



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 4XGU / pdb_00004xgu
Title : Structure of C. elegans PCH-2
Authors : Ye, Q.; Corbett, K.D.
Deposited on : 2015-01-02
Resolution : 2.30 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

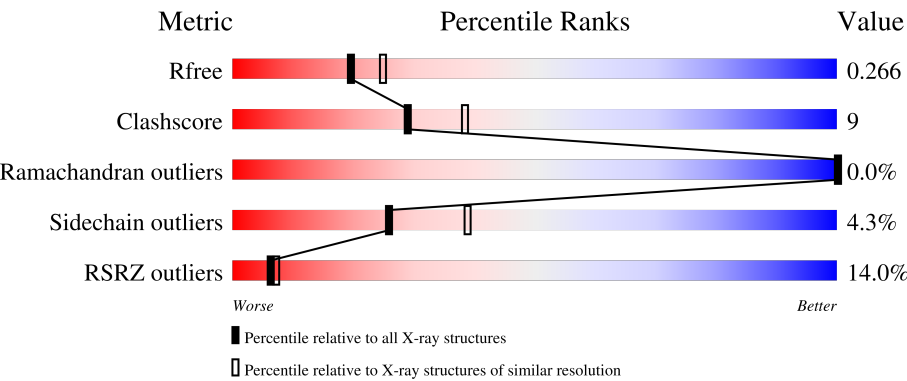
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	424	19% 65%22%•11%
1	B	424	11% 66%22%•10%
1	C	424	15% 65%22%•12%
1	D	424	7% 74%14%•11%
1	E	424	12% 70%18%•11%

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Mol	Chain	Length	Quality of chain
1	F	424	12% 64% 21% • 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17995 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 Putative pachytene checkpoint protein 2.

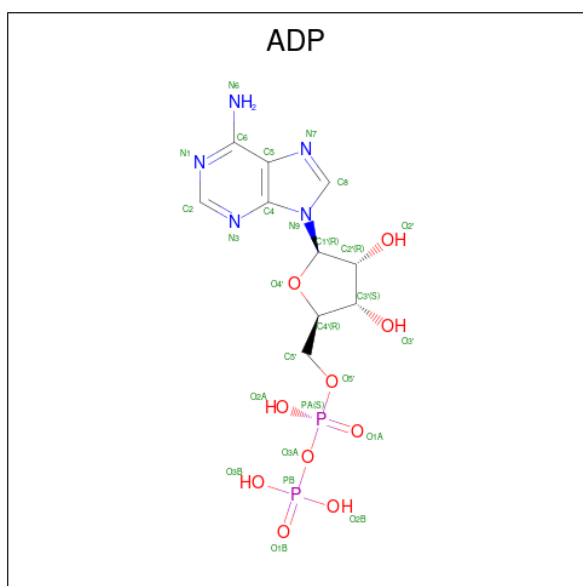
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2984	1885	516	565	18			
1	B	382	Total	C	N	O	S	0	0	0
			3020	1912	514	577	17			
1	C	374	Total	C	N	O	S	0	0	0
			2936	1853	505	561	17			
1	D	377	Total	C	N	O	S	0	0	0
			2981	1881	513	570	17			
1	E	379	Total	C	N	O	S	0	0	0
			2982	1884	511	570	17			
1	F	376	Total	C	N	O	S	0	0	0
			2948	1860	507	564	17			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	8	Total O 8 8	0	0

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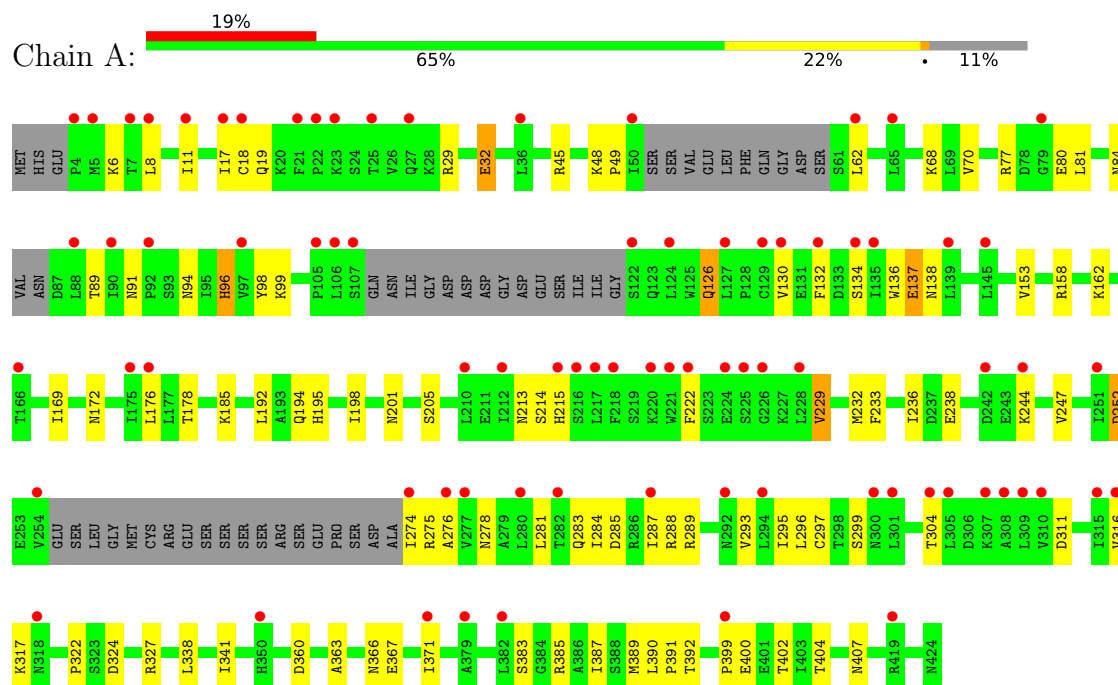
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	13	Total 13	O 13	0	0
4	D	16	Total 16	O 16	0	0
4	E	11	Total 11	O 11	0	0
4	F	7	Total 7	O 7	0	0

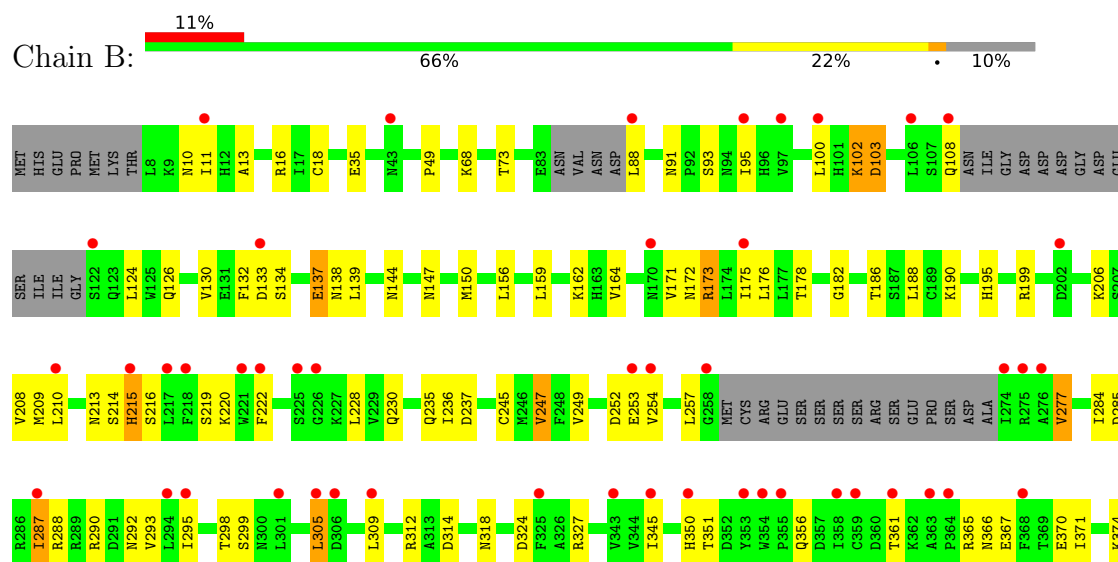
3 Residue-property plots [i](#)

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: Putative pachytene checkpoint protein 2

