



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 04:46 PM EDT

PDB ID : 4M9X
Title : Crystal structure of CED-4 bound CED-3 fragment
Authors : Huang, W.J.; Jinag, T.Y.; Choi, W.Y.; Wang, J.W.; Shi, Y.G.
Deposited on : 2013-08-15
Resolution : 3.34 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

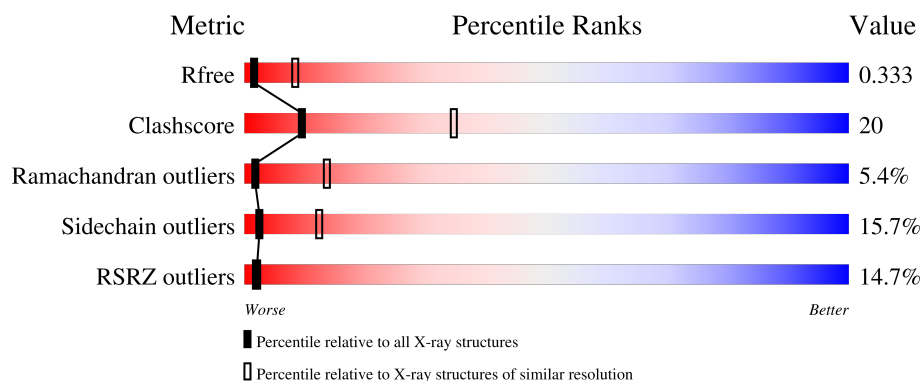
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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	549	
1	B	549	
2	C	8	
2	D	8	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8349 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 Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4088	2606	685	767	30			
1	B	511	Total	C	N	O	S	0	0	0
			4094	2607	688	768	31			

- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			57	41	8	8			
2	D	5	Total	C	N	O	0	0	0
			46	34	6	6			

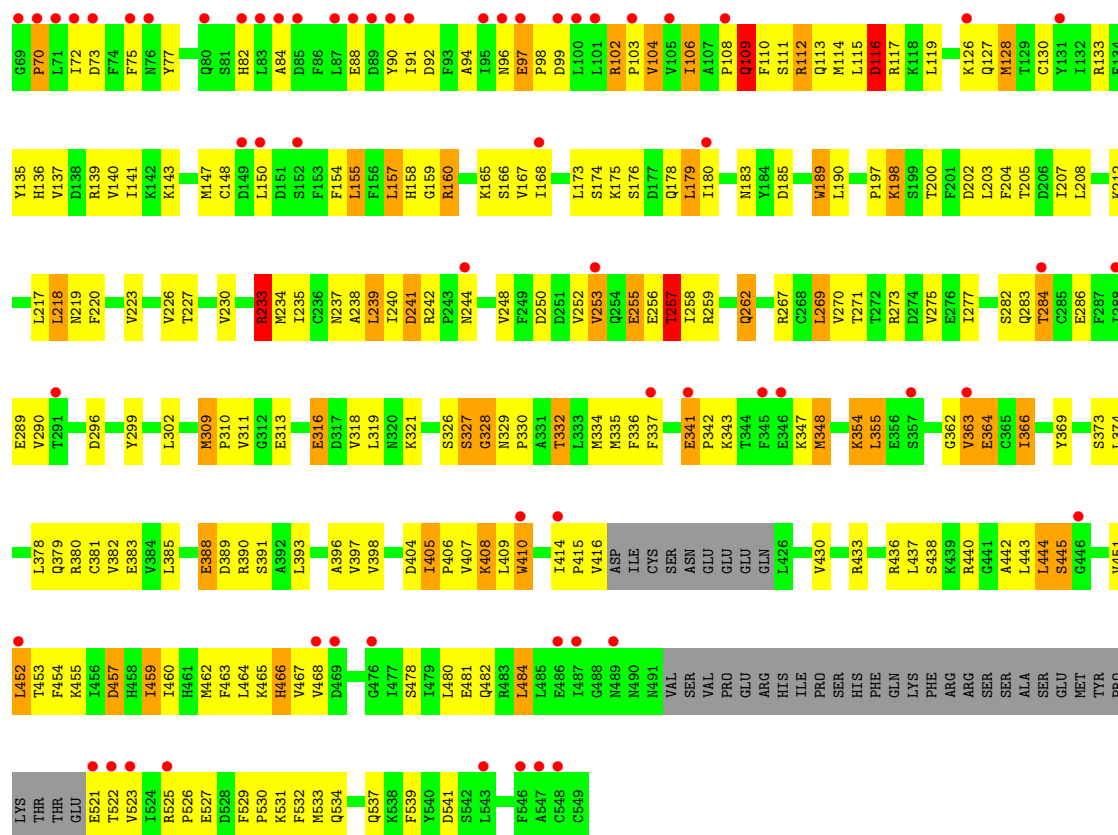
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



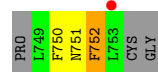
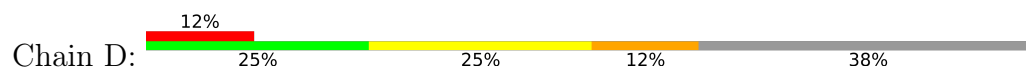
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



• Molecule 2: CED-3 fragment



• Molecule 2: CED-3 fragment



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.80Å 182.80Å 202.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.64 – 3.34 41.64 – 3.34	Depositor EDS
% Data completeness (in resolution range)	66.4 (41.64-3.34) 66.4 (41.64-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.272 , 0.333 0.272 , 0.333	Depositor DCC
R_{free} test set	858 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 199.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8349	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: MG, ATP

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	0.33	0/4163	0.68	0/5625
1	B	0.32	0/4169	0.69	2/5633 (0.0%)
2	C	0.38	0/59	0.53	0/78
2	D	0.38	0/47	0.47	0/62
All	All	0.32	0/8438	0.68	2/11398 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	233	ARG	NE-CZ-NH1	5.45	123.02	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	LEU	Peptide

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	4088	0	4107	156	0
1	B	4094	0	4116	171	0
2	C	57	0	54	1	0
2	D	46	0	45	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	3	0
All	All	8349	0	8346	327	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 20.

