



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 AM UTC

PDB ID : 3DGE / pdb_00003dge
Title : Structure of a histidine kinase-response regulator complex reveals insights into Two-component signaling and a novel cis-autophosphorylation mechanism
Authors : Casino, P.; Marina, A.
Deposited on : 2008-06-13
Resolution : 2.80 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

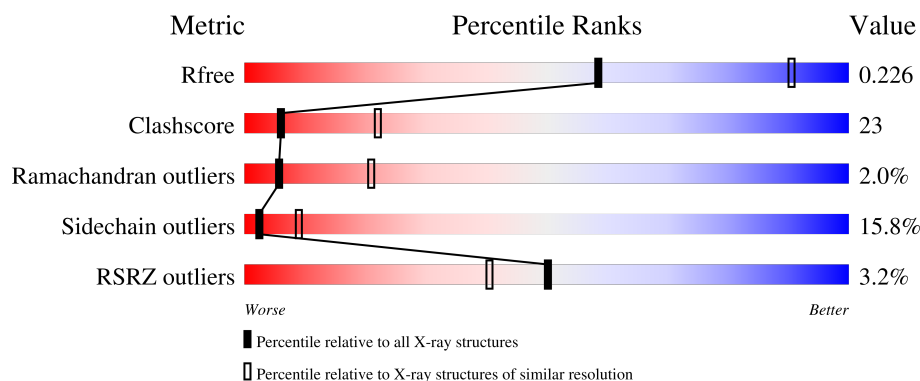
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	258	
1	B	258	
2	C	122	
2	D	122	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5951 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.

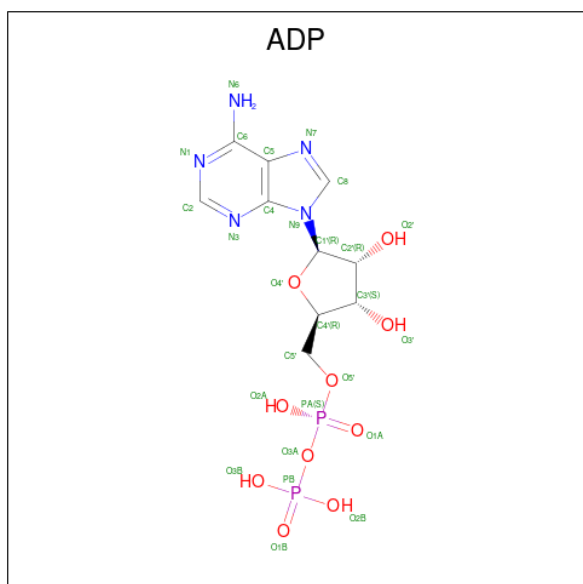
- Molecule 1 is a protein called Sensor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1886	1202	319	362	3			
1	B	237	Total	C	N	O	S	0	0	0
			1886	1202	319	362	3			

- Molecule 2 is a protein called Response regulator.

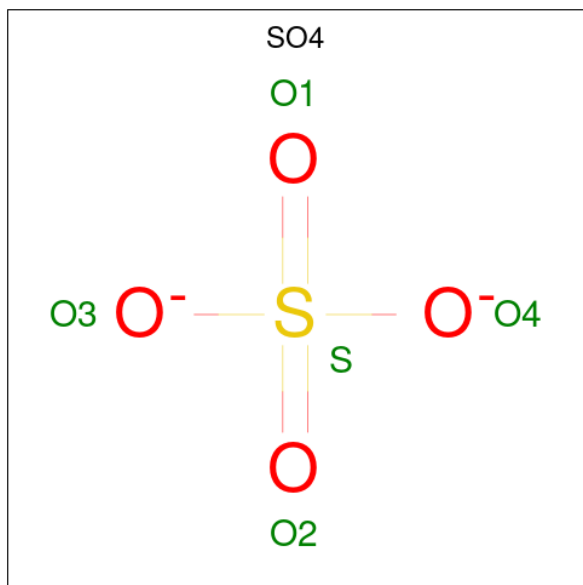
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	122	Total	C	N	O	S	0	0	0
			970	625	157	183	5			
2	D	122	Total	C	N	O	S	0	0	0
			970	625	157	183	5			

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



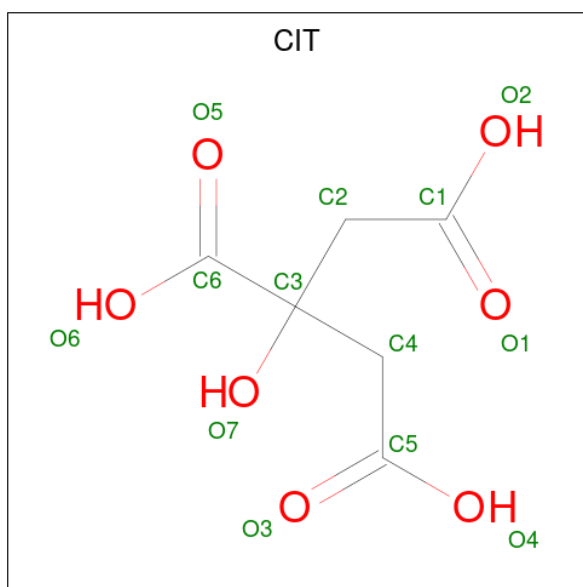
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	N	1	Total	C	O	0	0
			13	6	7		

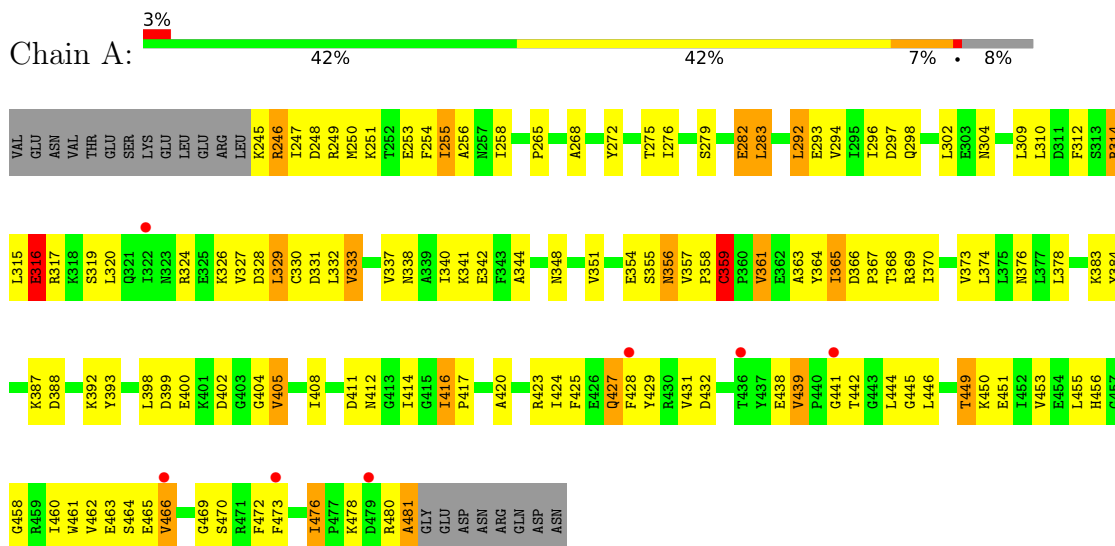
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	C	27	Total	O	0	0
			27	27		
6	B	60	Total	O	0	0
			60	60		
6	D	36	Total	O	0	0
			36	36		
6	N	2	Total	O	0	0
			2	2		