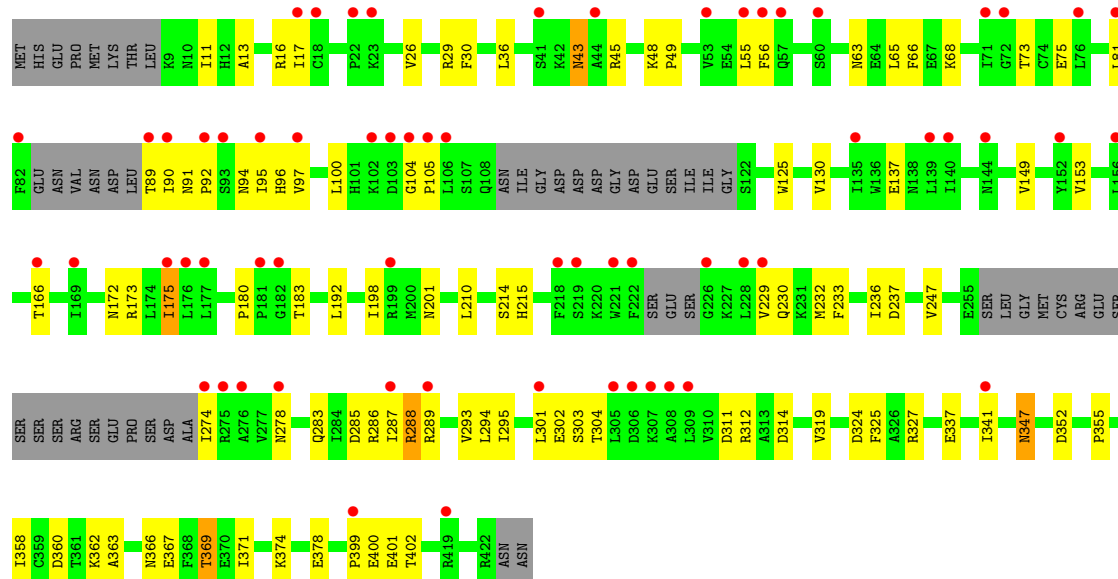


• Molecule 1: Putative pachytene checkpoint protein 2

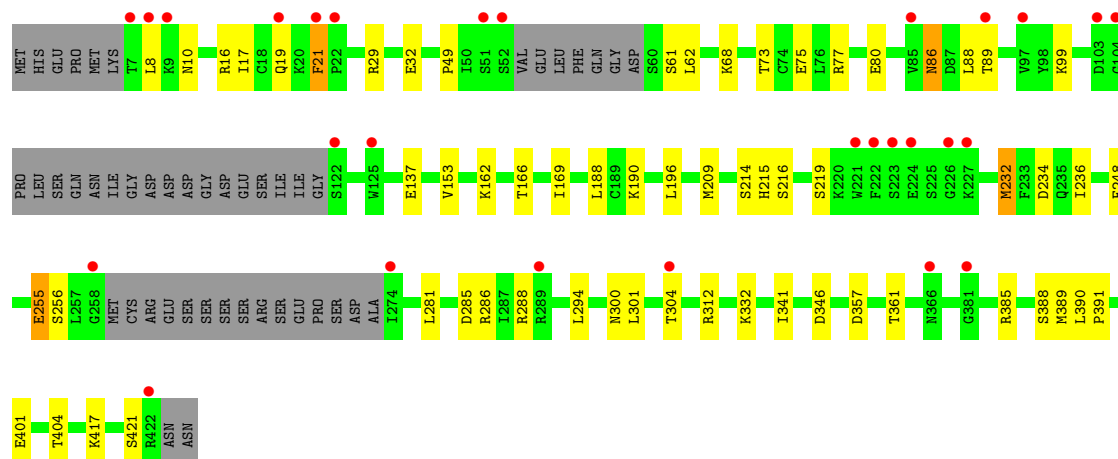
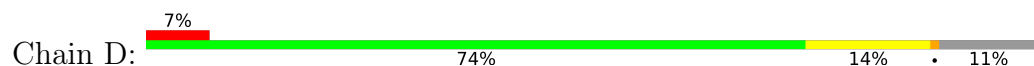




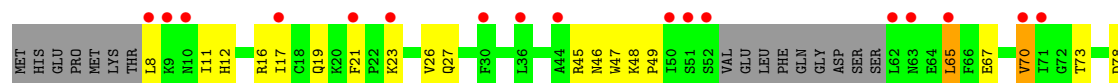
• Molecule 1: Putative pachytene checkpoint protein 2

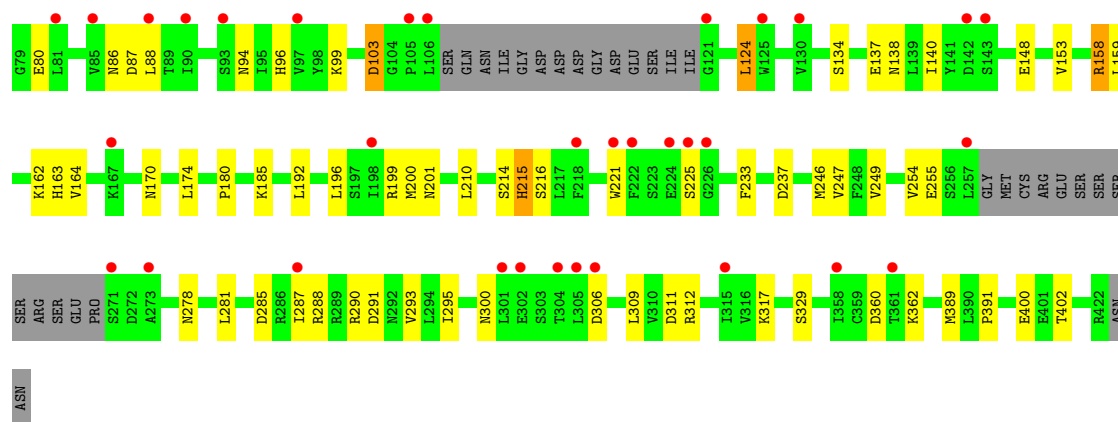


• Molecule 1: Putative pachytene checkpoint protein 2

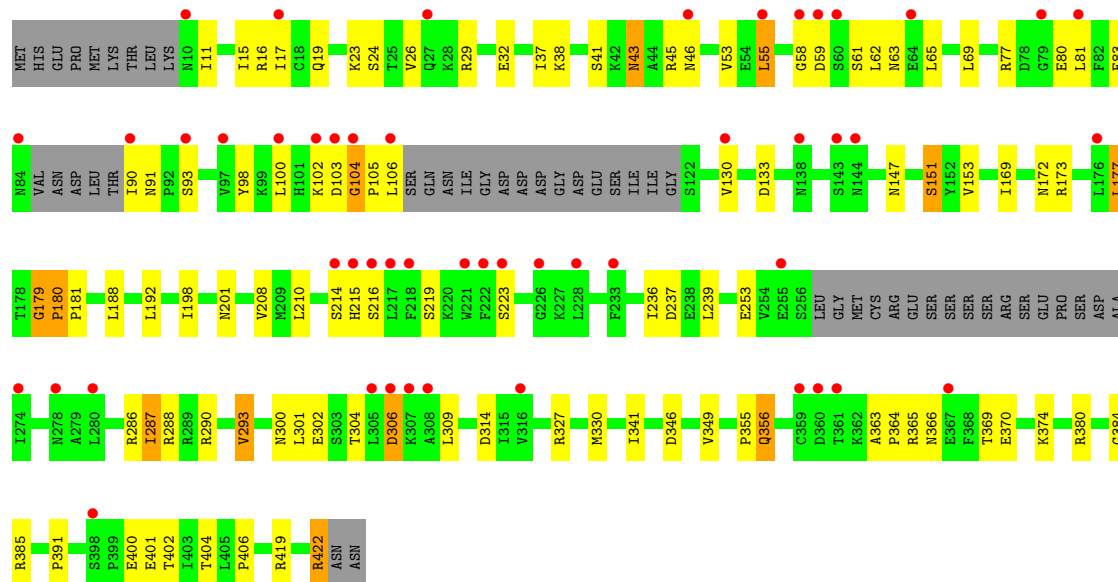


• Molecule 1: Putative pachytene checkpoint protein 2





• Molecule 1: Putative pachytene checkpoint protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	126.71Å 240.97Å 197.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.30 39.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	71.8 (39.36-2.30) 71.8 (39.36-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.264 0.234 , 0.266	Depositor DCC
R_{free} test set	4884 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17995	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.57% 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: ADP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/3028	0.72	1/4085 (0.0%)
1	B	0.28	0/3066	0.70	0/4139
1	C	0.31	0/2978	0.73	4/4024 (0.1%)
1	D	0.32	0/3025	0.70	0/4085
1	E	0.32	0/3027	0.74	2/4092 (0.0%)
1	F	0.31	0/2992	0.77	6/4044 (0.1%)
All	All	0.31	0/18116	0.73	13/24469 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	PRO	CA-C-N	6.62	127.15	119.47
1	E	180	PRO	C-N-CA	6.62	127.15	119.47
1	F	104	GLY	CA-C-N	-6.06	113.70	119.76
1	F	104	GLY	C-N-CA	-6.06	113.70	119.76
1	A	130	VAL	N-CA-C	5.61	115.80	110.53
1	C	104	GLY	CA-C-N	-5.51	112.95	119.84
1	C	104	GLY	C-N-CA	-5.51	112.95	119.84
1	C	180	PRO	CA-C-N	5.47	126.68	119.84
1	C	180	PRO	C-N-CA	5.47	126.68	119.84
1	F	180	PRO	CA-C-N	5.46	126.66	119.84
1	F	180	PRO	C-N-CA	5.46	126.66	119.84
1	F	179	GLY	CA-C-N	5.24	123.48	119.66
1	F	179	GLY	C-N-CA	5.24	123.48	119.66

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	2984	0	3024	63	0
1	B	3020	0	3047	57	0
1	C	2936	0	2938	58	0
1	D	2981	0	3000	40	0
1	E	2982	0	2989	51	0
1	F	2948	0	2938	60	0
2	A	5	0	0	1	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
3	B	27	0	12	0	0
3	E	27	0	12	0	0
4	B	8	0	0	0	0
4	C	13	0	0	0	0
4	D	16	0	0	0	0
4	E	11	0	0	0	0
4	F	7	0	0	0	0
All	All	17995	0	17960	313	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 9.