All (327) 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:B:20:ASP:OD2	1:B:82:HIS:NE2	2.12	0.83
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.61	0.81
1:A:262:GLN:HE21	1:A:283:GLN:HB2	1.46	0.80
1:A:63:ARG:HE	1:A:240:ILE:HD11	1.46	0.80
1:B:366:ILE:HD12	1:B:366:ILE:H	1.49	0.77
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.66	0.76
1:A:47:MET:HB2	1:A:53:ARG:HG3	1.68	0.75
1:A:366:ILE:HD12	1:A:366:ILE:H	1.49	0.75
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.74	0.70
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.73	0.69
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.75	0.68
1:B:406:PRO:HA	1:B:453:THR:HG22	1.74	0.68
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.76	0.68
1:A:96:ASN:O	1:A:98:PRO:HD3	1.95	0.67
1:B:24:ARG:HH22	1:B:53:ARG:HH11	1.42	0.67
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.76	0.67
1:B:72:ILE:HG21	1:B:88:GLU:HG3	1.76	0.67
2:C:750:PHE:O	2:C:752:PHE:N	2.28	0.66
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.77	0.66
1:B:478:SER:O	1:B:482:GLN:HG2	1.95	0.66
1:A:414:ILE:HG21	1:A:430:VAL:HG13	1.78	0.65
1:B:135:TYR:O	1:B:139:ARG:HG3	1.95	0.65
1:A:443:LEU:HD23	1:A:460:ILE:HD11	1.79	0.65
1:A:58:LEU:O	1:A:62:ARG:HG3	1.97	0.65
1:B:112:ARG:HA	1:B:116:ASP:HB2	1.79	0.64
1:A:406:PRO:HA	1:A:453:THR:HG22	1.80	0.64
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.79	0.64
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.80	0.64
1:A:67:GLU:HG2	1:A:69:GLY:H	1.64	0.63
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.80	0.62
1:B:342:PRO:O	1:B:343:LYS:HB3	1.99	0.62
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.80	0.62
1:A:452:LEU:HD23	1:A:452:LEU:H	1.65	0.62
1:B:443:LEU:HD23	1:B:460:ILE:HD11	1.80	0.62
1:A:204:PHE:HA	1:A:207:ILE:HD12	1.81	0.62
1:B:255:GLU:O	1:B:259:ARG:HG3	2.00	0.61
1:B:334:MET:HE3	1:B:337:PHE:HD2	1.65	0.61
1:B:108:PRO:O	1:B:109:GLN:HB2	2.00	0.61
1:B:8:ARG:HH11	1:B:8:ARG:HG2	1.63	0.61
1:A:205:THR:HA	1:A:231:LEU:HD11	1.83	0.60
1:B:154:PHE:HE1	1:B:262:GLN:HG3	1.65	0.60
1:A:255:GLU:O	1:A:259:ARG:HG3	2.00	0.60
1:A:309:MET:HG3	1:A:310:PRO:HD2	1.84	0.60
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.83	0.60
1:B:464:LEU:O	1:B:468:VAL:HG22	2.02	0.60
1:A:457:ASP:OD1	1:A:457:ASP:N	2.35	0.59
1:B:309:MET:HG3	1:B:310:PRO:HD2	1.84	0.59
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.33	0.59
1:A:262:GLN:NE2	1:A:283:GLN:HB2	2.18	0.59
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.85	0.59
1:A:464:LEU:O	1:A:468:VAL:HG22	2.03	0.58
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.85	0.58
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.84	0.58
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.84	0.58
1:B:166:SER:HA	1:B:271:THR:HG21	1.86	0.58
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.85	0.58
1:B:457:ASP:N	1:B:457:ASP:OD1	2.36	0.58
1:B:50:ARG:HA	1:B:53:ARG:HE	1.69	0.57
1:B:59:ARG:HH11	1:B:63:ARG:HH22	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:O	1:A:53:ARG:HG2	2.05	0.57
1:A:91:ILE:O	1:A:95:ILE:HG13	2.04	0.57
1:A:342:PRO:O	1:A:343:LYS:HB3	2.05	0.57
1:B:437:LEU:HB3	1:B:444:LEU:HD22	1.86	0.57
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.70	0.56
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.70	0.56
1:A:463:PHE:O	1:A:467:VAL:HB	2.05	0.56
1:B:226:VAL:HG11	1:B:234:MET:HE1	1.86	0.56
1:A:477:ILE:HG21	1:A:544:LYS:HE3	1.88	0.56
1:B:157:LEU:HD11	1:B:168:ILE:HG22	1.87	0.56
1:B:327:SER:HB2	1:B:459:ILE:HG13	1.88	0.56
1:B:150:LEU:O	1:B:267:ARG:NH1	2.39	0.56
1:A:150:LEU:O	1:A:267:ARG:NH1	2.38	0.56
1:A:143:LYS:O	1:A:147:MET:HG3	2.05	0.56
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.86	0.56
1:B:40:HIS:HD2	1:B:60:ILE:HG23	1.71	0.56
1:A:410:TRP:HD1	1:A:414:ILE:HD13	1.70	0.55
1:B:165:LYS:N	4:B:602:ATP:O2B	2.38	0.55
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.87	0.55
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.88	0.55
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.88	0.55
1:A:332:THR:HG23	1:A:374:LEU:HB2	1.88	0.55
1:A:159:GLY:N	1:A:165:LYS:HD3	2.21	0.55
1:B:128:MET:HG3	1:B:167:VAL:HG22	1.88	0.54
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.90	0.54
1:B:452:LEU:HD23	1:B:452:LEU:H	1.72	0.54
1:B:47:MET:HB2	1:B:53:ARG:HG3	1.88	0.54
1:A:415:PRO:O	1:A:416:VAL:HG23	2.06	0.54
1:B:204:PHE:HA	1:B:207:ILE:HD12	1.89	0.54
1:B:529:PHE:N	1:B:530:PRO:HD3	2.23	0.53
1:A:137:VAL:O	1:A:141:ILE:HG13	2.09	0.53
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.73	0.53
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.41	0.53
1:A:283:GLN:HG2	1:A:284:THR:H	1.72	0.53
1:A:354:LYS:HD3	1:A:362:GLY:O	2.08	0.53
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.91	0.53
1:A:391:SER:OG	1:A:415:PRO:HG2	2.08	0.53
1:A:326:SER:O	1:A:328:GLY:N	2.42	0.53
1:B:44:ILE:O	1:B:53:ARG:HG2	2.09	0.53
1:B:109:GLN:C	1:B:111:SER:H	2.12	0.53
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MET:HE3	1:B:364:GLU:HA	1.90	0.53
1:B:4:GLU:O	1:B:8:ARG:HB2	2.09	0.52
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.44	0.52
1:A:437:LEU:HB3	1:A:444:LEU:HD22	1.90	0.52
1:B:4:GLU:HG3	1:B:5:ILE:N	2.24	0.52
1:B:111:SER:O	1:B:115:LEU:HB3	2.09	0.52
1:B:143:LYS:O	1:B:147:MET:HG3	2.10	0.52
1:A:272:THR:HG21	1:A:277:ILE:HD11	1.92	0.52
1:B:257:THR:HG22	1:B:258:ILE:N	2.24	0.52
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.45	0.52
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.91	0.52
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.92	0.52
1:B:527:GLU:N	1:B:527:GLU:OE1	2.42	0.52
1:B:23:PRO:HG2	1:B:53:ARG:C	2.31	0.52
1:A:67:GLU:HG2	1:A:69:GLY:N	2.25	0.51
1:A:136:HIS:O	1:A:140:VAL:HG23	2.10	0.51
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.10	0.51
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.90	0.51
1:B:318:VAL:O	1:B:321:LYS:HB3	2.10	0.51
1:A:257:THR:HG22	1:A:258:ILE:N	2.25	0.51
1:B:269:LEU:HD22	1:B:270:VAL:H	1.76	0.51
1:A:313:GLU:O	1:A:316:GLU:HG3	2.10	0.51
1:B:24:ARG:HH22	1:B:53:ARG:NH1	2.07	0.51
1:A:368:PRO:HG3	1:B:282:SER:HB3	1.92	0.51
1:B:173:LEU:HD23	1:B:179:LEU:HD23	1.93	0.51
1:B:88:GLU:HA	1:B:91:ILE:HG22	1.92	0.51
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.92	0.51
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.11	0.51
1:A:529:PHE:N	1:A:530:PRO:HD3	2.26	0.50
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.42	0.50
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.75	0.50
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.93	0.50
1:B:521:GLU:C	1:B:523:VAL:H	2.14	0.50
1:A:252:VAL:HG11	1:A:258:ILE:HD13	1.93	0.50
1:A:102:ARG:HG2	1:A:182:ILE:HG22	1.94	0.50
1:A:521:GLU:C	1:A:523:VAL:H	2.15	0.50
1:B:5:ILE:HD13	1:B:94:ALA:HB1	1.93	0.50
1:B:415:PRO:O	1:B:416:VAL:HG23	2.12	0.49
1:A:235:ILE:O	1:A:239:LEU:HB2	2.12	0.49
1:B:336:PHE:HE1	1:B:348:MET:HG2	1.77	0.49
1:B:463:PHE:O	1:B:467:VAL:HB	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.47	0.49
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.94	0.49
2:D:751:ASN:O	2:D:751:ASN:ND2	2.45	0.49
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.94	0.49
1:B:56:ASN:O	1:B:60:ILE:HB	2.13	0.49
1:B:1:MET:HA	1:B:62:ARG:O	2.13	0.49
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.95	0.49
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.46	0.49
1:B:379:GLN:O	1:B:383:GLU:HG3	2.12	0.48
1:B:481:GLU:O	1:B:484:LEU:HG	2.12	0.48
1:B:23:PRO:HG2	1:B:53:ARG:O	2.14	0.48
1:A:343:LYS:O	1:A:343:LYS:HG2	2.13	0.48
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.96	0.48
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.49	0.48
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.79	0.48
1:B:115:LEU:O	1:B:119:LEU:HB2	2.14	0.48
1:B:159:GLY:N	1:B:165:LYS:HD3	2.28	0.48
1:B:158:HIS:HE1	1:B:289:GLU:HB2	1.79	0.48
1:B:233:ARG:HH11	1:B:233:ARG:CG	2.27	0.48
1:B:49:THR:HG22	1:B:50:ARG:N	2.29	0.48