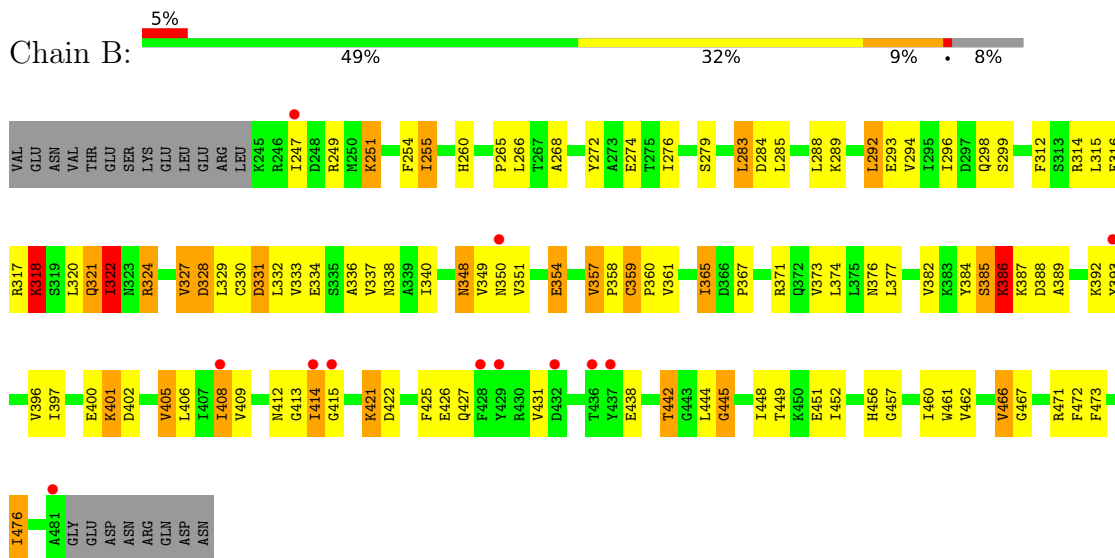
3 Residue-property plots [i](#)

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: Sensor protein

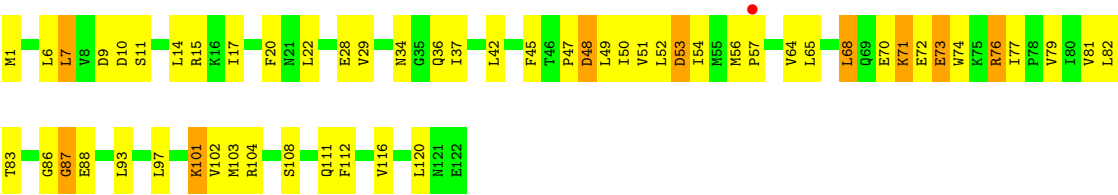


- Molecule 1: Sensor protein

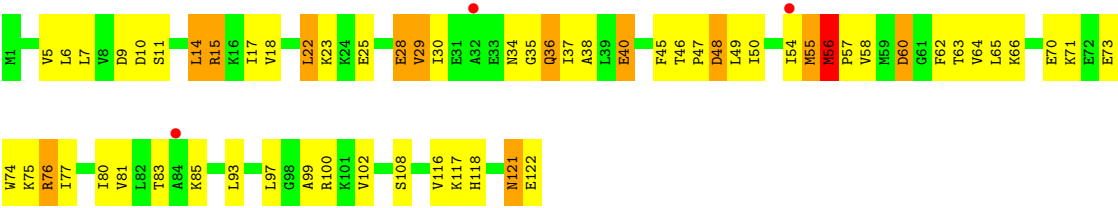


- Molecule 2: Response regulator





● Molecule 2: Response regulator



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.96Å 90.67Å 68.98Å 90.00° 108.42° 90.00°	Depositor
Resolution (Å)	43.64 – 2.80 43.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.64-2.80) 99.6 (43.64-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.234 , 0.284 0.227 , 0.226	Depositor DCC
R_{free} test set	1502 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5951	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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, CIT

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	1.12	7/1918 (0.4%)	1.02	5/2597 (0.2%)
1	B	1.08	11/1918 (0.6%)	1.00	2/2597 (0.1%)
2	C	0.80	0/983	1.02	1/1318 (0.1%)
2	D	0.89	1/983 (0.1%)	1.13	5/1318 (0.4%)
All	All	1.02	19/5802 (0.3%)	1.03	13/7830 (0.2%)

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
1	B	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	ARG	CZ-NH1	25.24	1.68	1.32
1	B	324	ARG	CZ-NH2	11.87	1.48	1.33
1	A	388	ASP	CG-OD1	10.65	1.45	1.25
1	B	422	ASP	CG-OD1	10.18	1.44	1.25
1	A	314	ARG	CZ-NH2	9.76	1.46	1.33
1	B	466	VAL	C-O	9.26	1.35	1.24
1	B	354	GLU	CD-OE2	9.03	1.42	1.25
1	A	388	ASP	CG-OD2	8.77	1.42	1.25
2	D	76	ARG	CZ-NH1	8.31	1.44	1.32
1	B	318	LYS	CG-CD	8.24	1.77	1.52
1	B	426	GLU	CD-OE1	8.12	1.40	1.25
1	A	348	ASN	CG-OD1	7.25	1.37	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	354	GLU	CD-OE1	7.17	1.39	1.25
1	B	422	ASP	CG-OD2	6.50	1.37	1.25
1	B	466	VAL	C-N	6.43	1.42	1.33
1	A	314	ARG	CD-NE	6.21	1.54	1.46
1	B	386	LYS	CE-NZ	5.99	1.67	1.49
1	B	324	ARG	NE-CZ	5.85	1.39	1.33
1	A	481	ALA	C-O	5.59	1.34	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ARG	NE-CZ-NH2	-9.23	110.89	119.20
2	D	56	MET	N-CA-C	8.14	115.46	108.13
1	B	324	ARG	NE-CZ-NH1	-7.58	113.92	121.50
1	A	392	LYS	N-CA-C	7.27	120.86	109.96
1	A	314	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	B	324	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	A	314	ARG	CD-NE-CZ	-6.00	116.00	124.40
1	A	462	VAL	N-CA-C	5.86	117.13	108.45
2	D	56	MET	CA-C-N	5.62	126.86	119.84
2	D	56	MET	C-N-CA	5.62	126.86	119.84
2	D	83	THR	N-CA-C	5.32	118.23	109.72
2	C	56	MET	N-CA-C	5.12	114.19	108.25
2	D	15	ARG	N-CA-C	-5.07	105.64	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	CYS	Peptide
1	B	359	CYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1886	0	1896	109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1886	0	1896	98	0
2	C	970	0	1024	42	0
2	D	970	0	1024	38	0
3	A	27	0	12	5	0
3	B	27	0	12	3	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
5	N	13	0	5	0	0
6	A	37	0	0	5	0
6	B	60	0	0	3	0
6	C	27	0	0	1	0
6	D	36	0	0	2	0
6	N	2	0	0	0	0
All	All	5951	0	5869	264	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 23.