All (313) 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:287:ILE:HG22	1:E:293:VAL:HG11	1.59	0.85
1:C:355:PRO:HA	1:C:369:THR:HG22	1.61	0.82
1:A:198:ILE:O	1:A:201:ASN:ND2	2.14	0.81
1:D:281:LEU:HB3	1:D:312:ARG:HH12	1.47	0.79
1:D:190:LYS:HG2	1:D:209:MET:HE1	1.66	0.78
1:A:287:ILE:HG22	1:A:293:VAL:HG11	1.63	0.77
1:A:77:ARG:HB2	1:A:80:GLU:HG3	1.66	0.77
1:F:198:ILE:O	1:F:201:ASN:ND2	2.18	0.77
1:C:49:PRO:HD3	1:C:137:GLU:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ILE:HD13	1:C:26:VAL:HG21	1.68	0.75
1:A:176:LEU:HD21	1:A:316:VAL:HG12	1.69	0.73
1:E:49:PRO:HB3	1:E:70:VAL:HG22	1.68	0.73
1:A:222:PHE:HE1	1:A:229:VAL:HG21	1.52	0.72
1:E:11:ILE:HG12	1:E:73:THR:HB	1.71	0.72
1:C:324:ASP:OD1	1:C:327:ARG:NH2	2.22	0.71
1:D:73:THR:HG22	1:D:75:GLU:H	1.55	0.71
1:D:19:GLN:HA	1:D:99:LYS:HD2	1.73	0.71
1:C:301:LEU:HD13	1:C:304:THR:HB	1.72	0.70
1:B:134:SER:O	1:B:138:ASN:ND2	2.24	0.69
1:B:49:PRO:HD3	1:B:137:GLU:HG2	1.75	0.69
1:C:153:VAL:HG22	1:C:175:ILE:HD12	1.73	0.69
1:E:16:ARG:HG2	1:E:67:GLU:HB2	1.74	0.69
1:F:29:ARG:HH12	1:F:61:SER:HB2	1.58	0.69
1:E:45:ARG:HB2	1:E:48:LYS:HB2	1.76	0.68
1:B:385:ARG:NH2	1:C:311:ASP:O	2.26	0.67
1:A:49:PRO:HD3	1:A:137:GLU:HG2	1.75	0.67
1:B:249:VAL:HB	1:B:295:ILE:HG22	1.75	0.67
1:B:16:ARG:NH2	1:B:133:ASP:OD2	2.26	0.67
1:C:153:VAL:HG21	1:C:192:LEU:HD21	1.76	0.67
1:A:8:LEU:HB3	1:A:11:ILE:HD11	1.76	0.66
1:C:283:GLN:OE1	1:C:286:ARG:NH1	2.28	0.66
1:E:17:ILE:HD13	1:E:26:VAL:HG11	1.77	0.66
1:F:404:THR:HG22	1:F:406:PRO:HD2	1.77	0.65
1:E:134:SER:O	1:E:138:ASN:ND2	2.29	0.65
1:A:45:ARG:HH22	1:A:360:ASP:HB2	1.62	0.65
1:C:17:ILE:HD11	1:C:26:VAL:HG11	1.78	0.64
1:B:237:ASP:OD1	1:B:290:ARG:NH2	2.30	0.64
1:F:173:ARG:NH1	1:F:288:ARG:O	2.30	0.64
1:C:13:ALA:HB3	1:C:95:ILE:HG13	1.80	0.63
1:D:49:PRO:HD3	1:D:137:GLU:HG2	1.80	0.63
1:D:401:GLU:OE1	1:E:158:ARG:NH2	2.32	0.62
1:C:91:ASN:HB2	1:C:94:ASN:HB2	1.82	0.62
1:B:13:ALA:HB3	1:B:95:ILE:HG22	1.81	0.62
1:E:96:HIS:ND1	1:E:201:ASN:OD1	2.27	0.61
1:A:324:ASP:OD1	1:A:327:ARG:NH1	2.32	0.61
1:D:388:SER:OG	1:E:170:ASN:ND2	2.33	0.61
1:D:385:ARG:NH2	1:E:311:ASP:O	2.33	0.61
1:A:132:PHE:HB3	1:A:194:GLN:HB2	1.83	0.61
1:D:234:ASP:OD1	1:D:286:ARG:NH2	2.34	0.61
1:A:400:GLU:OE2	1:A:400:GLU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:HG21	1:C:289:ARG:HH12	1.66	0.60
1:F:15:ILE:HD11	1:F:37:ILE:HD11	1.84	0.60
1:A:134:SER:O	1:A:138:ASN:ND2	2.33	0.60
1:B:178:THR:OG1	1:B:318:ASN:ND2	2.34	0.60
1:C:366:ASN:HB2	1:C:369:THR:HG23	1.84	0.60
1:F:17:ILE:HD13	1:F:26:VAL:HG21	1.84	0.59
1:F:58:GLY:HA2	1:F:59:ASP:HB2	1.83	0.59
1:A:19:GLN:HA	1:A:99:LYS:HD2	1.84	0.59
1:D:32:GLU:HB3	1:D:62:LEU:HD21	1.84	0.59
1:B:172:ASN:OD1	1:B:288:ARG:NH2	2.36	0.58
1:A:222:PHE:CE1	1:A:229:VAL:HG21	2.38	0.58
1:C:36:LEU:HD11	1:C:55:LEU:HD11	1.85	0.58
1:E:12:HIS:HA	1:E:94:ASN:HB3	1.86	0.58
1:C:285:ASP:OD1	1:C:312:ARG:NH1	2.37	0.58
1:D:285:ASP:OD1	1:D:288:ARG:NH1	2.36	0.58
1:E:19:GLN:HA	1:E:99:LYS:HE2	1.84	0.58
1:C:183:THR:HB	1:C:319:VAL:HG11	1.85	0.57
1:D:255:GLU:OE2	1:D:300:ASN:ND2	2.37	0.57
1:E:103:ASP:N	1:E:103:ASP:OD1	2.37	0.57
1:E:23:LYS:O	1:E:27:GLN:HG3	2.04	0.57
1:F:38:LYS:O	1:F:41:SER:OG	2.21	0.57
1:A:233:PHE:HD1	1:A:236:ILE:HD12	1.69	0.57
1:B:351:THR:O	1:B:356:GLN:NE2	2.37	0.57
1:C:347:ASN:OD1	1:C:347:ASN:N	2.37	0.56
1:A:252:ASP:OD1	1:A:252:ASP:N	2.38	0.56
1:A:322:PRO:O	1:A:327:ARG:NH2	2.38	0.56
1:A:399:PRO:O	1:B:10:ASN:HB2	2.05	0.56
1:F:356:GLN:H	1:F:369:THR:HG22	1.70	0.56
1:A:247:VAL:HB	1:A:293:VAL:HG22	1.88	0.56
1:B:324:ASP:OD1	1:B:327:ARG:NH2	2.36	0.56
1:B:126:GLN:HE22	1:B:206:LYS:HE3	1.71	0.56
1:F:29:ARG:HD3	1:F:65:LEU:HD11	1.87	0.56
1:E:391:PRO:HG2	1:F:169:ILE:HG23	1.87	0.56
1:E:140:ILE:HG21	1:E:329:SER:HB2	1.87	0.56
1:F:32:GLU:HB3	1:F:62:LEU:HD11	1.88	0.56
1:E:163:HIS:ND1	1:E:291:ASP:OD2	2.40	0.55
1:F:45:ARG:HG2	1:F:81:LEU:HD23	1.88	0.55
1:F:287:ILE:HG22	1:F:293:VAL:HG21	1.88	0.55
1:E:185:LYS:NZ	1:E:300:ASN:OD1	2.33	0.55
1:A:311:ASP:OD1	1:F:385:ARG:NH2	2.40	0.55
1:B:210:LEU:HD13	1:B:236:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:GLN:HA	1:C:283:GLN:HE21	1.71	0.55
1:C:352:ASP:O	1:C:366:ASN:ND2	2.40	0.55
1:E:285:ASP:OD1	1:E:288:ARG:NH1	2.39	0.54
1:A:178:THR:HG22	1:A:299:SER:HB3	1.88	0.54
1:C:43:ASN:OD1	1:C:43:ASN:N	2.40	0.54
1:F:237:ASP:OD2	1:F:286:ARG:NH1	2.40	0.54
1:C:17:ILE:CD1	1:C:26:VAL:HG11	2.37	0.54
1:E:86:ASN:OD1	1:E:87:ASP:N	2.36	0.54
1:A:172:ASN:OD1	1:A:288:ARG:NH2	2.40	0.54
1:B:285:ASP:OD1	1:B:312:ARG:NE	2.33	0.54
1:C:360:ASP:HB3	1:C:363:ALA:HB2	1.89	0.54
1:B:247:VAL:HG22	1:B:293:VAL:HG22	1.89	0.54
1:D:346:ASP:OD2	1:D:404:THR:OG1	2.25	0.53
1:C:237:ASP:OD2	1:C:286:ARG:NH2	2.41	0.53
1:A:45:ARG:HB2	1:A:48:LYS:HB2	1.90	0.53
1:B:139:LEU:HD13	1:B:188:LEU:HD23	1.90	0.53
1:E:153:VAL:HG12	1:E:196:LEU:HD11	1.89	0.53
1:F:219:SER:O	1:F:223:SER:N	2.40	0.53
1:F:43:ASN:OD1	1:F:43:ASN:N	2.42	0.53
1:F:147:ASN:O	1:F:151:SER:OG	2.27	0.52
1:F:90:ILE:HG12	1:F:91:ASN:H	1.74	0.52
1:F:330:MET:HE1	1:F:384:GLY:HA2	1.92	0.52
1:C:287:ILE:HG22	1:C:293:VAL:HG21	1.90	0.52
1:A:400:GLU:HG2	1:A:402:THR:O	2.10	0.52
1:C:302:GLU:OE2	1:C:302:GLU:N	2.41	0.52
1:A:389:MET:O	1:A:392:THR:HG22	2.10	0.52
1:C:210:LEU:HD22	1:C:236:ILE:HD11	1.91	0.52
1:F:419:ARG:NH2	1:F:422:ARG:O	2.43	0.52
1:B:144:ASN:HD21	1:B:147:ASN:HD22	1.58	0.52
1:C:173:ARG:HB2	1:C:294:LEU:HD23	1.92	0.52
1:F:19:GLN:OE1	1:F:19:GLN:N	2.42	0.52
1:A:96:HIS:HB2	1:A:201:ASN:HD21	1.76	0.51
1:E:237:ASP:OD1	1:E:290:ARG:NE	2.42	0.51
1:F:366:ASN:HB2	1:F:369:THR:HG23	1.91	0.51
1:F:301:LEU:HD13	1:F:304:THR:HB	1.92	0.51
1:E:148:GLU:OE1	1:E:317:LYS:NZ	2.41	0.51
1:E:249:VAL:HB	1:E:295:ILE:HG22	1.92	0.51
1:F:91:ASN:HD21	1:F:93:SER:HB2	1.75	0.51
1:A:136:TRP:CD1	1:A:195:HIS:HE2	2.29	0.51
1:C:400:GLU:C	1:C:402:THR:H	2.19	0.50
1:E:174:LEU:HD12	1:E:295:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:PHE:HE2	1:E:65:LEU:HB2	1.77	0.50
1:A:213:ASN:ND2	1:A:252:ASP:O	2.44	0.50
1:D:301:LEU:HD13	1:D:304:THR:HG23	1.94	0.50
1:D:153:VAL:HG12	1:D:196:LEU:HD11	1.93	0.50
1:D:332:LYS:NZ	1:D:357:ASP:OD1	2.45	0.50
1:F:210:LEU:HD22	1:F:236:ILE:HD11	1.93	0.50
1:E:159:LEU:O	1:E:164:VAL:HG23	2.12	0.49
1:B:216:SER:OG	1:B:253:GLU:OE1	2.30	0.49
1:C:29:ARG:HH11	1:C:65:LEU:HD11	1.76	0.49
1:C:100:LEU:HD13	1:C:130:VAL:HA	1.95	0.49
1:A:233:PHE:CD2	1:A:283:GLN:HB3	2.48	0.49
1:C:105:PRO:HB3	1:C:125:TRP:CZ3	2.47	0.49
1:B:16:ARG:NH2	1:B:68:LYS:HD3	2.27	0.49
1:E:254:VAL:HG11	1:E:309:LEU:HD22	1.95	0.49
1:F:15:ILE:HG12	1:F:69:LEU:HD13	1.94	0.49
1:F:400:GLU:C	1:F:402:THR:H	2.21	0.49
1:A:98:TYR:HB3	1:A:198:ILE:HG23	1.95	0.48
1:B:103:ASP:N	1:B:103:ASP:OD1	2.43	0.48
1:D:86:ASN:OD1	1:D:86:ASN:N	2.46	0.48
1:A:385:ARG:O	1:A:389:MET:HG2	2.13	0.48
1:B:132:PHE:CZ	1:B:190:LYS:HD2	2.48	0.48
1:B:190:LYS:HD3	1:B:209:MET:HE1	1.94	0.48
1:F:355:PRO:HA	1:F:369:THR:HG22	1.95	0.48
1:A:284:ILE:HG13	1:A:295:ILE:HD13	1.95	0.48
1:B:91:ASN:ND2	1:B:93:SER:HB3	2.28	0.48
1:A:6:LYS:HD2	1:A:84:ASN:HB2	1.94	0.48
1:B:213:ASN:ND2	1:B:252:ASP:O	2.43	0.48
1:B:150:MET:HE1	1:B:195:HIS:HB3	1.96	0.48
1:C:45:ARG:HB2	1:C:48:LYS:HB2	1.96	0.48
1:B:156:LEU:HD22	1:B:171:VAL:HG13	1.95	0.48
1:D:216:SER:O	1:D:219:SER:OG	2.32	0.48
1:A:172:ASN:HA	1:A:288:ARG:HH21	1.79	0.47