1:A:341:GLU:CB	1:A:342:PRO:HD3	2.44	0.47
1:A:269:LEU:HD22	1:A:270:VAL:H	1.79	0.47
1:A:385:LEU:HD22	1:A:389:ASP:HB3	1.96	0.47
1:A:116:ASP:OD1	1:A:116:ASP:N	2.48	0.47
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.49	0.47
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.74	0.47
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.50	0.47
1:A:30:LEU:HD21	1:A:70:PRO:O	2.14	0.47
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.49	0.47
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.96	0.47
1:A:160:ARG:HG2	1:A:161:ALA:H	1.80	0.47
1:A:443:LEU:HA	1:A:460:ILE:HG12	1.97	0.47
1:B:35:ILE:CD1	1:B:70:PRO:HG2	2.45	0.47
1:B:237:ASN:C	1:B:239:LEU:H	2.18	0.47
1:A:253:VAL:HG11	1:A:380:ARG:HD3	1.96	0.47
1:A:160:ARG:NH1	1:A:442:ALA:O	2.48	0.47
1:A:527:GLU:OE1	1:A:527:GLU:N	2.47	0.47
1:B:385:LEU:HD11	1:B:393:LEU:HD12	1.96	0.47
1:B:326:SER:O	1:B:328:GLY:N	2.47	0.47
1:A:478:SER:O	1:A:482:GLN:HG2	2.15	0.46
1:B:248:VAL:HG22	1:B:269:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:O	1:A:440:ARG:HG3	2.15	0.46
1:B:484:LEU:HD13	1:B:531:LYS:O	2.15	0.46
1:B:537:GLN:O	1:B:541:ASP:N	2.44	0.46
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.97	0.46
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.50	0.46
1:B:133:ARG:O	1:B:137:VAL:HG23	2.16	0.46
1:B:332:THR:HG23	1:B:374:LEU:HB2	1.97	0.46
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.80	0.46
1:A:274:ASP:OD2	1:A:440:ARG:NH1	2.49	0.46
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.98	0.46
1:A:178:GLN:O	1:A:182:ILE:HB	2.16	0.46
1:B:21:PHE:CG	1:B:22:GLU:N	2.84	0.46
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.79	0.46
1:B:136:HIS:O	1:B:140:VAL:HG23	2.16	0.46
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.29	0.46
1:A:233:ARG:HA	1:A:236:CYS:SG	2.55	0.46
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.51	0.46
1:B:385:LEU:O	1:B:390:ARG:NH2	2.49	0.46
1:A:142:LYS:O	1:A:146:GLU:HG3	2.15	0.46
1:A:347:LYS:HA	1:A:350:GLN:HB2	1.97	0.45
1:A:111:SER:C	1:A:113:GLN:H	2.20	0.45
1:A:115:LEU:HD21	1:A:180:ILE:HB	1.97	0.45
1:B:532:PHE:C	1:B:534:GLN:H	2.19	0.45
1:A:79:ASN:ND2	1:B:36:PHE:O	2.48	0.45
1:B:313:GLU:O	1:B:316:GLU:HG3	2.15	0.45
1:B:444:LEU:HD12	1:B:444:LEU:HA	1.74	0.45
1:A:21:PHE:CG	1:A:22:GLU:N	2.85	0.45
1:A:335:MET:HE3	1:A:364:GLU:HA	1.99	0.45
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.51	0.45
1:B:379:GLN:NE2	2:D:752:PHE:O	2.50	0.45
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.52	0.45
1:B:250:ASP:HA	1:B:271:THR:OG1	2.16	0.45
1:B:343:LYS:HB3	1:B:343:LYS:HE3	1.74	0.45
1:B:459:ILE:HG13	1:B:459:ILE:H	1.46	0.45
1:A:40:HIS:O	1:A:44:ILE:HG13	2.17	0.45
1:B:109:GLN:C	1:B:111:SER:N	2.69	0.45
1:B:230:VAL:HG12	1:B:234:MET:CE	2.47	0.44
1:B:40:HIS:O	1:B:44:ILE:HG13	2.17	0.44
1:B:88:GLU:O	1:B:91:ILE:HG22	2.18	0.44
1:A:160:ARG:HB3	1:A:163:SER:HB3	1.99	0.44
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.52	0.44
1:B:436:ARG:O	1:B:440:ARG:HG3	2.16	0.44
1:B:235:ILE:O	1:B:239:LEU:HB2	2.16	0.44
1:A:8:ARG:HD3	1:A:90:TYR:OH	2.18	0.44
1:A:160:ARG:NH2	1:A:457:ASP:OD2	2.50	0.44
1:A:379:GLN:O	1:A:383:GLU:HG3	2.17	0.44
1:B:32:GLY:C	1:B:34:ASN:H	2.21	0.44
1:B:481:GLU:HA	1:B:484:LEU:CD2	2.48	0.44
1:A:525:ARG:HD3	1:A:535:LEU:HD13	1.99	0.44
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.99	0.44
1:A:36:PHE:HD2	1:A:40:HIS:HB3	1.83	0.43
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.59	0.43
1:B:391:SER:OG	1:B:415:PRO:HG2	2.17	0.43
1:A:332:THR:O	1:A:336:PHE:HB2	2.18	0.43
1:B:354:LYS:HD3	1:B:362:GLY:O	2.18	0.43
1:A:250:ASP:HA	1:A:271:THR:OG1	2.18	0.43
1:A:527:GLU:C	1:A:530:PRO:HD3	2.39	0.43
1:B:527:GLU:HA	1:B:530:PRO:HG3	2.01	0.43
1:A:47:MET:HB2	1:A:53:ARG:CG	2.44	0.43
1:A:167:VAL:HG11	4:A:602:ATP:C5	2.54	0.43
1:A:466:HIS:ND1	1:A:466:HIS:N	2.67	0.43
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.74	0.43
1:B:397:VAL:HG22	1:B:464:LEU:HB3	2.00	0.43
1:B:525:ARG:HA	1:B:526:PRO:HD3	1.89	0.43
1:B:49:THR:HG22	1:B:51:LEU:H	1.83	0.43
1:B:406:PRO:CA	1:B:453:THR:HG22	2.47	0.43
1:B:481:GLU:HA	1:B:484:LEU:HG	2.01	0.43
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.58	0.43
1:A:527:GLU:HA	1:A:530:PRO:HG3	2.00	0.43
1:B:167:VAL:HG11	4:B:602:ATP:C6	2.54	0.43
1:A:102:ARG:HG2	1:A:182:ILE:CG2	2.48	0.43
1:A:187:ILE:HD13	1:A:246:LEU:HB3	2.01	0.43
1:A:252:VAL:HG11	1:A:258:ILE:CD1	2.49	0.43
1:A:26:ALA:HB2	1:A:74:PHE:CE1	2.53	0.42
1:A:115:LEU:CD2	1:A:180:ILE:HB	2.49	0.42
1:A:349:ALA:HA	1:A:352:ASN:HB2	2.01	0.42
1:A:444:LEU:HB3	1:A:445:SER:H	1.57	0.42
1:B:237:ASN:O	1:B:240:ILE:HG23	2.19	0.42
1:B:390:ARG:HE	1:B:390:ARG:HB2	1.58	0.42
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.78	0.42
1:B:438:SER:O	1:B:442:ALA:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:SER:O	1:A:113:GLN:N	2.52	0.42
1:B:240:ILE:HG13	1:B:241:ASP:OD1	2.19	0.42
1:B:445:SER:HB3	1:B:455:LYS:O	2.19	0.42
1:A:13:ALA:HB2	1:A:86:PHE:CE1	2.54	0.42
1:B:408:LYS:HD2	1:B:408:LYS:HA	1.76	0.42
1:A:24:ARG:HH21	1:A:53:ARG:NH1	2.17	0.42
1:A:141:ILE:HD11	1:A:175:LYS:HB3	2.01	0.42
1:B:374:LEU:HD13	1:B:378:LEU:HG	2.01	0.42
1:A:133:ARG:O	1:A:137:VAL:HG23	2.19	0.42
1:A:163:SER:C	1:A:330:PRO:HG2	2.40	0.42
1:A:314:LYS:HA	1:A:317:ASP:HB2	2.01	0.42
1:B:18:ILE:O	1:B:50:ARG:NH2	2.53	0.42
1:A:437:LEU:HD22	1:A:437:LEU:HA	1.84	0.42
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.85	0.42
1:A:167:VAL:O	1:A:171:GLN:HG3	2.20	0.42
1:B:160:ARG:NH1	1:B:442:ALA:O	2.53	0.42
1:A:336:PHE:HE2	1:A:348:MET:SD	2.43	0.42
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.73	0.42
1:A:46:LYS:H	1:A:46:LYS:HG3	1.56	0.42
1:A:92:ASP:C	1:A:94:ALA:H	2.23	0.42
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.49	0.41
1:A:347:LYS:O	1:A:347:LYS:HD3	2.19	0.41
1:A:408:LYS:HD2	1:A:408:LYS:HA	1.77	0.41
1:B:252:VAL:HG22	1:B:257:THR:HG21	2.01	0.41
1:B:407:VAL:HG23	1:B:452:LEU:O	2.20	0.41
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.55	0.41
1:A:406:PRO:CA	1:A:453:THR:HG22	2.49	0.41
1:B:30:LEU:HD13	1:B:36:PHE:CE1	2.56	0.41
1:B:110:PHE:HA	1:B:113:GLN:HB2	2.01	0.41
1:B:218:LEU:HG	1:B:219:ASN:N	2.36	0.41
1:B:240:ILE:HG13	1:B:241:ASP:N	2.35	0.41
1:A:240:ILE:HG13	1:A:241:ASP:N	2.35	0.41
1:B:97:GLU:HA	1:B:98:PRO:HD3	1.93	0.41
1:B:137:VAL:O	1:B:141:ILE:HG13	2.21	0.41
1:B:527:GLU:C	1:B:530:PRO:HD3	2.40	0.41
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.56	0.41
1:B:239:LEU:HD22	1:B:242:ARG:HB2	2.02	0.41
1:B:521:GLU:O	1:B:523:VAL:N	2.52	0.41
1:B:410:TRP:HD1	1:B:414:ILE:HD13	1.84	0.41
1:A:296:ASP:O	1:A:299:TYR:HB2	2.20	0.41
1:B:466:HIS:ND1	1:B:466:HIS:N	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:O	1:A:139:ARG:HG3	2.20	0.41
1:A:240:ILE:C	1:A:242:ARG:H	2.25	0.41
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.82	0.41
1:B:24:ARG:NH2	1:B:53:ARG:HH11	2.15	0.41
1:B:178:GLN:HB3	1:B:183:ASN:OD1	2.20	0.41
1:B:233:ARG:NH1	1:B:237:ASN:HD21	2.19	0.41
1:B:347:LYS:O	1:B:347:LYS:HD3	2.20	0.41
1:B:385:LEU:HD22	1:B:389:ASP:HB3	2.02	0.41
1:A:165:LYS:H	1:A:165:LYS:HG3	1.69	0.41
1:A:188:VAL:HB	1:A:247:PHE:HD1	1.85	0.41
1:A:430:VAL:O	1:A:434:LEU:HG	2.20	0.41
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.88	0.40
1:B:212:LYS:HE2	1:B:212:LYS:HA	2.01	0.40
1:A:484:LEU:CD1	1:A:533:MET:HG2	2.42	0.40
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.40
1:A:410:TRP:CD1	1:A:414:ILE:HD13	2.51	0.40
1:B:269:LEU:HD22	1:B:270:VAL:N	2.37	0.40
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.67	0.40
1:B:252:VAL:CG2	1:B:257:THR:HG21	2.52	0.40
1:B:202:ASP:O	1:B:205:THR:HB	2.22	0.40
1:B:204:PHE:O	1:B:235:ILE:HD11	2.22	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	504/549 (92%)	406 (81%)	73 (14%)	25 (5%)	2	15
1	B	505/549 (92%)	407 (81%)	71 (14%)	27 (5%)	2	14
2	C	5/8 (62%)	2 (40%)	1 (20%)	2 (40%)	0	0
2	D	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1017/1114 (91%)	816 (80%)	146 (14%)	55 (5%)	2	13

