



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 1H1S / pdb_00001h1s
Title : Structure of human Thr160-phospho CDK2/cyclin A complexed with the inhibitor NU6102
Authors : Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.
Deposited on : 2002-07-21
Resolution : 2.00 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

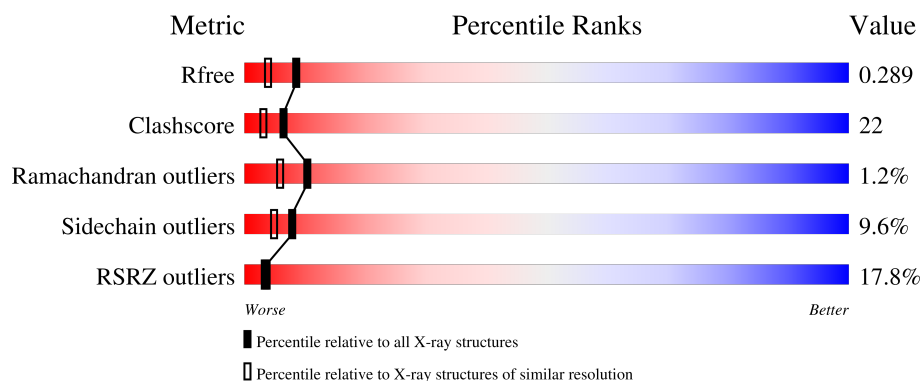
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	303	
1	C	303	
2	B	258	
2	D	258	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9701 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.

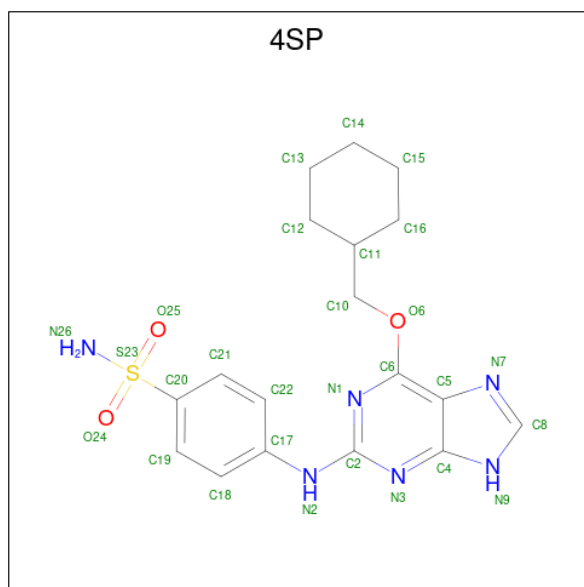
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (CCD ID: 4SP) (formula: C₁₈H₂₂N₆O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			28	18	6	3	1		

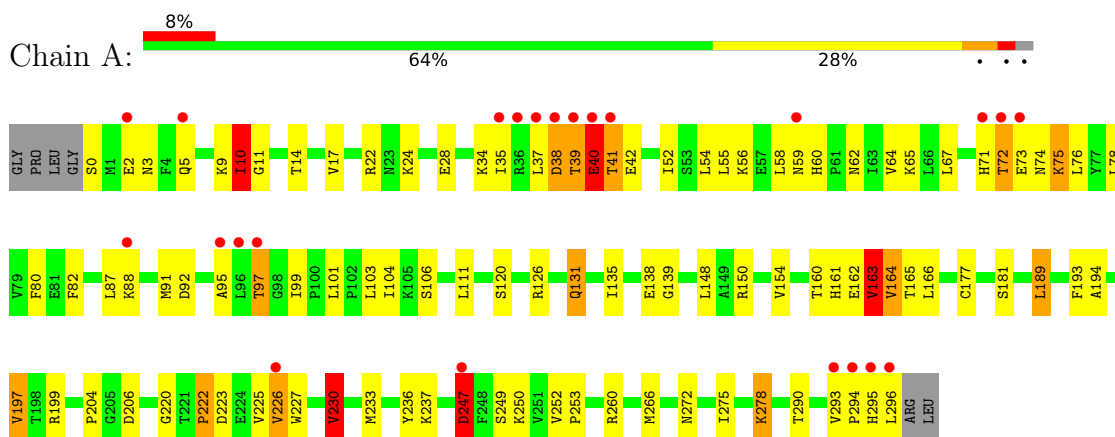
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	B	182	Total	O	0	0
			182	182		
4	C	138	Total	O	0	0
			138	138		
4	D	112	Total	O	0	0
			112	112		