1:A:338:LEU:HA	1:A:341:ILE:HD12	1.95	0.47
1:B:361:THR:HG22	1:B:365:ARG:HH21	1.80	0.47
1:E:153:VAL:HG21	1:E:192:LEU:HD21	1.97	0.47
1:A:360:ASP:OD1	1:A:363:ALA:N	2.46	0.47
1:C:11:ILE:HG12	1:C:73:THR:HB	1.96	0.47
1:D:77:ARG:HB2	1:D:80:GLU:HB2	1.97	0.47
1:E:247:VAL:HB	1:E:293:VAL:HG22	1.97	0.47
1:B:284:ILE:O	1:B:288:ARG:HG2	2.14	0.47
1:D:214:SER:HA	1:D:215:HIS:HA	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:ILE:HG13	1:F:90:ILE:HG13	1.96	0.47
1:B:345:ILE:HB	1:B:402:THR:HG21	1.97	0.46
1:E:285:ASP:OD2	1:E:312:ARG:NH1	2.48	0.46
1:F:306:ASP:OD1	1:F:306:ASP:N	2.47	0.46
1:A:205:SER:HB3	1:A:244:LYS:HE3	1.97	0.46
1:C:247:VAL:HB	1:C:293:VAL:HG12	1.95	0.46
1:F:214:SER:HA	1:F:215:HIS:HA	1.55	0.46
1:B:11:ILE:HG23	1:B:73:THR:HB	1.98	0.46
1:A:383:SER:O	1:A:387:ILE:HG13	2.16	0.46
1:C:29:ARG:HD2	1:C:65:LEU:HD11	1.97	0.46
1:F:346:ASP:OD1	1:F:349:VAL:N	2.39	0.46
1:E:8:LEU:HD21	1:E:11:ILE:HG13	1.98	0.46
1:B:366:ASN:HD22	1:B:366:ASN:H	1.63	0.46
1:A:317:LYS:HA	1:A:317:LYS:HD3	1.73	0.45
1:F:17:ILE:HD11	1:F:26:VAL:HG11	1.97	0.45
1:B:182:GLY:HA3	1:B:383:SER:HB2	1.97	0.45
1:E:360:ASP:O	1:E:362:LYS:HG3	2.16	0.45
1:B:176:LEU:HD21	1:B:305:LEU:HD21	1.98	0.45
1:E:285:ASP:OD1	1:E:312:ARG:HD3	2.16	0.45
1:F:16:ARG:HB2	1:F:98:TYR:CZ	2.51	0.45
1:E:21:PHE:CE2	1:E:65:LEU:HB2	2.52	0.45
1:F:59:ASP:N	1:F:59:ASP:OD1	2.49	0.45
1:F:100:LEU:HD13	1:F:130:VAL:HA	1.98	0.45
1:F:214:SER:O	1:F:214:SER:OG	2.34	0.45
1:B:178:THR:HG22	1:B:299:SER:HB3	1.98	0.45
1:D:166:THR:HA	1:D:169:ILE:O	2.16	0.45
1:A:281:LEU:O	1:A:284:ILE:HG22	2.16	0.45
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.84	0.45
1:A:341:ILE:HD11	1:B:164:VAL:HG22	1.99	0.45
1:B:124:LEU:HD11	1:B:208:VAL:HB	1.98	0.45
1:B:214:SER:HA	1:B:215:HIS:HA	1.59	0.45
1:C:173:ARG:N	1:C:314:ASP:OD2	2.50	0.45
1:C:233:PHE:HA	1:C:236:ILE:HD12	1.99	0.45
1:E:23:LYS:H	1:E:23:LYS:HD2	1.82	0.45
1:E:281:LEU:HD13	1:E:312:ARG:NH2	2.31	0.45
1:A:32:GLU:H	1:A:32:GLU:HG2	1.42	0.45
1:F:327:ARG:CZ	1:F:380:ARG:HA	2.47	0.45
1:B:254:VAL:HG11	1:B:309:LEU:HD22	1.98	0.44
1:E:185:LYS:NZ	1:E:300:ASN:HA	2.32	0.44
1:E:214:SER:HA	1:E:215:HIS:HA	1.56	0.44
1:A:68:LYS:NZ	1:A:137:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ASN:ND2	1:F:93:SER:HB2	2.32	0.44
1:A:367:GLU:O	1:A:371:ILE:HG13	2.18	0.44
1:D:341:ILE:HD13	1:E:164:VAL:HG22	1.98	0.44
1:B:159:LEU:O	1:B:164:VAL:HG23	2.17	0.44
1:B:245:CYS:O	1:B:292:ASN:ND2	2.50	0.44
1:C:288:ARG:HG3	1:C:295:ILE:HD12	1.99	0.44
1:D:255:GLU:OE1	1:D:300:ASN:N	2.32	0.44
1:B:91:ASN:HD21	1:B:93:SER:HB3	1.82	0.44
1:C:400:GLU:HA	1:D:10:ASN:ND2	2.32	0.44
1:F:302:GLU:H	1:F:302:GLU:CD	2.25	0.44
1:B:366:ASN:O	1:B:370:GLU:N	2.47	0.44
1:D:417:LYS:O	1:D:421:SER:OG	2.32	0.44
1:B:108:GLN:HG2	1:B:235:GLN:HE22	1.83	0.43
1:C:374:LYS:O	1:C:378:GLU:HG2	2.18	0.43
1:E:159:LEU:HD22	1:E:164:VAL:HG21	1.98	0.43
1:F:153:VAL:HG21	1:F:192:LEU:HD21	1.98	0.43
1:F:179:GLY:O	1:F:300:ASN:HA	2.17	0.43
1:C:30:PHE:HZ	1:C:92:PRO:HA	1.83	0.43
1:C:274:ILE:O	1:C:278:ASN:ND2	2.51	0.43
1:D:21:PHE:HD1	1:D:21:PHE:N	2.16	0.43
1:E:158:ARG:O	1:E:162:LYS:HG2	2.18	0.43
1:B:375:ILE:HG12	1:B:413:LEU:HD13	2.01	0.43
1:C:73:THR:OG1	1:C:75:GLU:HG2	2.18	0.43
1:E:88:LEU:HD12	1:E:88:LEU:HA	1.85	0.43
1:B:178:THR:HG21	1:B:305:LEU:HD11	2.01	0.43
1:C:232:MET:O	1:C:236:ILE:HG13	2.18	0.43
1:F:55:LEU:O	1:F:63:ASN:ND2	2.51	0.43
1:A:169:ILE:HG23	1:F:391:PRO:HG2	2.00	0.43
1:D:21:PHE:N	1:D:21:PHE:CD1	2.86	0.43
1:A:126:GLN:HE21	1:A:126:GLN:HB3	1.55	0.43
1:A:153:VAL:HG21	1:A:192:LEU:HD21	2.01	0.43
1:A:176:LEU:HA	1:A:297:CYS:O	2.17	0.43
1:A:275:ARG:HA	1:A:278:ASN:HD22	1.84	0.43
1:D:21:PHE:O	1:D:99:LYS:NZ	2.51	0.43
1:E:317:LYS:HA	1:E:317:LYS:HD3	1.79	0.43
1:F:216:SER:N	1:F:253:GLU:OE1	2.51	0.43
1:A:45:ARG:HD3	1:A:81:LEU:HG	2.00	0.43
1:A:274:ILE:HG22	1:A:276:ALA:H	1.84	0.43
1:B:11:ILE:HD12	1:B:88:LEU:HD11	2.00	0.43
1:C:198:ILE:O	1:C:201:ASN:HB2	2.18	0.43
1:C:367:GLU:O	1:C:371:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LEU:HD11	1:F:188:LEU:HD23	2.01	0.42
1:F:208:VAL:HG11	1:F:239:LEU:HD13	2.01	0.42
1:B:374:LYS:O	1:B:378:GLU:HG2	2.19	0.42
1:C:16:ARG:HH21	1:C:68:LYS:HE2	1.84	0.42
1:A:17:ILE:HG22	1:A:18:CYS:O	2.19	0.42
1:A:91:ASN:HD22	1:A:94:ASN:ND2	2.18	0.42
1:D:390:LEU:N	1:D:391:PRO:HD2	2.35	0.42
1:A:185:LYS:HG3	2:A:501:SO4:O3	2.20	0.42
1:C:229:VAL:O	1:C:233:PHE:HD2	2.01	0.42
1:B:222:PHE:CE2	1:B:277:VAL:HG12	2.55	0.42
1:F:370:GLU:O	1:F:374:LYS:HG2	2.18	0.42
1:E:200:MET:HG3	1:E:246:MET:HE1	2.01	0.42
1:A:404:THR:HG22	1:A:407:ASN:HB2	2.02	0.42
1:E:46:ASN:HB3	1:E:78:ASP:O	2.19	0.42
1:A:158:ARG:NH2	1:F:401:GLU:HG3	2.34	0.42
1:D:16:ARG:NH2	1:D:68:LYS:HE3	2.35	0.42
1:E:47:TRP:HH2	1:E:199:ARG:HH21	1.67	0.42
1:E:124:LEU:HD12	1:E:210:LEU:HD21	2.01	0.42
1:E:221:TRP:O	1:E:225:SER:N	2.53	0.42
1:A:285:ASP:O	1:A:289:ARG:HG3	2.20	0.42
1:A:390:LEU:N	1:A:391:PRO:HD2	2.34	0.42
1:B:287:ILE:CG2	1:B:293:VAL:HG11	2.50	0.42
1:C:341:ILE:HG23	1:D:162:LYS:HB3	2.01	0.42
1:D:62:LEU:HD12	1:D:62:LEU:H	1.85	0.42
1:D:255:GLU:HG2	1:D:256:SER:N	2.34	0.42
1:F:46:ASN:ND2	1:F:77:ARG:O	2.40	0.42
1:A:232:MET:O	1:A:236:ILE:HG13	2.20	0.41
1:C:172:ASN:O	1:C:288:ARG:HG2	2.20	0.41
1:A:49:PRO:HB3	1:A:70:VAL:HG22	2.03	0.41
1:B:186:THR:O	1:B:190:LYS:HG2	2.21	0.41
1:C:325:PHE:HE1	1:C:358:ILE:HG21	1.84	0.41
1:F:309:LEU:HD23	1:F:309:LEU:HA	1.93	0.41
1:C:149:VAL:O	1:C:153:VAL:HG23	2.21	0.41
1:B:102:LYS:HB3	1:B:102:LYS:HE2	1.79	0.41
1:D:29:ARG:NH2	1:D:61:SER:OG	2.54	0.41
1:F:365:ARG:HB3	1:F:369:THR:OG1	2.20	0.41
1:A:162:LYS:HB3	1:F:341:ILE:HB	2.03	0.41
1:B:367:GLU:O	1:B:371:ILE:N	2.41	0.41
1:C:63:ASN:HA	1:C:66:PHE:CE1	2.55	0.41
1:C:90:ILE:HG23	1:C:95:ILE:HD13	2.03	0.41
1:F:172:ASN:H	1:F:314:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:HG23	1:B:162:LYS:HB3	2.03	0.41
1:B:219:SER:HA	1:B:257:LEU:HD23	2.03	0.41
1:C:214:SER:HA	1:C:215:HIS:HA	1.64	0.41
1:C:362:LYS:HA	1:C:362:LYS:HD3	1.89	0.41
1:D:281:LEU:HB3	1:D:312:ARG:NH1	2.25	0.41
1:A:214:SER:HA	1:A:215:HIS:HA	1.55	0.41
1:B:254:VAL:HG23	1:B:298:THR:O	2.21	0.41
1:D:248:PHE:HE1	1:D:294:LEU:HD23	1.86	0.41
1:F:237:ASP:OD1	1:F:290:ARG:NE	2.53	0.41
1:D:232:MET:O	1:D:236:ILE:HG13	2.21	0.40
1:F:180:PRO:HA	1:F:181:PRO:HD3	1.93	0.40
1:B:173:ARG:N	1:B:314:ASP:OD2	2.54	0.40
1:D:8:LEU:HD23	1:D:88:LEU:HD22	2.02	0.40
1:E:233:PHE:HD1	1:E:287:ILE:HD11	1.85	0.40
1:F:363:ALA:HA	1:F:364:PRO:HD3	1.99	0.40
1:F:104:GLY:N	1:F:105:PRO:HD3	2.36	0.40
1:C:399:PRO:C	1:D:10:ASN:HD22	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/424 (86%)	358 (98%)	8 (2%)	0	100	100
1	B	374/424 (88%)	366 (98%)	8 (2%)	0	100	100
1	C	364/424 (86%)	354 (97%)	9 (2%)	1 (0%)	36	46
1	D	369/424 (87%)	362 (98%)	7 (2%)	0	100	100
1	E	371/424 (88%)	363 (98%)	8 (2%)	0	100	100
1	F	368/424 (87%)	358 (97%)	10 (3%)	0	100	100
All	All	2212/2544 (87%)	2161 (98%)	50 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	303	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/386 (88%)	326 (96%)	13 (4%)	29	44
1	B	343/386 (89%)	324 (94%)	19 (6%)	19	28
1	C	329/386 (85%)	317 (96%)	12 (4%)	31	47
1	D	338/386 (88%)	329 (97%)	9 (3%)	39	58
1	E	336/386 (87%)	321 (96%)	15 (4%)	24	37
1	F	329/386 (85%)	311 (94%)	18 (6%)	19	28
All	All	2014/2316 (87%)	1928 (96%)	86 (4%)	26	39