All (264) 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:318:LYS:CD	1:B:318:LYS:CG	1.77	1.54
1:A:314:ARG:NH1	1:A:314:ARG:CZ	1.68	1.51
1:A:314:ARG:NH2	6:A:151:HOH:O	1.83	1.12
1:A:357:VAL:HG22	1:A:358:PRO:HD2	1.31	1.11
1:A:255:ILE:HD11	1:B:254:PHE:CZ	1.97	1.00
1:A:387:LYS:HE2	2:C:57:PRO:HB3	1.43	1.00
1:B:376:ASN:HD21	1:B:445:GLY:C	1.70	0.99
2:C:10:ASP:OD1	6:C:177:HOH:O	1.81	0.97
1:A:258:ILE:HD11	1:A:309:LEU:HD21	1.49	0.94
1:A:376:ASN:ND2	1:A:449:THR:OG1	2.06	0.88
1:A:316:GLU:HG3	1:A:427:GLN:HE22	1.41	0.85
1:A:431:VAL:HB	3:A:500:ADP:O2'	1.77	0.84
2:C:73:GLU:CD	2:C:73:GLU:H	1.87	0.83
1:A:255:ILE:HD11	1:B:254:PHE:HZ	1.42	0.82
2:D:28:GLU:OE1	2:D:28:GLU:HA	1.81	0.81
2:D:100:ARG:NH1	2:D:122:GLU:OE1	2.13	0.81
1:B:387:LYS:HE3	2:D:57:PRO:HB3	1.62	0.80
2:C:49:LEU:HD23	2:C:116:VAL:HG13	1.62	0.79
1:B:318:LYS:CG	1:B:318:LYS:CE	2.60	0.79
1:B:376:ASN:ND2	1:B:445:GLY:O	2.16	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LYS:CD	1:B:318:LYS:CB	2.61	0.78
2:C:101:LYS:HD3	2:C:102:VAL:N	2.00	0.76
1:A:314:ARG:CZ	6:A:151:HOH:O	2.27	0.76
1:B:365:ILE:HG22	1:B:456:HIS:HD2	1.50	0.76
1:A:255:ILE:CD1	1:B:254:PHE:HZ	1.99	0.75
1:B:414:ILE:HG22	1:B:415:GLY:H	1.51	0.74
1:B:316:GLU:HG3	1:B:427:GLN:HE22	1.51	0.74
1:B:357:VAL:HG21	1:B:400:GLU:HG3	1.68	0.74
1:A:258:ILE:CD1	1:A:309:LEU:HD21	2.20	0.72
1:B:376:ASN:ND2	1:B:449:THR:OG1	2.22	0.72
1:A:333:VAL:O	1:A:337:VAL:HG23	1.90	0.70
2:D:55:MET:O	6:D:196:HOH:O	2.08	0.70
1:B:334:GLU:HA	1:B:337:VAL:HB	1.74	0.70
1:A:327:VAL:HG11	1:A:332:LEU:HD12	1.73	0.70
1:A:428:PHE:CE2	1:B:251:LYS:HE2	2.27	0.69
1:B:337:VAL:HG13	1:B:351:VAL:CG1	2.22	0.69
1:A:431:VAL:HB	3:A:500:ADP:HO2'	1.57	0.68
1:B:327:VAL:HG11	1:B:332:LEU:HD12	1.74	0.68
1:A:315:LEU:HD21	1:A:320:LEU:HD23	1.74	0.67
1:B:324:ARG:HD3	1:B:324:ARG:H	1.57	0.67
1:A:316:GLU:OE1	1:A:427:GLN:NE2	2.28	0.67
1:B:329:LEU:O	1:B:333:VAL:HG23	1.94	0.66
1:B:387:LYS:CE	2:D:57:PRO:HB3	2.23	0.66
1:B:431:VAL:HB	3:B:600:ADP:O2'	1.94	0.66
1:A:387:LYS:CE	2:C:57:PRO:HB3	2.22	0.66
1:B:386:LYS:HE2	1:B:388:ASP:H	1.61	0.65
1:A:316:GLU:CG	1:A:427:GLN:HE22	2.08	0.65
1:A:365:ILE:HG22	1:A:456:HIS:HD2	1.62	0.65
2:D:30:ILE:HD13	2:D:45:PHE:CZ	2.32	0.64
2:D:10:ASP:OD1	6:D:196:HOH:O	2.14	0.64
2:C:49:LEU:CD2	2:C:116:VAL:HG13	2.28	0.63
1:A:428:PHE:HE2	1:B:251:LYS:HE2	1.62	0.63
2:C:82:LEU:HD23	2:C:103:MET:HB3	1.80	0.63
1:B:442:THR:HG22	1:B:444:LEU:HD13	1.80	0.62
2:D:5:VAL:O	2:D:29:VAL:HA	1.99	0.62
2:C:93:LEU:O	2:C:97:LEU:HB2	2.00	0.62
1:B:324:ARG:HD3	1:B:324:ARG:N	2.14	0.62
2:D:74:TRP:O	2:D:77:ILE:HG12	1.98	0.62
1:A:254:PHE:CE2	1:B:255:ILE:HD11	2.35	0.62
1:A:312:PHE:HE1	1:A:427:GLN:NE2	1.98	0.62
1:A:355:SER:C	1:A:356:ASN:HD22	2.09	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:LYS:HG3	2:C:73:GLU:OE2	2.01	0.61
1:B:314:ARG:HB3	1:B:320:LEU:HD13	1.83	0.60
2:D:34:ASN:OD1	2:D:37:ILE:HG12	2.02	0.60
1:B:337:VAL:HG13	1:B:351:VAL:HG12	1.84	0.60
1:A:423:ARG:NH2	1:A:429:TYR:CE1	2.70	0.60
1:B:373:VAL:HG13	1:B:449:THR:HG23	1.84	0.59
1:A:317:ARG:HB3	1:A:319:SER:OG	2.03	0.59
2:C:49:LEU:HB2	2:C:120:LEU:HD21	1.84	0.59
1:B:321:GLN:O	1:B:322:ILE:HG13	2.03	0.58
1:B:385:SER:HA	1:B:413:GLY:HA3	1.85	0.58
1:A:272:TYR:CE1	2:C:17:ILE:HB	2.39	0.58
1:A:340:ILE:HD13	1:A:378:LEU:HB3	1.85	0.58
1:B:442:THR:CG2	1:B:444:LEU:HD13	2.34	0.58
2:D:63:THR:O	2:D:64:VAL:C	2.47	0.57
1:A:376:ASN:HD21	1:A:445:GLY:C	2.11	0.57
2:C:93:LEU:O	2:C:93:LEU:HD12	2.05	0.57
1:B:330:CYS:SG	1:B:361:VAL:HG23	2.44	0.57
1:B:349:VAL:HG11	1:B:382:VAL:HG22	1.86	0.56
1:B:315:LEU:HD22	1:B:451:GLU:HG2	1.86	0.56
1:A:276:ILE:HD13	1:A:292:LEU:HD13	1.87	0.56
2:C:48:ASP:OD1	2:C:48:ASP:N	2.38	0.56
1:B:322:ILE:HG22	1:B:324:ARG:HD2	1.88	0.56
1:A:312:PHE:CE1	1:A:427:GLN:NE2	2.74	0.56
1:A:304:ASN:HD22	1:A:304:ASN:N	2.02	0.55
1:A:316:GLU:HG3	1:A:427:GLN:NE2	2.17	0.55
1:A:328:ASP:HA	1:A:361:VAL:O	2.07	0.55
1:B:284:ASP:O	1:B:285:LEU:C	2.50	0.55
1:A:292:LEU:HD21	1:B:276:ILE:HG22	1.87	0.54
2:C:73:GLU:CD	2:C:73:GLU:N	2.62	0.54
2:D:36:GLN:O	2:D:40:GLU:HG3	2.07	0.54
1:A:246:ARG:HE	1:A:250:MET:CE	2.20	0.54
2:C:101:LYS:HD3	2:C:101:LYS:C	2.29	0.54
1:A:365:ILE:HG22	1:A:456:HIS:CD2	2.41	0.54
1:A:329:LEU:O	1:A:333:VAL:HG22	2.07	0.54
2:C:88:GLU:CD	1:B:321:GLN:HE22	2.14	0.54
2:C:53:ASP:OD1	4:C:150:SO4:O3	2.25	0.54
1:B:289:LYS:O	1:B:293:GLU:HG2	2.08	0.54
1:B:279:SER:O	1:B:283:LEU:HB2	2.07	0.53
1:A:420:ALA:O	1:A:424:ILE:HG23	2.09	0.53
2:C:34:ASN:OD1	2:C:37:ILE:HG12	2.08	0.53
1:B:327:VAL:HG11	1:B:332:LEU:CD1	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HG13	1:B:351:VAL:HG11	1.89	0.53
1:B:438:GLU:HA	2:D:55:MET:HG2	1.92	0.53
2:D:18:VAL:HG12	2:D:22:LEU:HD22	1.91	0.53
1:A:315:LEU:C	1:A:317:ARG:H	2.17	0.52
1:A:458:GLY:HA3	1:A:476:ILE:HD13	1.92	0.52
2:D:60:ASP:OD2	2:D:62:PHE:HB2	2.09	0.52
1:A:446:LEU:HG	3:A:500:ADP:O1A	2.09	0.52
1:A:423:ARG:NH2	1:A:429:TYR:HE1	2.08	0.52
1:B:421:LYS:NZ	6:B:153:HOH:O	2.43	0.52
1:A:340:ILE:CD1	1:A:378:LEU:HD13	2.40	0.52
1:B:333:VAL:O	1:B:337:VAL:HG23	2.10	0.52
1:A:314:ARG:CZ	6:A:152:HOH:O	2.56	0.52
1:A:429:TYR:O	3:A:500:ADP:H5'1	2.11	0.51
1:B:260:HIS:HB2	6:B:98:HOH:O	2.11	0.51
1:B:312:PHE:HB2	1:B:444:LEU:HD23	1.92	0.51
1:A:324:ARG:HD3	1:A:364:TYR:O	2.09	0.51
1:A:332:LEU:HD11	1:A:367:PRO:HA	1.91	0.51
2:C:45:PHE:CZ	2:C:47:PRO:HG3	2.45	0.51
1:A:255:ILE:CD1	1:B:254:PHE:CZ	2.76	0.51
1:A:265:PRO:HG2	1:A:302:LEU:HD13	1.93	0.51
1:B:408:ILE:HA	1:B:472:PHE:O	2.10	0.51
2:D:93:LEU:O	2:D:97:LEU:HB2	2.11	0.51
1:A:316:GLU:CD	1:A:427:GLN:NE2	2.68	0.51
1:A:383:LYS:HD3	1:A:439:VAL:HG13	1.93	0.51
1:A:255:ILE:HD11	1:B:254:PHE:CE2	2.43	0.50
1:A:356:ASN:HD22	1:A:356:ASN:N	2.10	0.50
1:A:432:ASP:HA	6:A:125:HOH:O	2.11	0.50
2:D:49:LEU:CD2	2:D:116:VAL:HG13	2.41	0.50
2:C:108:SER:HB3	2:C:111:GLN:HB2	1.93	0.50
1:B:448:ILE:HG22	1:B:452:ILE:HD11	1.94	0.50
1:B:373:VAL:HG13	1:B:449:THR:CG2	2.41	0.50
2:D:121:ASN:C	2:D:121:ASN:HD22	2.18	0.50
2:C:112:PHE:O	2:C:116:VAL:HG23	2.11	0.49
1:B:389:ALA:HB3	1:B:392:LYS:HD3	1.94	0.49