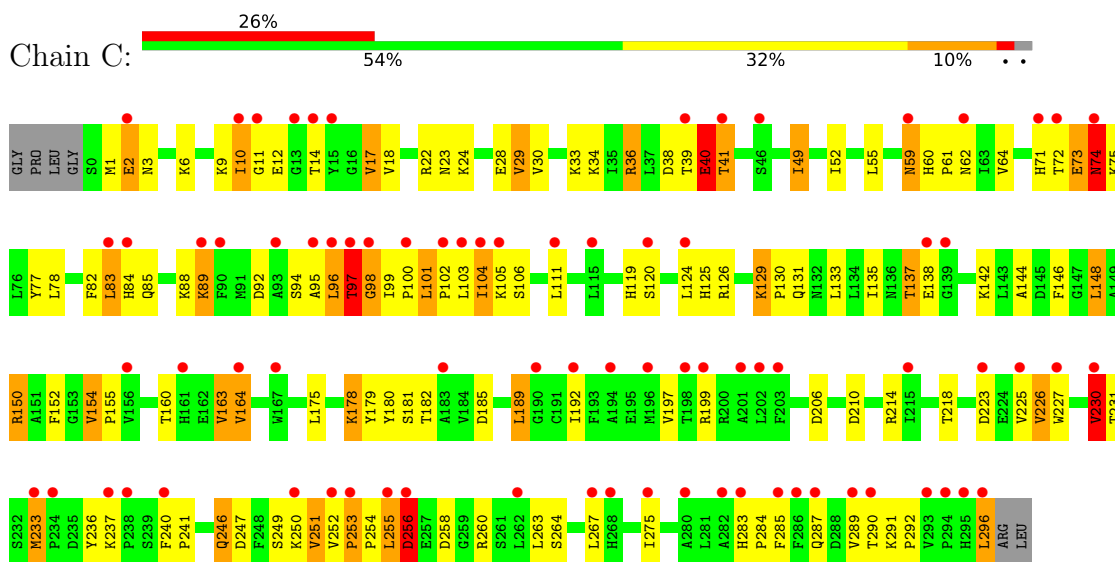
3 Residue-property plots [i](#)

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.

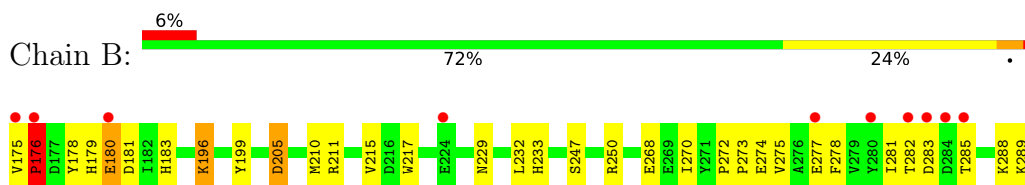
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 1: CELL DIVISION PROTEIN KINASE 2