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	32	GLU
1	A	62	LEU
1	A	89	THR
1	A	96	HIS
1	A	126	GLN
1	A	137	GLU
1	A	229	VAL
1	A	238	GLU
1	A	252	ASP
1	A	296	LEU
1	A	304	THR
1	A	366	ASN
1	B	18	CYS
1	B	35	GLU
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	102	LYS
1	B	103	ASP
1	B	130	VAL
1	B	137	GLU
1	B	173	ARG
1	B	175	ILE
1	B	199	ARG
1	B	215	HIS
1	B	220	LYS
1	B	228	LEU
1	B	230	GLN
1	B	247	VAL
1	B	277	VAL
1	B	287	ILE
1	B	305	LEU
1	B	350	HIS
1	C	43	ASN
1	C	56	PHE
1	C	81	LEU
1	C	89	THR
1	C	96	HIS
1	C	97	VAL
1	C	175	ILE
1	C	288	ARG
1	C	337	GLU
1	C	347	ASN
1	C	369	THR
1	C	401	GLU
1	D	17	ILE
1	D	21	PHE
1	D	86	ASN
1	D	89	THR
1	D	188	LEU
1	D	232	MET
1	D	255	GLU
1	D	361	THR
1	D	389	MET
1	E	65	LEU
1	E	70	VAL
1	E	80	GLU
1	E	103	ASP
1	E	124	LEU