1:A:384:TYR:CZ	3:A:500:ADP:H2'	2.48	0.49
2:C:86:GLY:O	2:C:87:GLY:C	2.55	0.49
1:B:328:ASP:HA	1:B:361:VAL:O	2.12	0.49
1:A:404:GLY:HA2	1:A:478:LYS:H	1.78	0.49
1:B:268:ALA:HB3	1:B:298:GLN:HG3	1.94	0.49
1:A:393:TYR:CE1	1:A:412:ASN:HB3	2.48	0.49
2:C:9:ASP:OD1	2:C:11:SER:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD23	1:B:266:LEU:HD13	1.94	0.49
2:D:71:LYS:O	2:D:75:LYS:HB2	2.12	0.49
1:A:365:ILE:HD13	1:A:370:ILE:HG13	1.95	0.49
1:A:256:ALA:O	6:A:38:HOH:O	2.20	0.48
1:A:411:ASP:OD1	1:A:470:SER:N	2.43	0.48
1:B:348:ASN:N	1:B:348:ASN:HD22	2.12	0.48
1:A:316:GLU:CD	1:A:427:GLN:HE22	2.21	0.48
2:D:71:LYS:HG3	2:D:74:TRP:CE3	2.48	0.48
2:D:6:LEU:HD23	2:D:50:ILE:HG12	1.95	0.48
1:B:333:VAL:O	1:B:337:VAL:N	2.47	0.48
1:A:480:ARG:O	1:A:481:ALA:CB	2.61	0.48
1:A:254:PHE:CZ	1:B:255:ILE:HD11	2.49	0.48
1:A:408:ILE:HA	1:A:472:PHE:O	2.13	0.48
2:D:63:THR:O	2:D:66:LYS:N	2.47	0.48
1:A:324:ARG:HH21	1:A:456:HIS:HA	1.78	0.47
1:A:464:SER:HB2	1:A:469:GLY:O	2.14	0.47
1:A:428:PHE:CD1	1:A:444:LEU:HD11	2.50	0.47
1:B:251:LYS:HA	1:B:254:PHE:HB3	1.97	0.47
1:B:316:GLU:HG3	1:B:427:GLN:NE2	2.23	0.47
1:B:401:LYS:HE3	1:B:402:ASP:H	1.80	0.47
1:B:315:LEU:C	1:B:317:ARG:H	2.21	0.47
2:D:60:ASP:OD2	2:D:62:PHE:N	2.46	0.47
2:C:54:ILE:HG12	2:C:83:THR:HB	1.97	0.47
1:B:268:ALA:CB	1:B:298:GLN:HG3	2.45	0.47
1:A:366:ASP:OD2	1:A:369:ARG:HG2	2.15	0.47
2:D:14:LEU:O	2:D:18:VAL:HG23	2.14	0.47
1:A:251:LYS:HA	1:A:254:PHE:HB3	1.96	0.46
1:B:357:VAL:HG13	1:B:358:PRO:HD2	1.97	0.46
1:A:357:VAL:HG22	1:A:358:PRO:CD	2.23	0.46
1:A:480:ARG:O	1:A:481:ALA:HB3	2.16	0.46
1:B:384:TYR:CZ	3:B:600:ADP:H2'	2.51	0.46
1:A:272:TYR:CZ	1:A:294:VAL:HG11	2.50	0.46
2:C:52:LEU:CD2	2:C:65:LEU:HG	2.46	0.46
1:B:272:TYR:CE1	2:D:17:ILE:HB	2.51	0.46
2:D:75:LYS:HB3	2:D:76:ARG:HD2	1.97	0.46
1:B:476:ILE:HD13	1:B:476:ILE:HA	1.75	0.46
1:B:425:PHE:CZ	1:B:460:ILE:HG12	2.50	0.45
1:A:254:PHE:HE2	1:B:255:ILE:HD11	1.79	0.45
1:A:246:ARG:HG3	1:A:249:ARG:NH2	2.31	0.45
1:A:268:ALA:HB3	1:A:298:GLN:HG3	1.97	0.45
1:A:357:VAL:CG2	1:A:358:PRO:HD2	2.22	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:28:GLU:HA	2:C:28:GLU:OE1	2.17	0.45
2:C:74:TRP:O	2:C:77:ILE:HG12	2.15	0.45
1:B:374:LEU:HD12	1:B:374:LEU:HA	1.85	0.45
1:B:367:PRO:O	1:B:371:ARG:HB2	2.17	0.45
2:D:30:ILE:HD13	2:D:45:PHE:HZ	1.82	0.45
1:B:396:VAL:HG22	1:B:409:VAL:HG22	1.99	0.45
2:D:48:ASP:N	2:D:48:ASP:OD1	2.50	0.45
1:A:258:ILE:HD11	1:A:309:LEU:CD2	2.33	0.45
1:A:310:LEU:HD21	1:A:314:ARG:HH21	1.82	0.45
2:C:7:LEU:HD13	2:C:15:ARG:HG2	1.99	0.45
1:B:272:TYR:CZ	1:B:294:VAL:HG11	2.52	0.45
1:B:373:VAL:O	1:B:374:LEU:C	2.59	0.45
2:D:121:ASN:C	2:D:121:ASN:ND2	2.74	0.45
1:A:283:LEU:HD13	2:C:20:PHE:CZ	2.52	0.45
1:B:365:ILE:HG22	1:B:456:HIS:CD2	2.40	0.45
2:D:11:SER:O	2:D:15:ARG:HG3	2.17	0.45
2:D:35:GLY:O	2:D:38:ALA:HB3	2.17	0.44
1:A:246:ARG:HH21	1:A:250:MET:HE1	1.83	0.44
2:C:6:LEU:HB3	2:C:50:ILE:HG12	1.99	0.44
1:A:341:LYS:HA	1:A:344:ALA:HB3	1.98	0.44
1:A:373:VAL:HG13	1:A:449:THR:CG2	2.47	0.44
1:B:265:PRO:HA	1:B:298:GLN:HE21	1.83	0.44
1:A:445:GLY:O	1:A:449:THR:OG1	2.33	0.44
2:D:23:LYS:C	2:D:25:GLU:H	2.26	0.44
1:A:399:ASP:O	1:A:405:VAL:HG12	2.18	0.44
2:C:64:VAL:O	2:C:68:LEU:HD23	2.18	0.44
1:A:268:ALA:CB	1:A:298:GLN:HG3	2.48	0.43
1:B:397:ILE:HB	1:B:408:ILE:HG23	2.00	0.43
1:A:326:LYS:HA	1:A:363:ALA:O	2.18	0.43
1:B:457:GLY:HA2	6:B:57:HOH:O	2.18	0.43
2:D:10:ASP:HB3	2:D:56:MET:HB3	2.00	0.43
1:A:446:LEU:HA	1:A:449:THR:OG1	2.18	0.43
2:C:7:LEU:HD23	2:C:51:VAL:HB	2.01	0.43
1:B:431:VAL:HB	3:B:600:ADP:HO2'	1.82	0.43
2:D:65:LEU:HD21	2:D:99:ALA:HB2	2.00	0.43
1:A:275:THR:CB	2:C:17:ILE:HD11	2.48	0.43
1:B:334:GLU:C	1:B:336:ALA:N	2.74	0.43
1:B:292:LEU:O	1:B:296:ILE:HG13	2.19	0.43
2:D:11:SER:HB3	2:D:14:LEU:HB2	2.01	0.43
2:C:50:ILE:HB	2:C:79:VAL:HG22	2.01	0.42
1:B:421:LYS:O	1:B:462:VAL:CG1	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD21	1:A:314:ARG:NH2	2.33	0.42
1:A:416:ILE:CG2	1:A:417:PRO:HD2	2.49	0.42
1:B:386:LYS:H	1:B:413:GLY:HA2	1.84	0.42
2:D:81:VAL:HB	2:D:102:VAL:HG22	2.00	0.42
1:A:411:ASP:OD1	1:A:411:ASP:C	2.61	0.42
1:A:376:ASN:ND2	1:A:445:GLY:O	2.52	0.42
1:A:428:PHE:HD1	1:A:444:LEU:HD11	1.84	0.42
1:A:316:GLU:CG	1:A:427:GLN:NE2	2.80	0.42
1:A:465:GLU:HG3	1:A:466:VAL:H	1.84	0.42
1:A:315:LEU:CD2	1:A:320:LEU:HD23	2.45	0.42
1:A:449:THR:O	1:A:453:VAL:HG23	2.19	0.42
1:B:338:ASN:C	1:B:340:ILE:H	2.26	0.42
2:C:52:LEU:O	2:C:81:VAL:HA	2.20	0.42
1:B:312:PHE:CB	1:B:444:LEU:HD23	2.48	0.42
1:A:245:LYS:C	1:A:247:ILE:H	2.28	0.41
1:A:330:CYS:SG	1:A:361:VAL:HG23	2.60	0.41
1:A:425:PHE:CE2	1:A:460:ILE:HG12	2.55	0.41
2:C:71:LYS:HE3	2:C:72:GLU:H	1.85	0.41
1:B:288:LEU:HG	1:B:292:LEU:HD22	2.02	0.41
1:B:405:VAL:N	1:B:476:ILE:O	2.43	0.41
1:B:444:LEU:O	1:B:445:GLY:C	2.63	0.41
1:B:461:TRP:CE2	1:B:473:PHE:HB2	2.55	0.41
1:B:408:ILE:HD12	1:B:473:PHE:CE2	2.56	0.41
1:A:296:ILE:HD13	1:B:274:GLU:HG2	2.02	0.41
1:B:385:SER:HA	1:B:413:GLY:CA	2.50	0.41
2:C:9:ASP:O	2:C:15:ARG:NH1	2.46	0.41
2:C:9:ASP:C	2:C:11:SER:H	2.29	0.41
2:C:76:ARG:HA	2:C:76:ARG:HD3	1.70	0.41
1:B:331:ASP:OD1	1:B:331:ASP:C	2.63	0.41
2:D:9:ASP:O	2:D:15:ARG:HD3	2.21	0.41
2:C:36:GLN:O	2:C:37:ILE:C	2.64	0.41
2:D:46:THR:HA	2:D:47:PRO:HD3	1.80	0.41
1:A:292:LEU:O	1:A:296:ILE:HG13	2.21	0.40
2:C:11:SER:O	2:C:15:ARG:HG3	2.21	0.40
1:B:473:PHE:CD1	1:B:473:PHE:N	2.89	0.40
1:A:279:SER:HB3	1:A:282:GLU:HG2	2.03	0.40
1:A:461:TRP:CE2	1:A:473:PHE:HB2	2.55	0.40
1:A:451:GLU:O	1:A:455:LEU:HG	2.21	0.40
1:B:393:TYR:CD1	1:B:393:TYR:C	2.99	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	235/258 (91%)	209 (89%)	21 (9%)	5 (2%)	5	20
1	B	235/258 (91%)	204 (87%)	23 (10%)	8 (3%)	3	11
2	C	120/122 (98%)	105 (88%)	14 (12%)	1 (1%)	16	44
2	D	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
All	All	710/760 (93%)	626 (88%)	70 (10%)	14 (2%)	6	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	GLY
2	C	87	GLY
1	B	318	LYS
1	B	322	ILE
1	B	466	VAL
1	B	360	PRO
1	B	467	GLY
1	A	361	VAL
1	B	421	LYS
1	A	359	CYS
1	B	359	CYS
1	A	316	GLU
1	A	466	VAL
1	B	445	GLY