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER
2	C	751	ASN
1	B	109	GLN
1	B	127	GLN
1	B	327	SER
1	B	341	GLU
1	B	398	VAL
1	B	445	SER
1	A	112	ARG
1	A	208	LEU
1	A	244	ASN
1	A	396	ALA
1	A	465	LYS
1	A	522	THR
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	B	522	THR
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	238	ALA
1	A	284	THR
2	C	750	PHE
1	B	2	LEU
1	B	73	ASP
1	B	104	VAL
1	B	160	ARG
1	B	176	SER
1	B	208	LEU
1	B	238	ALA
1	B	284	THR
1	A	485	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	750	PHE
1	A	33	LYS
1	A	237	ASN
1	B	35	ILE
1	B	116	ASP
1	B	257	THR
1	B	328	GLY
1	B	354	LYS
1	A	484	LEU
1	B	102	ARG
1	A	311	VAL
1	B	311	VAL
1	A	70	PRO
1	A	108	PRO
1	B	70	PRO
1	B	106	ILE
1	A	35	ILE
1	A	416	VAL

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	462/501 (92%)	393 (85%)	69 (15%)	3	13
1	B	464/501 (93%)	388 (84%)	76 (16%)	2	10
2	C	6/7 (86%)	5 (83%)	1 (17%)	2	10
2	D	5/7 (71%)	4 (80%)	1 (20%)	1	5
All	All	937/1016 (92%)	790 (84%)	147 (16%)	2	12