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Mol	Chain	Res	Type
1	E	137	GLU
1	E	158	ARG
1	E	215	HIS
1	E	216	SER
1	E	255	GLU
1	E	278	ASN
1	E	306	ASP
1	E	389	MET
1	E	400	GLU
1	E	402	THR
1	F	23	LYS
1	F	24	SER
1	F	43	ASN
1	F	53	VAL
1	F	55	LEU
1	F	80	GLU
1	F	83	GLU
1	F	102	LYS
1	F	103	ASP
1	F	106	LEU
1	F	133	ASP
1	F	151	SER
1	F	177	LEU
1	F	287	ILE
1	F	293	VAL
1	F	306	ASP
1	F	356	GLN
1	F	422	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	91	ASN
1	A	123	GLN
1	A	215	HIS
1	A	278	ASN
1	A	366	ASN
1	B	57	GLN
1	B	101	HIS
1	B	123	GLN
1	B	126	GLN

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	144	ASN
1	B	235	GLN
1	B	318	ASN
1	B	366	ASN
1	C	63	ASN
1	C	172	ASN
1	C	278	ASN
1	C	407	ASN
1	D	10	ASN
1	D	63	ASN
1	D	123	GLN
1	D	147	ASN
1	D	215	HIS
1	D	410	ASN
1	E	170	ASN
1	E	195	HIS
1	E	215	HIS
1	E	356	GLN
1	E	410	ASN
1	F	12	HIS
1	F	27	GLN
1	F	94	ASN
1	F	138	ASN
1	F	170	ASN
1	F	201	ASN
1	F	283	GLN
1	F	318	ASN
1	F	356	GLN
1	F	407	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	E	501	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.11	0
3	ADP	B	501	-	28,29,29	1.45	5 (17%)	43,45,45	1.82	8 (18%)
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.10	0
3	ADP	E	503	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	E	502	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	F	501	-	4,4,4	0.25	0	6,6,6	0.08	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
3	ADP	B	501	-	-	6/16/32/32	0/3/3/3
3	ADP	E	503	-	-	6/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ADP	C5-C4	4.89	1.47	1.39
3	E	503	ADP	C5-C4	4.72	1.47	1.39
3	B	501	ADP	C5-C6	2.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	ADP	C5-C6	2.50	1.48	1.41
3	E	503	ADP	C5-N7	-2.41	1.34	1.39
3	B	501	ADP	C5-N7	-2.36	1.34	1.39
3	B	501	ADP	C8-N7	2.34	1.36	1.31
3	E	503	ADP	C8-N7	2.29	1.36	1.31
3	B	501	ADP	PA-O3A	2.28	1.62	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ADP	C5-C4-N3	-5.94	118.54	126.72
3	E	503	ADP	C5-C4-N3	-5.64	118.96	126.72
3	B	501	ADP	N3-C4-N9	4.76	135.26	127.17
3	E	503	ADP	N3-C4-N9	4.63	135.04	127.17
3	B	501	ADP	C2-N3-C4	3.65	120.76	111.83
3	E	503	ADP	C2-N3-C4	3.53	120.45	111.83
3	B	501	ADP	C4-C5-N7	-3.27	106.85	110.58
3	E	503	ADP	C4-C5-N7	-3.25	106.86	110.58
3	B	501	ADP	N3-C2-N1	-3.15	123.81	128.58
3	E	503	ADP	N3-C2-N1	-3.10	123.89	128.58
3	E	503	ADP	C4-N9-C8	2.83	108.71	105.74
3	E	503	ADP	C5-N7-C8	2.46	107.31	103.45
3	B	501	ADP	C5-N7-C8	2.38	107.19	103.45
3	E	503	ADP	C3'-C2'-C1'	2.37	105.94	101.46
3	B	501	ADP	C4-N9-C8	2.36	108.21	105.74
3	B	501	ADP	C3'-C2'-C1'	2.35	105.90	101.46
3	E	503	ADP	C2'-C1'-N9	-2.23	107.76	113.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	ADP	C5'-O5'-PA-O1A
3	B	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	C5'-O5'-PA-O3A
3	E	503	ADP	C5'-O5'-PA-O2A
3	E	503	ADP	O4'-C4'-C5'-O5'
3	E	503	ADP	C3'-C4'-C5'-O5'
3	B	501	ADP	O4'-C4'-C5'-O5'
3	E	503	ADP	C5'-O5'-PA-O1A
3	E	503	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	PA-O3A-PB-O1B

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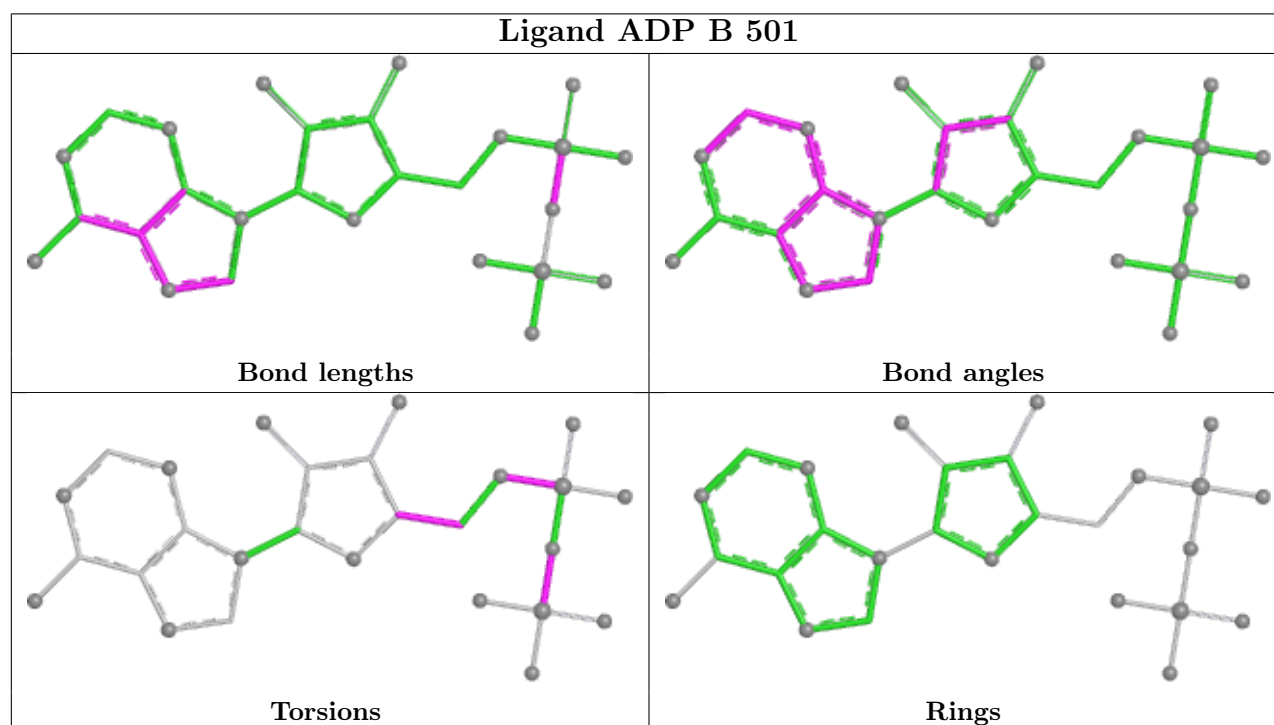
Mol	Chain	Res	Type	Atoms
3	B	501	ADP	C3'-C4'-C5'-O5'
3	E	503	ADP	PA-O3A-PB-O1B