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	210/232 (90%)	174 (83%)	36 (17%)	2	7
1	B	210/232 (90%)	181 (86%)	29 (14%)	3	12
2	C	110/110 (100%)	95 (86%)	15 (14%)	3	13
2	D	110/110 (100%)	89 (81%)	21 (19%)	1	5
All	All	640/684 (94%)	539 (84%)	101 (16%)	2	9

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	ARG
1	A	248	ASP
1	A	253	GLU
1	A	255	ILE
1	A	282	GLU
1	A	283	LEU
1	A	292	LEU
1	A	293	GLU
1	A	297	ASP
1	A	316	GLU
1	A	329	LEU
1	A	331	ASP
1	A	333	VAL
1	A	338	ASN
1	A	342	GLU
1	A	351	VAL
1	A	354	GLU
1	A	356	ASN
1	A	359	CYS
1	A	365	ILE
1	A	368	THR
1	A	374	LEU
1	A	398	LEU
1	A	400	GLU
1	A	402	ASP
1	A	405	VAL
1	A	414	ILE
1	A	416	ILE
1	A	427	GLN
1	A	438	GLU
1	A	439	VAL
1	A	442	THR
1	A	449	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	450	LYS
1	A	463	GLU
1	A	476	ILE
2	C	1	MET
2	C	7	LEU
2	C	14	LEU
2	C	22	LEU
2	C	29	VAL
2	C	42	LEU
2	C	48	ASP
2	C	53	ASP
2	C	68	LEU
2	C	70	GLU
2	C	71	LYS
2	C	73	GLU
2	C	76	ARG
2	C	101	LYS
2	C	104	ARG
1	B	247	ILE
1	B	249	ARG
1	B	251	LYS
1	B	255	ILE
1	B	283	LEU
1	B	292	LEU
1	B	299	SER
1	B	321	GLN
1	B	322	ILE
1	B	327	VAL
1	B	328	ASP
1	B	331	ASP
1	B	348	ASN
1	B	350	ASN
1	B	354	GLU
1	B	357	VAL
1	B	365	ILE
1	B	377	LEU
1	B	385	SER
1	B	386	LYS
1	B	401	LYS
1	B	405	VAL
1	B	406	LEU
1	B	408	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	412	ASN
1	B	414	ILE
1	B	442	THR
1	B	471	ARG
1	B	476	ILE
2	D	7	LEU
2	D	14	LEU
2	D	22	LEU
2	D	28	GLU
2	D	29	VAL
2	D	36	GLN
2	D	40	GLU
2	D	48	ASP
2	D	54	ILE
2	D	55	MET
2	D	56	MET
2	D	58	VAL
2	D	60	ASP
2	D	70	GLU
2	D	73	GLU
2	D	80	ILE
2	D	85	LYS
2	D	108	SER
2	D	117	LYS
2	D	118	HIS
2	D	121	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	HIS
1	A	278	ASN
1	A	304	ASN
1	A	350	ASN
1	A	356	ASN
1	A	376	ASN
1	A	379	ASN
1	A	427	GLN
2	C	36	GLN
2	C	69	GLN
1	B	278	ASN
1	B	298	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	300	ASN
1	B	321	GLN
1	B	348	ASN
1	B	376	ASN
1	B	379	ASN
1	B	380	ASN
1	B	412	ASN
2	D	121	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
5	CIT	N	3	-	12,12,12	1.13	0	17,17,17	1.34	1 (5%)
3	ADP	B	600	-	28,29,29	1.66	6 (21%)	43,45,45	1.85	9 (20%)
4	SO4	D	160	-	4,4,4	0.25	0	6,6,6	0.34	0
4	SO4	C	150	-	4,4,4	0.32	0	6,6,6	0.38	0
3	ADP	A	500	-	28,29,29	1.69	5 (17%)	43,45,45	1.90	11 (25%)