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	15	THR
1	A	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	46	LYS
1	A	51	LEU
1	A	52	GLU
1	A	67	GLU
1	A	68	LEU
1	A	77	TYR
1	A	95	ILE
1	A	113	GLN
1	A	115	LEU
1	A	117	ARG
1	A	126	LYS
1	A	128	MET
1	A	130	CYS
1	A	131	TYR
1	A	155	LEU
1	A	157	LEU
1	A	174	SER
1	A	179	LEU
1	A	180	ILE
1	A	185	ASP
1	A	189	TRP
1	A	198	LYS
1	A	203	LEU
1	A	217	LEU
1	A	218	LEU
1	A	220	PHE
1	A	223	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	241	ASP
1	A	253	VAL
1	A	255	GLU
1	A	262	GLN
1	A	269	LEU
1	A	284	THR
1	A	286	GLU
1	A	296	ASP
1	A	309	MET
1	A	316	GLU
1	A	332	THR
1	A	348	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
1	A	374	LEU
1	A	379	GLN
1	A	381	CYS
1	A	387	ASP
1	A	404	ASP
1	A	405	ILE
1	A	408	LYS
1	A	409	LEU
1	A	410	TRP
1	A	437	LEU
1	A	444	LEU
1	A	451	VAL
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	466	HIS
1	A	485	LEU
1	A	525	ARG
1	A	533	MET
2	C	750	PHE
1	B	1	MET
1	B	4	GLU
1	B	15	THR
1	B	17	LEU
1	B	46	LYS
1	B	52	GLU
1	B	67	GLU
1	B	68	LEU
1	B	77	TYR
1	B	97	GLU
1	B	99	ASP
1	B	104	VAL
1	B	106	ILE
1	B	109	GLN
1	B	112	ARG
1	B	114	MET
1	B	116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	ARG
1	B	126	LYS
1	B	128	MET
1	B	130	CYS
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	174	SER
1	B	175	LYS
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU
1	B	217	LEU
1	B	218	LEU
1	B	220	PHE
1	B	223	VAL
1	B	227	THR
1	B	233	ARG
1	B	239	LEU
1	B	241	ASP
1	B	253	VAL
1	B	255	GLU
1	B	257	THR
1	B	262	GLN
1	B	269	LEU
1	B	283	GLN
1	B	284	THR
1	B	286	GLU
1	B	296	ASP
1	B	309	MET
1	B	316	GLU
1	B	332	THR
1	B	348	MET
1	B	355	LEU
1	B	363	VAL
1	B	364	GLU
1	B	366	ILE
1	B	369	TYR
1	B	381	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	382	VAL
1	B	388	GLU
1	B	404	ASP
1	B	405	ILE
1	B	408	LYS
1	B	409	LEU
1	B	410	TRP
1	B	444	LEU
1	B	451	VAL
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	462	MET
1	B	466	HIS
1	B	480	LEU
1	B	533	MET
1	B	539	PHE
2	D	752	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	A	602	3	26,33,33	0.94	1 (3%)	31,52,52	1.37	4 (12%)
4	ATP	B	602	3	26,33,33	1.01	2 (7%)	31,52,52	1.51	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	602	3	-	0/18/38/38	0/3/3/3
4	ATP	B	602	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	ATP	C5-C4	2.66	1.48	1.40
4	A	602	ATP	C5-C4	2.58	1.47	1.40
4	B	602	ATP	C2-N3	2.02	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	PA-O3A-PB	-3.87	119.54	132.83
4	B	602	ATP	N3-C2-N1	-3.49	123.22	128.68
4	B	602	ATP	PB-O3B-PG	-3.47	120.91	132.83
4	A	602	ATP	N3-C2-N1	-3.10	123.84	128.68
4	A	602	ATP	PA-O3A-PB	-3.04	122.39	132.83
4	A	602	ATP	PB-O3B-PG	-2.92	122.80	132.83
4	A	602	ATP	C4-C5-N7	-2.46	106.84	109.40
4	B	602	ATP	C4-C5-N7	-2.31	106.99	109.40