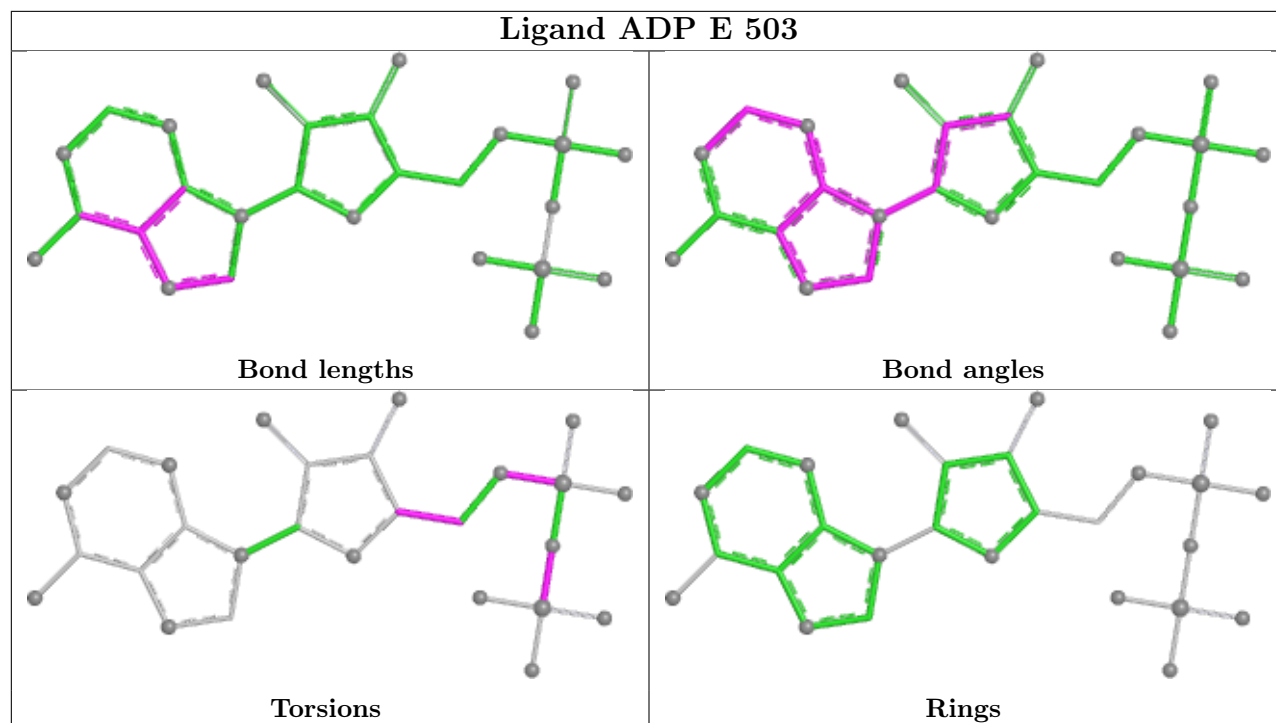
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/424 (88%)	1.29	79 (21%) 2 3	61, 95, 158, 197	0
1	B	382/424 (90%)	1.01	47 (12%) 8 9	48, 84, 137, 160	0
1	C	374/424 (88%)	1.05	63 (16%) 4 5	42, 85, 129, 150	0
1	D	377/424 (88%)	0.57	28 (7%) 20 22	37, 64, 111, 147	0
1	E	379/424 (89%)	0.78	50 (13%) 7 8	38, 77, 140, 166	0
1	F	376/424 (88%)	0.94	50 (13%) 7 8	39, 80, 133, 203	0
All	All	2264/2544 (88%)	0.94	317 (14%) 6 7	37, 83, 139, 203	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	50	ILE	5.8
1	E	305	LEU	5.5
1	D	52	SER	5.0
1	F	222	PHE	5.0
1	A	65	LEU	5.0
1	A	62	LEU	4.9
1	A	221	TRP	4.9
1	A	122	SER	4.7
1	A	50	ILE	4.6
1	A	130	VAL	4.4
1	B	221	TRP	4.4
1	D	258	GLY	4.4
1	C	274	ILE	4.3
1	C	218	PHE	4.3
1	A	4	PRO	4.3
1	A	222	PHE	4.2
1	C	305	LEU	4.2
1	E	301	LEU	4.2
1	C	90	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	274	ILE	4.1
1	A	309	LEU	4.0
1	A	280	LEU	4.0
1	E	62	LEU	4.0
1	F	308	ALA	4.0
1	A	218	PHE	4.0
1	C	56	PHE	4.0
1	B	363	ALA	4.0
1	F	10	ASN	3.9
1	C	341	ILE	3.9
1	F	221	TRP	3.9
1	F	305	LEU	3.8
1	E	221	TRP	3.8
1	B	218	PHE	3.8
1	E	52	SER	3.8
1	A	97	VAL	3.8
1	E	65	LEU	3.8
1	D	274	ILE	3.7
1	B	254	VAL	3.7
1	F	90	ILE	3.7
1	B	258	GLY	3.7
1	A	217	LEU	3.6
1	C	55	LEU	3.6
1	C	82	PHE	3.6
1	A	305	LEU	3.6
1	A	215	HIS	3.6
1	A	7	THR	3.6
1	E	143	SER	3.5
1	B	133	ASP	3.5
1	A	315	ILE	3.5
1	C	308	ALA	3.4
1	F	215	HIS	3.4
1	F	59	ASP	3.4
1	C	222	PHE	3.4
1	A	308	ALA	3.4
1	F	104	GLY	3.3
1	E	106	LEU	3.3
1	E	90	ILE	3.3
1	B	217	LEU	3.3
1	C	92	PRO	3.3
1	B	358	ILE	3.3
1	B	353	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	VAL	3.3
1	D	104	GLY	3.2
1	C	228	LEU	3.2
1	F	214	SER	3.2
1	F	223	SER	3.2
1	C	104	GLY	3.2
1	D	9	LYS	3.2
1	E	36	LEU	3.2
1	F	278	ASN	3.2
1	B	100	LEU	3.2
1	C	17	ILE	3.2
1	F	274	ILE	3.2
1	E	304	THR	3.2
1	C	226	GLY	3.1
1	F	228	LEU	3.1
1	F	102	LYS	3.1
1	E	222	PHE	3.1
1	E	257	LEU	3.1
1	C	152	TYR	3.1
1	A	132	PHE	3.1
1	E	97	VAL	3.1
1	B	305	LEU	3.1
1	F	306	ASP	3.0
1	A	129	CYS	3.0
1	A	310	VAL	3.0
1	E	224	GLU	3.0
1	A	25	THR	3.0
1	C	93	SER	3.0
1	C	53	VAL	3.0
1	C	278	ASN	3.0
1	C	166	THR	3.0
1	D	122	SER	3.0
1	E	51	SER	3.0
1	D	8	LEU	2.9
1	A	90	ILE	2.9
1	A	287	ILE	2.9
1	B	175	ILE	2.9
1	A	105	PRO	2.9
1	E	23	LYS	2.9
1	C	199	ARG	2.9
1	A	22	PRO	2.9
1	B	106	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	2.9
1	C	89	THR	2.9
1	D	222	PHE	2.8
1	B	287	ILE	2.8
1	A	92	PRO	2.8
1	A	228	LEU	2.8
1	F	81	LEU	2.8
1	A	242	ASP	2.8
1	B	306	ASP	2.8
1	F	100	LEU	2.8
1	F	217	LEU	2.8
1	E	358	ILE	2.8
1	D	51	SER	2.8
1	A	106	LEU	2.8
1	A	274	ILE	2.7
1	F	84	ASN	2.7
1	F	233	PHE	2.7
1	F	361	THR	2.7
1	C	135	ILE	2.7
1	B	226	GLY	2.7
1	A	220	LYS	2.7
1	C	289	ARG	2.7
1	A	277	VAL	2.7
1	A	316	VAL	2.7
1	F	27	GLN	2.7
1	F	138	ASN	2.7
1	A	79	GLY	2.7
1	C	219	SER	2.7
1	F	255	GLU	2.7
1	B	215	HIS	2.7
1	B	222	PHE	2.7
1	D	103	ASP	2.7
1	D	226	GLY	2.7
1	F	359	CYS	2.7
1	E	8	LEU	2.7
1	B	368	PHE	2.6
1	A	135	ILE	2.6
1	E	226	GLY	2.6
1	E	88	LEU	2.6
1	E	125	TRP	2.6
1	F	367	GLU	2.6
1	A	124	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	2.6
1	E	81	LEU	2.6
1	B	202	ASP	2.6
1	F	46	ASN	2.6
1	F	218	PHE	2.6
1	C	140	ILE	2.6
1	E	287	ILE	2.6
1	A	23	LYS	2.6
1	E	142	ASP	2.6
1	B	361	THR	2.6
1	F	58	GLY	2.6
1	B	343	VAL	2.6
1	D	85	VAL	2.6
1	F	130	VAL	2.6
1	A	371	ILE	2.6
1	A	350	HIS	2.6
1	D	19	GLN	2.5
1	B	309	LEU	2.5
1	F	307	LYS	2.5
1	A	8	LEU	2.5
1	C	309	LEU	2.5
1	B	276	ALA	2.5
1	B	364	PRO	2.5
1	C	102	LYS	2.5
1	A	254	VAL	2.5
1	D	97	VAL	2.5
1	E	225	SER	2.5
1	D	422	ARG	2.5
1	C	106	LEU	2.5
1	C	144	ASN	2.5
1	C	306	ASP	2.5
1	E	306	ASP	2.5
1	B	359	CYS	2.5
1	C	182	GLY	2.5
1	C	399	PRO	2.5
1	D	381	GLY	2.5
1	C	57	GLN	2.5
1	B	354	TRP	2.5
1	D	224	GLU	2.5
1	C	175	ILE	2.5
1	A	176	LEU	2.5
1	F	176	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	2.4
1	A	175	ILE	2.4
1	B	11	ILE	2.4
1	B	301	LEU	2.4
1	C	177	LEU	2.4
1	F	106	LEU	2.4
1	A	318	ASN	2.4
1	A	379	ALA	2.4
1	C	44	ALA	2.4
1	A	304	THR	2.4
1	D	304	THR	2.4
1	E	93	SER	2.4
1	F	216	SER	2.4
1	B	325	PHE	2.4
1	C	307	LYS	2.4
1	E	167	LYS	2.4
1	E	10	ASN	2.4
1	A	399	PRO	2.4
1	D	7	THR	2.4
1	D	223	SER	2.4
1	C	23	LYS	2.4
1	C	287	ILE	2.4
1	E	21	PHE	2.4
1	E	315	ILE	2.4
1	A	5	MET	2.4
1	C	221	TRP	2.4
1	C	72	GLY	2.4
1	E	44	ALA	2.4
1	D	89	THR	2.4
1	A	36	LEU	2.4
1	A	294	LEU	2.4
1	D	289	ARG	2.4
1	E	63	ASN	2.3
1	A	226	GLY	2.3
1	A	18	CYS	2.3
1	C	97	VAL	2.3
1	E	361	THR	2.3
1	E	218	PHE	2.3
1	A	382	LEU	2.3
1	C	301	LEU	2.3
1	C	103	ASP	2.3
1	A	107	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	216	SER	2.3
1	B	275	ARG	2.3
1	F	398	SER	2.3
1	A	27	GLN	2.3
1	A	145	LEU	2.3
1	B	43	ASN	2.3
1	F	360	ASP	2.3
1	F	226	GLY	2.3
1	B	88	LEU	2.2
1	C	176	LEU	2.2
1	E	70	VAL	2.3
1	F	55	LEU	2.2
1	B	355	PRO	2.2
1	B	122	SER	2.2
1	E	271	SER	2.2
1	B	345	ILE	2.2
1	C	71	ILE	2.2
1	A	21	PHE	2.2
1	F	97	VAL	2.2
1	F	103	ASP	2.2
1	E	302	GLU	2.2
1	B	225	SER	2.2
1	F	93	SER	2.2
1	C	95	ILE	2.2
1	C	76	LEU	2.2
1	C	81	LEU	2.2
1	E	85	VAL	2.2
1	A	300	ASN	2.2
1	C	22	PRO	2.2
1	C	18	CYS	2.2
1	A	282	THR	2.2
1	A	88	LEU	2.2
1	B	210	LEU	2.2
1	F	17	ILE	2.2
1	B	97	VAL	2.2
1	D	21	PHE	2.2
1	E	273	ALA	2.2
1	A	210	LEU	2.1
1	B	95	ILE	2.1
1	A	307	LYS	2.1
1	E	9	LYS	2.1
1	A	166	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	2.1
1	C	275	ARG	2.1
1	A	139	LEU	2.1
1	A	251	ILE	2.1
1	E	17	ILE	2.1
1	F	64	GLU	2.1
1	B	350	HIS	2.1
1	C	181	PRO	2.1
1	D	125	TRP	2.1
1	E	30	PHE	2.1
1	A	292	ASN	2.1
1	B	295	ILE	2.1
1	D	366	ASN	2.1
1	F	144	ASN	2.1
1	A	134	SER	2.1
1	C	41	SER	2.1
1	C	60	SER	2.1
1	F	60	SER	2.1
1	F	143	SER	2.1
1	A	11	ILE	2.1
1	A	212	ILE	2.1
1	C	169	ILE	2.1
1	E	198	ILE	2.1
1	D	22	PRO	2.1
1	E	130	VAL	2.1
1	E	121	GLY	2.1
1	F	79	GLY	2.1
1	A	419	ARG	2.1
1	D	221	TRP	2.1
1	A	244	LYS	2.0
1	A	225	SER	2.0
1	A	276	ALA	2.0
1	B	253	GLU	2.0
1	B	108	GLN	2.0
1	A	301	LEU	2.0
1	B	294	LEU	2.0
1	C	139	LEU	2.0
1	F	280	LEU	2.0
1	A	17	ILE	2.0
1	C	105	PRO	2.0
1	E	105	PRO	2.0
1	C	419	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	316	VAL	2.0
1	B	170	ASN	2.0
1	E	71	ILE	2.0
1	D	227	LYS	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 [i](#)