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	600	-	-	3/16/32/32	0/3/3/3
3	ADP	A	500	-	-	4/16/32/32	0/3/3/3
5	CIT	N	3	-	-	11/16/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	ADP	C5-C4	5.54	1.49	1.39
3	B	600	ADP	C5-C4	5.16	1.48	1.39
3	B	600	ADP	PA-O3A	3.32	1.63	1.59
3	A	500	ADP	PA-O3A	2.93	1.62	1.59
3	A	500	ADP	C8-N7	2.89	1.37	1.31
3	A	500	ADP	C5-C6	2.89	1.49	1.41
3	B	600	ADP	C5-C6	2.66	1.48	1.41
3	B	600	ADP	C5-N7	-2.64	1.34	1.39
3	B	600	ADP	C8-N7	2.44	1.36	1.31
3	A	500	ADP	C5-N7	-2.32	1.34	1.39
3	B	600	ADP	C4-N9	-2.10	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	ADP	C5-C4-N3	-5.37	119.33	126.72
3	B	600	ADP	C5-C4-N3	-5.27	119.47	126.72
3	B	600	ADP	N3-C4-N9	4.58	134.96	127.17
3	A	500	ADP	N3-C4-N9	4.42	134.69	127.17
3	A	500	ADP	O2A-PA-O3A	3.90	117.80	107.27
3	B	600	ADP	O2A-PA-O3A	3.76	117.44	107.27
5	N	3	CIT	O6-C6-C3	3.54	119.92	113.14
3	A	500	ADP	C4-C5-N7	-3.34	106.77	110.58
3	B	600	ADP	C2-N3-C4	3.17	119.56	111.83
3	B	600	ADP	N3-C2-N1	-3.05	123.97	128.58
3	B	600	ADP	C4-N9-C8	3.01	108.90	105.74
3	A	500	ADP	C2-N3-C4	2.95	119.04	111.83
3	B	600	ADP	C4-C5-N7	-2.86	107.31	110.58
3	A	500	ADP	C4-N9-C8	2.84	108.72	105.74
3	A	500	ADP	N3-C2-N1	-2.53	124.75	128.58
3	A	500	ADP	C5-N7-C8	2.45	107.29	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	ADP	O3B-PB-O3A	-2.35	96.76	104.64
3	A	500	ADP	O3B-PB-O2B	2.27	116.31	107.80
3	B	600	ADP	C5-N7-C8	2.19	106.89	103.45
3	A	500	ADP	C2-N1-C6	2.09	122.16	118.73
3	A	500	ADP	O3B-PB-O3A	-2.03	97.81	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	ADP	O4'-C4'-C5'-O5'
3	B	600	ADP	PA-O3A-PB-O2B
3	B	600	ADP	O4'-C4'-C5'-O5'
5	N	3	CIT	C1-C2-C3-O7
5	N	3	CIT	C1-C2-C3-C4
5	N	3	CIT	C1-C2-C3-C6
3	A	500	ADP	C3'-C4'-C5'-O5'
3	B	600	ADP	C3'-C4'-C5'-O5'
5	N	3	CIT	C2-C3-C6-O5
5	N	3	CIT	C4-C3-C6-O6
5	N	3	CIT	O7-C3-C6-O5
5	N	3	CIT	C2-C3-C6-O6
3	A	500	ADP	PA-O3A-PB-O3B
5	N	3	CIT	O7-C3-C6-O6
5	N	3	CIT	C4-C3-C6-O5
3	A	500	ADP	PB-O3A-PA-O2A
5	N	3	CIT	O2-C1-C2-C3
5	N	3	CIT	O1-C1-C2-C3