There are no chirality outliers.

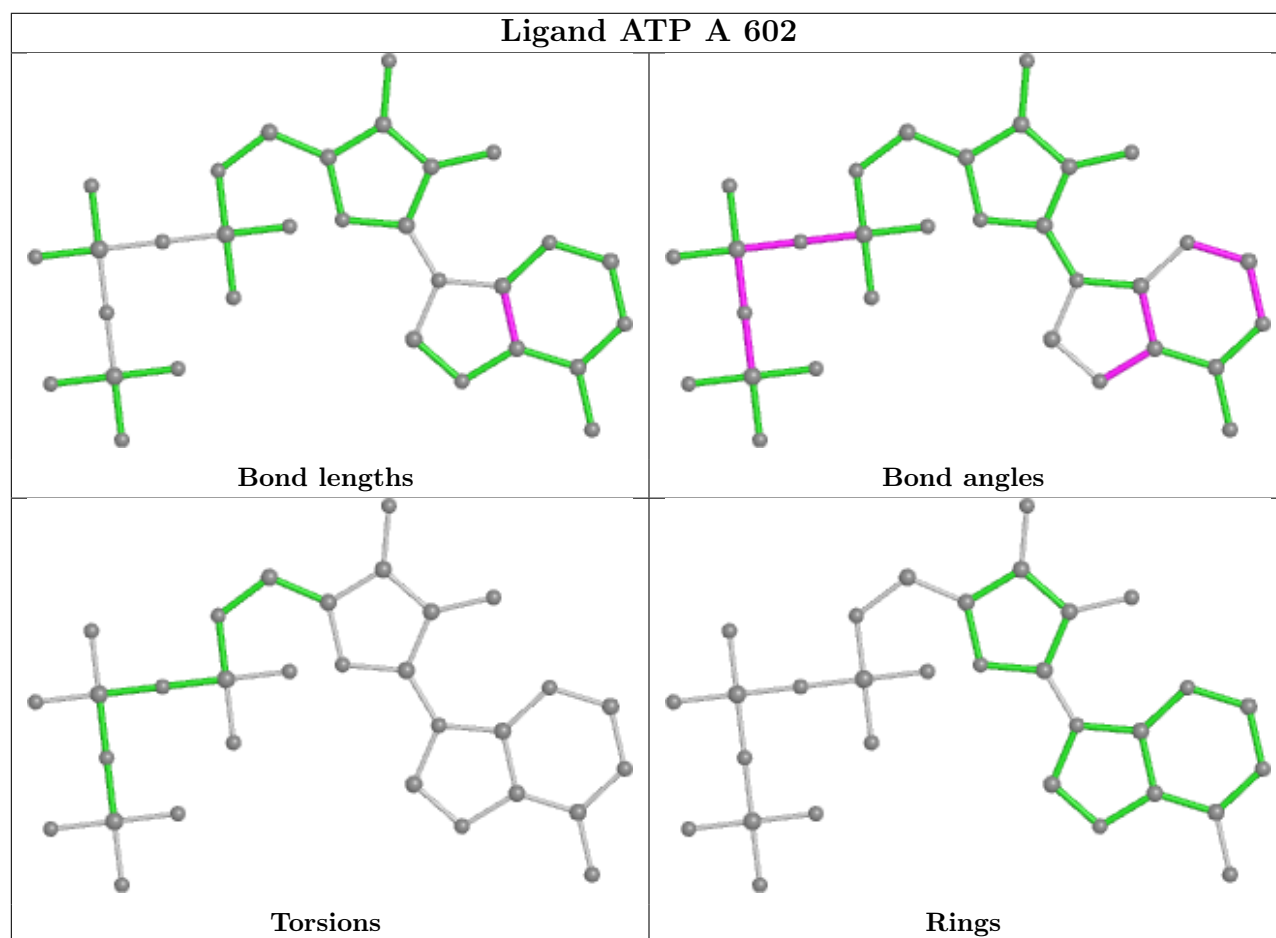
There are no torsion outliers.