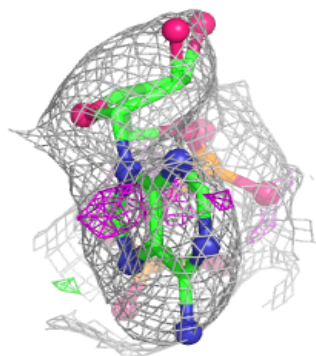
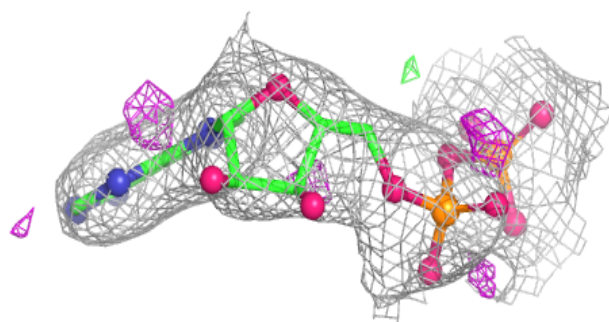
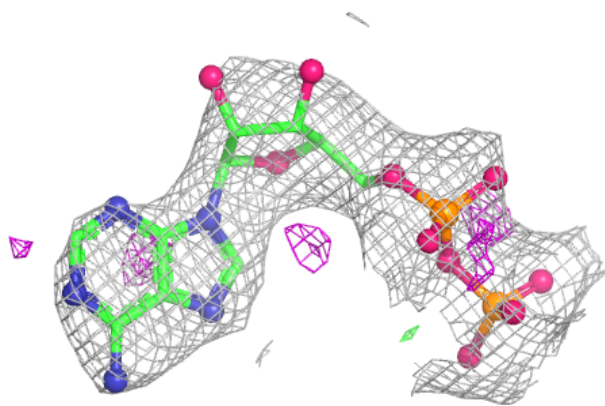
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	501	5/5	0.71	0.17	107,113,114,120	0
2	SO4	E	501	5/5	0.81	0.12	103,104,108,111	0
2	SO4	D	502	5/5	0.84	0.11	106,107,109,111	0
2	SO4	E	502	5/5	0.87	0.14	106,108,112,116	0
2	SO4	F	501	5/5	0.92	0.10	70,73,76,79	0
3	ADP	B	501	27/27	0.92	0.12	63,89,110,115	0
2	SO4	C	501	5/5	0.95	0.09	68,72,73,78	0
3	ADP	E	503	27/27	0.95	0.11	52,78,91,98	0
2	SO4	D	501	5/5	0.98	0.06	50,52,66,68	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.

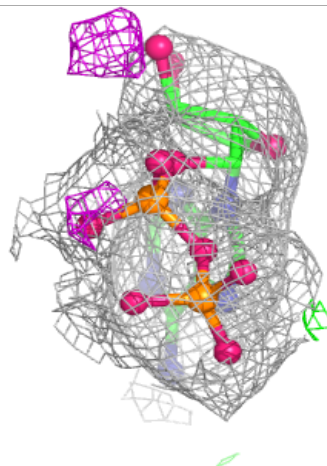
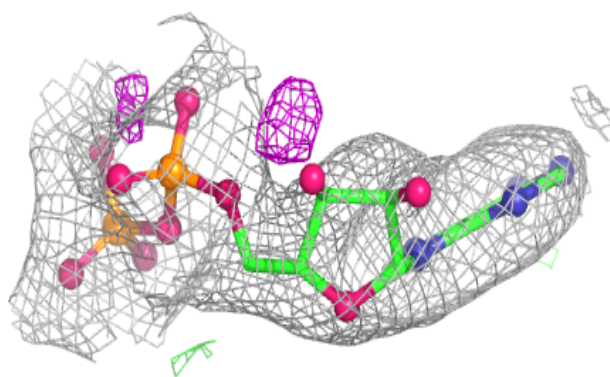
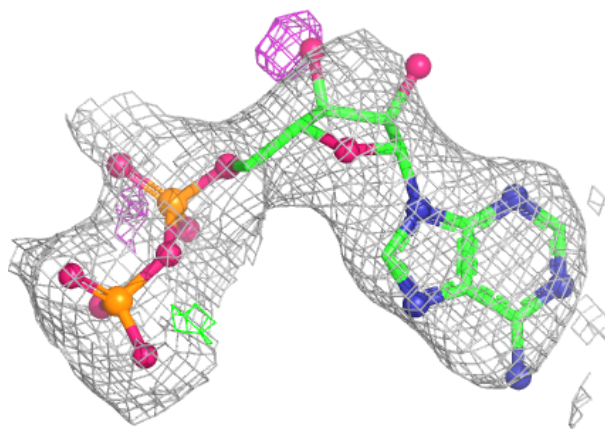
Electron density around ADP B 501:

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



Electron density around ADP E 503:

$2mF_o-DF_c$ (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.