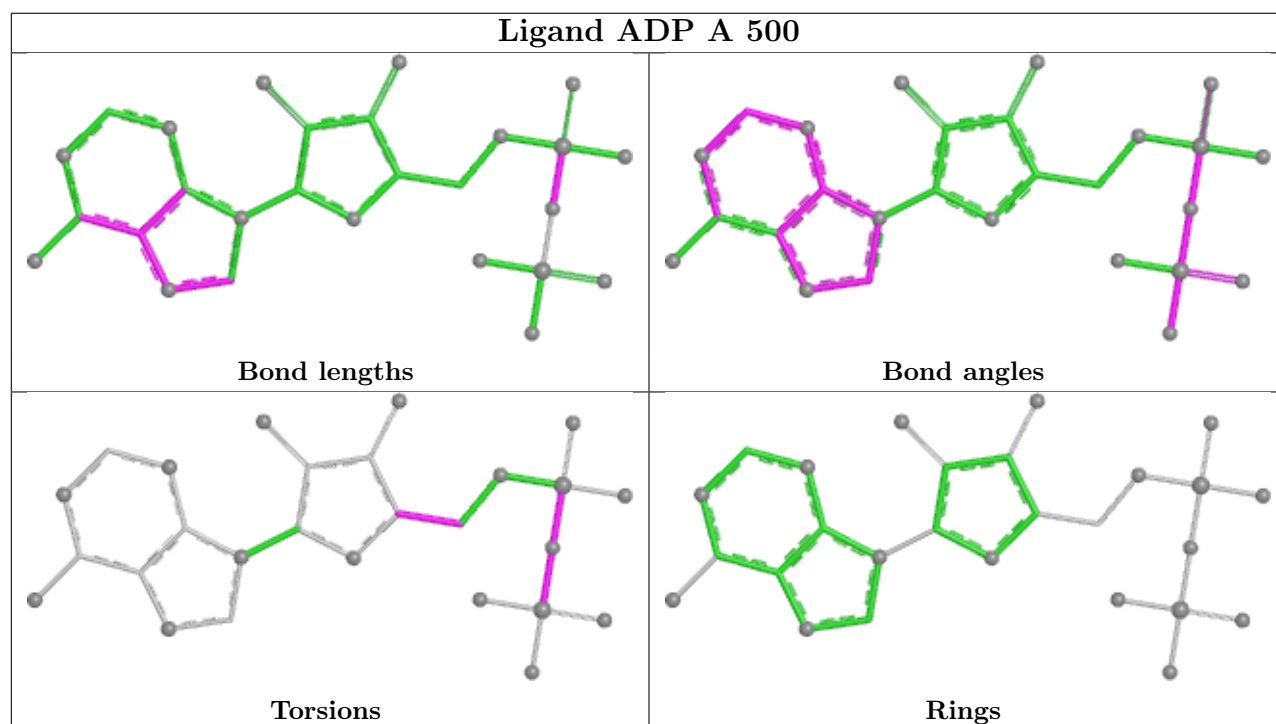
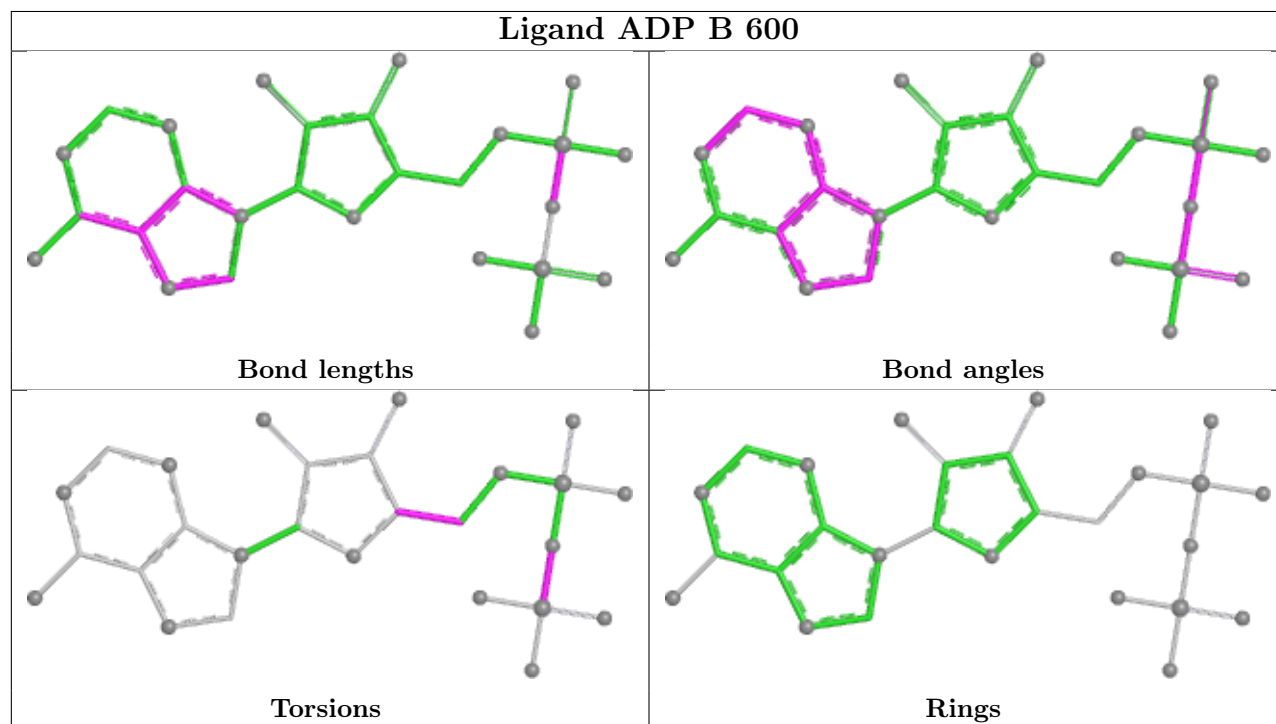
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	ADP	3	0
4	C	150	SO4	1	0
3	A	500	ADP	5	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	237/258 (91%)	0.51	7 (2%) 52 42	30, 86, 103, 108	0
1	B	237/258 (91%)	0.37	12 (5%) 33 25	33, 80, 102, 104	0
2	C	122/122 (100%)	0.23	1 (0%) 82 75	34, 70, 86, 88	0
2	D	122/122 (100%)	0.70	3 (2%) 58 48	45, 70, 84, 87	0
All	All	718/760 (94%)	0.45	23 (3%) 50 40	30, 77, 102, 108	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	84	ALA	3.2
1	A	428	PHE	3.2
2	D	32	ALA	3.0
1	B	393	TYR	2.6
1	A	436	THR	2.6
2	C	57	PRO	2.6
1	A	441	GLY	2.5
1	B	247	ILE	2.4
1	B	414	ILE	2.4
1	A	479	ASP	2.4
1	B	481	ALA	2.3
1	B	436	THR	2.2
1	B	429	TYR	2.2
1	A	322	ILE	2.2
1	A	473	PHE	2.2
1	B	428	PHE	2.1
1	B	408	ILE	2.1
2	D	54	ILE	2.1
1	B	415	GLY	2.1
1	B	432	ASP	2.0
1	B	437	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	350	ASN	2.0
1	A	466	VAL	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](#)