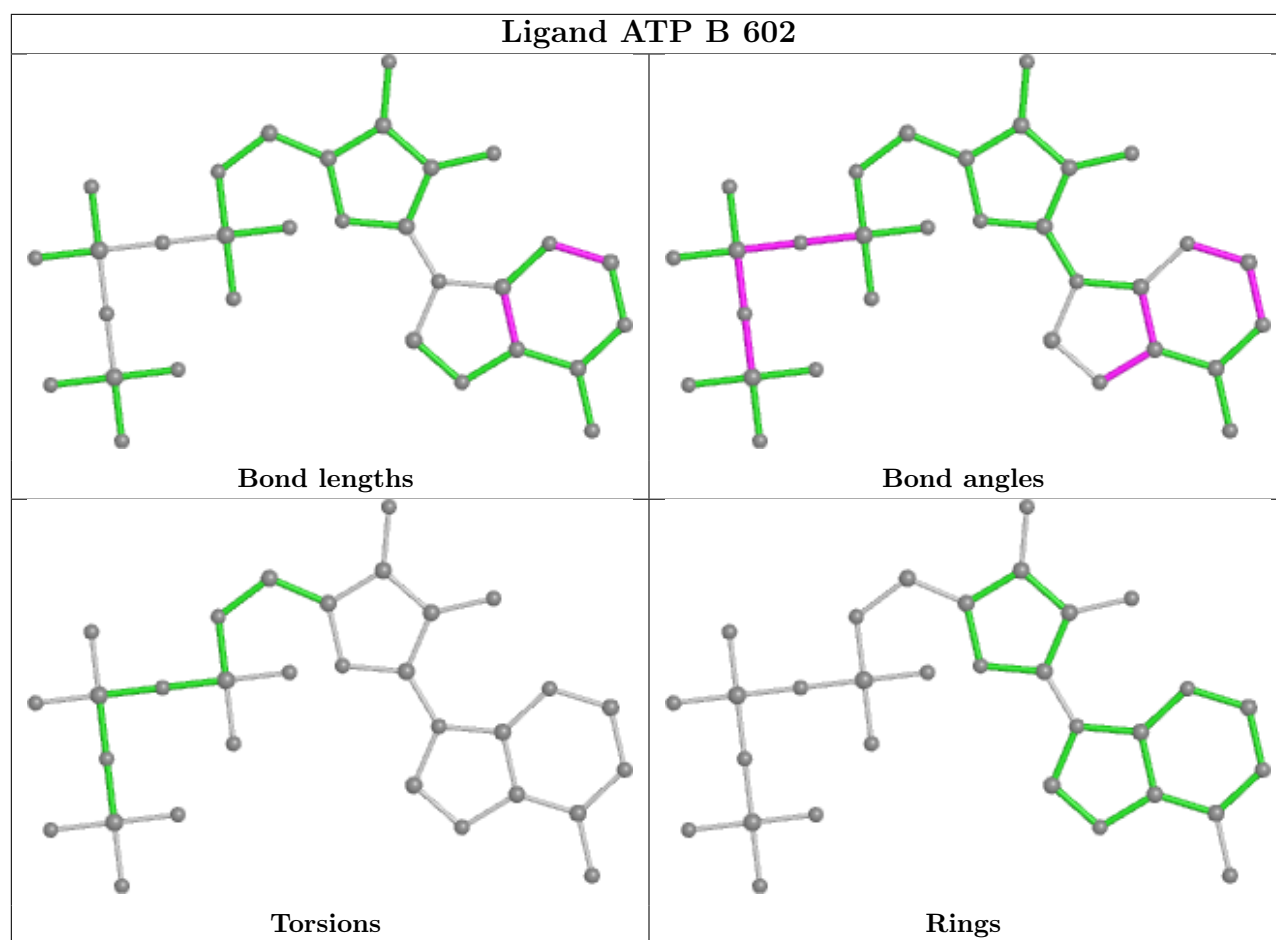
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	1	0
4	B	602	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	510/549 (92%)	0.76	63 (12%) 4 3	177, 244, 305, 345	0
1	B	511/549 (93%)	0.99	84 (16%) 1 1	178, 242, 352, 466	0
2	C	7/8 (87%)	2.35	4 (57%) 0 0	231, 274, 337, 344	0
2	D	5/8 (62%)	2.03	1 (20%) 1 1	228, 249, 302, 304	0
All	All	1033/1114 (92%)	0.89	152 (14%) 2 2	177, 244, 334, 466	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	12.2
1	B	101	LEU	11.5
1	B	34	ASN	9.8
1	B	13	ALA	9.3
1	B	521	GLU	8.6
1	A	31	GLU	8.1
1	B	73	ASP	7.6
1	B	72	ILE	7.6
1	B	36	PHE	7.6
1	B	69	GLY	6.5
1	A	78	ASN	6.1
1	B	68	LEU	6.0
1	B	27	LEU	5.9
1	A	64	GLN	5.7
1	B	14	HIS	5.5
2	C	754	CYS	5.5
1	B	82	HIS	5.4
2	D	753	LEU	5.3
1	B	284	THR	5.2
1	B	51	LEU	4.9
1	B	83	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	4.8
1	B	67	GLU	4.8
1	A	20	ASP	4.7
1	A	32	GLY	4.7
1	A	314	LYS	4.6
1	A	66	SER	4.5
1	B	71	LEU	4.4
1	A	27	LEU	4.3
1	B	52	GLU	4.3
1	B	26	ALA	4.3
1	B	469	ASP	4.2
1	A	35	ILE	4.2
1	A	77	TYR	4.1
1	B	84	ALA	4.1
1	B	487	ILE	4.1
1	A	102	ARG	4.0
1	A	87	LEU	4.0
1	B	150	LEU	4.0
1	A	46	LYS	4.0
1	B	29	TYR	3.9
1	A	23	PRO	3.9
1	B	37	THR	3.9
1	B	543	LEU	3.9
1	B	64	GLN	3.9
1	B	97	GLU	3.9
1	A	101	LEU	3.8
1	A	522	THR	3.8
1	B	23	PRO	3.7
1	B	105	VAL	3.7
1	B	410	TRP	3.6
1	B	149	ASP	3.6
1	A	110	PHE	3.6
1	B	363	VAL	3.6
1	A	49	THR	3.5
1	B	88	GLU	3.5
1	B	108	PRO	3.4
1	B	57	PHE	3.4
1	B	63	ARG	3.4
1	B	95	ILE	3.4
1	A	284	THR	3.4
1	B	525	ARG	3.4
1	B	61	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	86	PHE	3.3
1	A	345	PHE	3.3
1	B	33	LYS	3.3
1	B	346	GLU	3.3
1	B	99	ASP	3.3
1	A	1	MET	3.2
1	B	90	TYR	3.2
1	B	89	ASP	3.2
1	B	75	PHE	3.2
1	B	87	LEU	3.2
1	A	175	LYS	3.2
1	B	80	GLN	3.1
2	C	752	PHE	3.1
1	B	76	ASN	3.0
1	A	311	VAL	3.0
1	A	128	MET	2.9
1	A	319	LEU	2.9
1	A	452	LEU	2.9
1	B	126	LYS	2.9
1	A	346	GLU	2.9
1	B	337	PHE	2.8
1	B	70	PRO	2.8
1	B	152	SER	2.8
1	A	11	SER	2.8
1	B	244	ASN	2.8
1	A	63	ARG	2.8
1	B	103	PRO	2.8
1	B	452	LEU	2.8
1	B	476	GLY	2.8
1	A	106	ILE	2.8
1	B	291	THR	2.8
1	A	315	GLU	2.8
1	B	131	TYR	2.8
1	A	30	LEU	2.7
1	A	57	PHE	2.7
1	B	180	ILE	2.7
1	B	357	SER	2.7
1	B	96	ASN	2.7
1	A	109	GLN	2.6
1	A	100	LEU	2.6
1	B	288	ILE	2.6
1	B	446	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	476	GLY	2.6
1	B	85	ASP	2.6
1	A	303	GLU	2.5
1	B	21	PHE	2.5
1	A	318	VAL	2.5
1	B	253	VAL	2.5
2	C	748	PRO	2.5
1	A	173	LEU	2.5
1	A	521	GLU	2.5
1	A	104	VAL	2.5
1	B	66	SER	2.4
1	B	522	THR	2.4
1	B	414	ILE	2.4
1	B	341	GLU	2.4
1	A	19	HIS	2.4
1	B	168	ILE	2.3
1	B	91	ILE	2.3
1	A	407	VAL	2.3
1	B	468	VAL	2.3
1	B	489	ASN	2.3
1	A	530	PRO	2.3
1	A	88	GLU	2.2
1	A	34	ASN	2.2
1	A	174	SER	2.2
1	A	176	SER	2.2
1	A	472	THR	2.2
1	A	454	PHE	2.2
1	A	525	ARG	2.2
1	A	21	PHE	2.2
1	A	409	LEU	2.1
1	A	471	GLN	2.1
1	B	548	CYS	2.1
1	A	79	ASN	2.1
1	A	469	ASP	2.1
1	A	60	ILE	2.1
1	B	345	PHE	2.1
1	A	36	PHE	2.1
1	B	18	ILE	2.1
2	C	753	LEU	2.1
1	B	486	GLU	2.1
1	A	546	PHE	2.0
1	A	543	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	ARG	2.0
1	B	523	VAL	2.0
1	B	547	ALA	2.0
1	B	546	PHE	2.0
1	B	62	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

