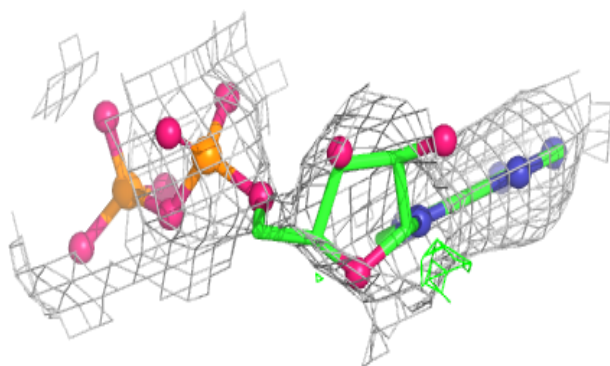
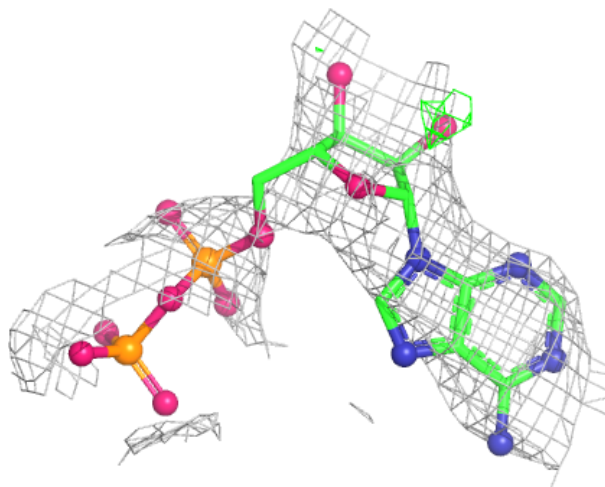
Electron density around ADP E 603:

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



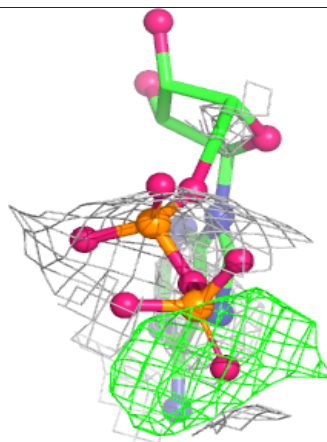
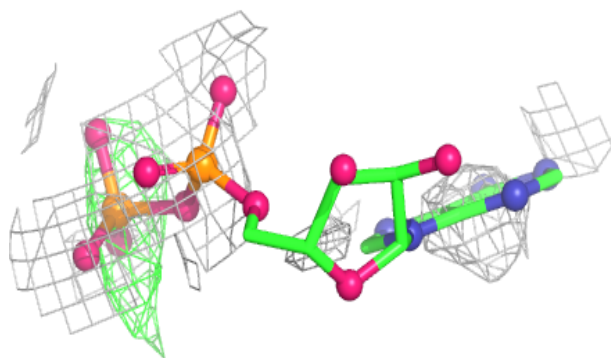
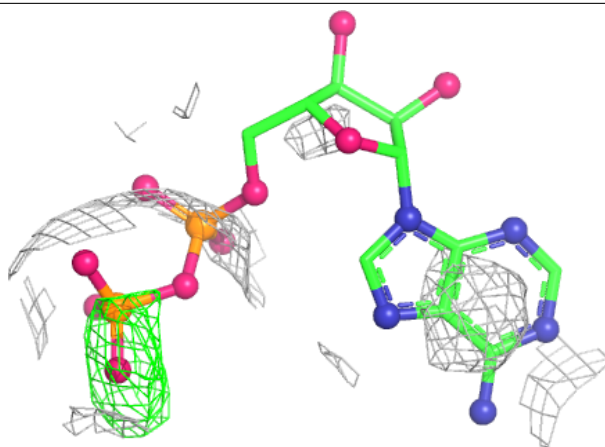
Electron density around ADP B 601:

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



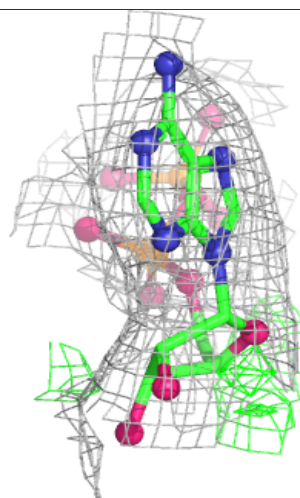
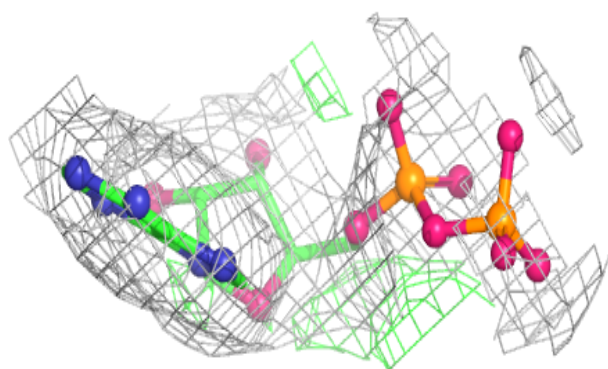
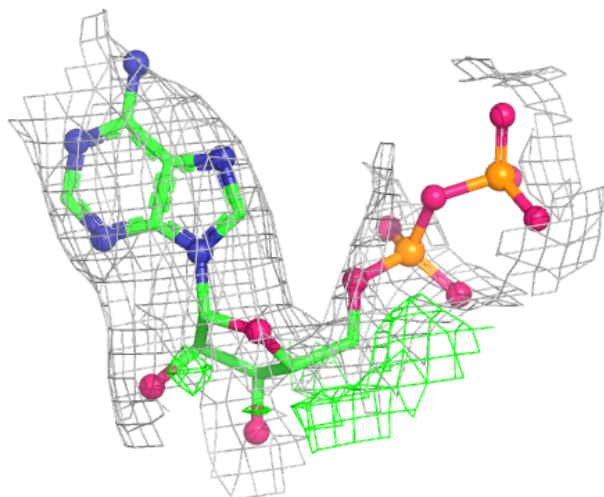
Electron density around ADP D 602:

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



Electron density around ADP A 600:

$2mF_o-DF_c$ (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.