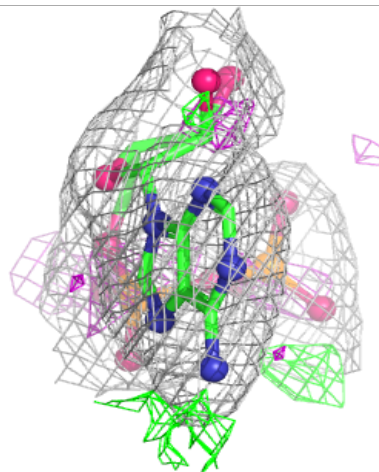
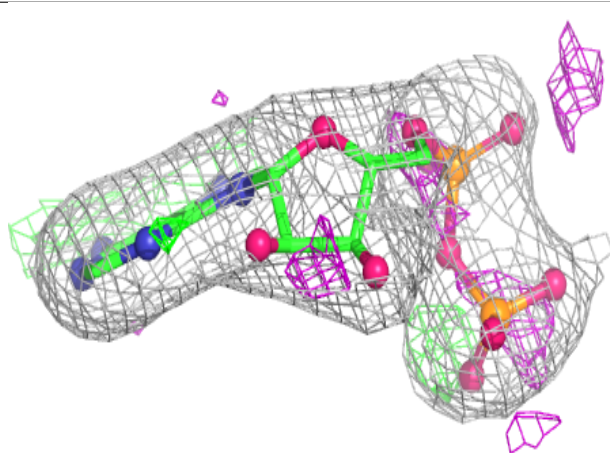
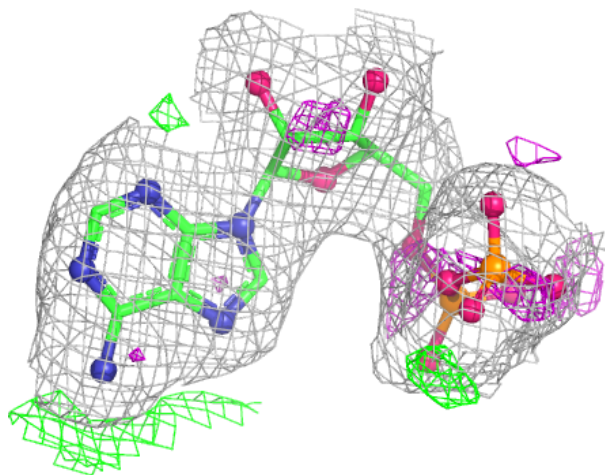
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CIT	N	3	13/13	0.70	0.13	107,108,109,110	0
4	SO4	D	160	5/5	0.88	0.13	101,102,103,103	0
3	ADP	A	500	27/27	0.91	0.09	48,65,71,73	0
3	ADP	B	600	27/27	0.93	0.10	48,61,66,68	0
4	SO4	C	150	5/5	0.95	0.11	99,100,100,101	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.

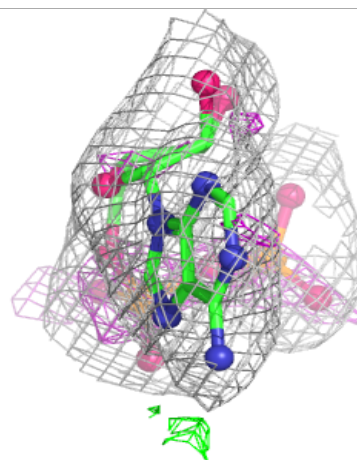
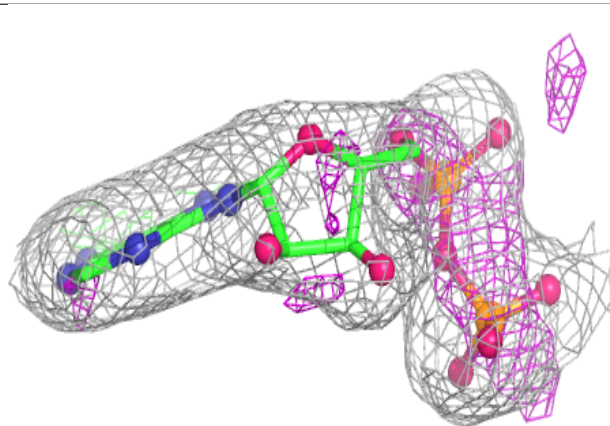
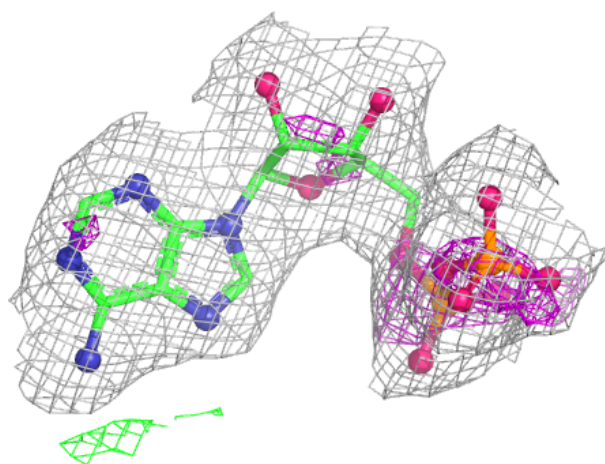
Electron density around ADP A 500:

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



Electron density around ADP B 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.