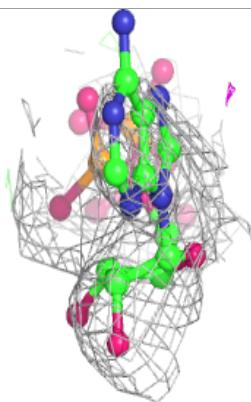
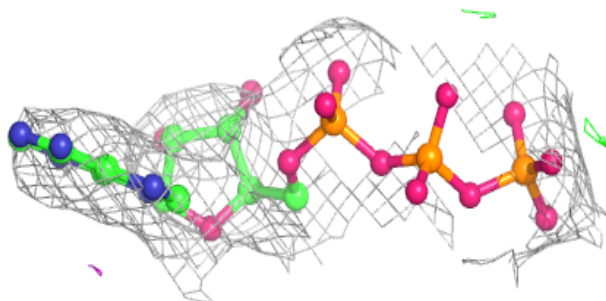
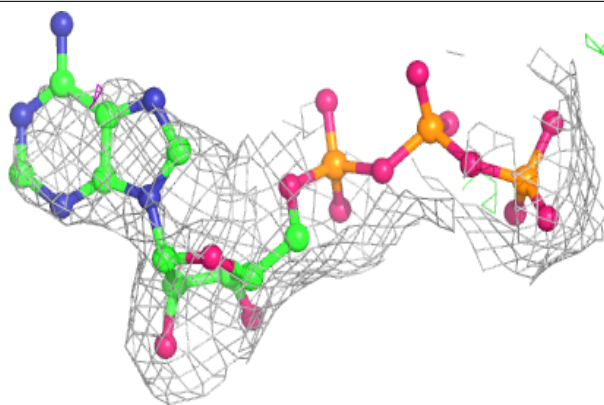
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	601	1/1	0.80	0.39	176,176,176,176	0
3	MG	B	601	1/1	0.83	0.28	168,168,168,168	0
4	ATP	A	602	31/31	0.90	0.24	157,214,239,249	0
4	ATP	B	602	31/31	0.92	0.23	184,209,243,250	0

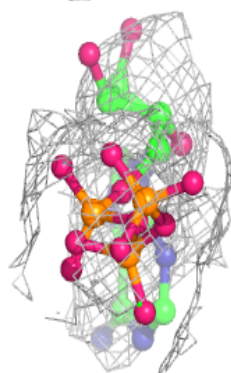
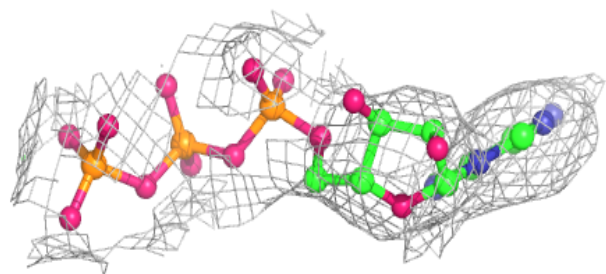
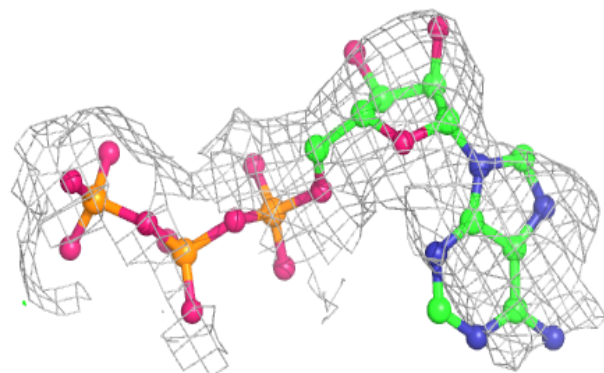
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 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 ATP B 602:**

$2mF_o-DF_c$ (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.