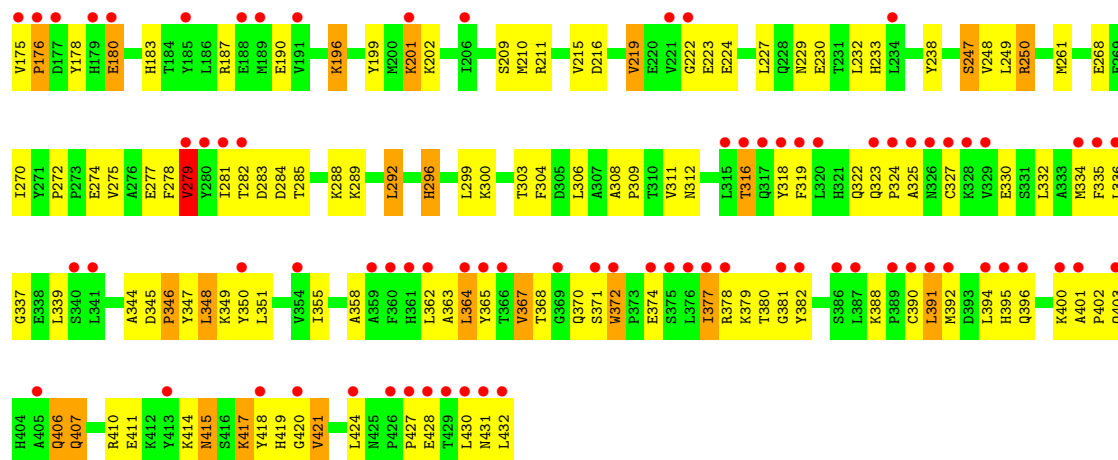


• Molecule 2: CYCLIN A2





● Molecule 2: CYCLIN A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.23Å 135.35Å 148.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.00) 94.1 (20.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.286 0.238 , 0.289	Depositor DCC
R_{free} test set	4974 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9701	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4SP, TPO

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	1.22	4/2438 (0.2%)	1.50	23/3308 (0.7%)
1	C	0.98	0/2438	1.51	29/3308 (0.9%)
2	B	1.15	2/2133 (0.1%)	1.39	15/2897 (0.5%)
2	D	0.90	0/2133	1.42	21/2897 (0.7%)
All	All	1.07	6/9142 (0.1%)	1.46	88/12410 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	272	PRO	CA-C	6.36	1.56	1.52
1	A	266	MET	CA-C	6.15	1.61	1.52
1	A	194	ALA	CA-CB	-5.50	1.44	1.53
1	A	162	GLU	CA-C	-5.12	1.47	1.53
2	B	272	PRO	CA-CB	-5.11	1.49	1.54
1	A	104	ILE	CA-CB	-5.03	1.48	1.54

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-14.29	92.86	112.14
1	C	36	ARG	NE-CZ-NH2	11.66	129.69	119.20
1	C	230	VAL	CB-CA-C	-11.14	97.44	111.70
1	C	84	HIS	N-CA-C	10.43	122.23	111.07
1	C	36	ARG	NE-CZ-NH1	-9.98	111.52	121.50
1	C	36	ARG	CG-CD-NE	9.79	133.55	112.00
1	C	36	ARG	CD-NE-CZ	9.53	137.74	124.40
1	A	38	ASP	N-CA-C	9.29	130.59	110.80
1	C	17	VAL	CB-CA-C	-9.23	94.74	110.71
1	C	73	GLU	N-CA-C	-8.28	102.33	111.36
1	A	97	THR	CB-CA-C	-8.08	97.33	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	VAL	N-CA-CB	7.89	118.90	110.62
1	A	230	VAL	N-CA-CB	7.74	121.06	110.54
1	A	163	VAL	N-CA-CB	-7.72	97.48	111.92
2	B	176	PRO	N-CA-C	7.65	128.23	112.47
1	C	11	GLY	N-CA-C	7.58	119.89	111.85
1	A	166	LEU	N-CA-C	7.55	119.15	111.07
2	D	285	THR	N-CA-C	-7.49	103.19	111.36
2	B	316	THR	N-CA-CB	-7.45	99.17	110.12
1	A	72	THR	N-CA-CB	-7.14	99.74	110.60
1	C	225	VAL	N-CA-C	-7.01	104.15	111.58
2	D	367	VAL	N-CA-C	6.90	117.69	110.72
2	D	347	TYR	N-CA-C	6.88	120.94	112.54
1	C	129	LYS	N-CA-C	-6.84	101.98	108.13
2	D	199	TYR	N-CA-C	6.77	118.66	111.28
2	B	422	SER	CA-C-N	-6.70	112.02	122.67
2	B	422	SER	C-N-CA	-6.70	112.02	122.67
2	B	268	GLU	N-CA-C	6.66	121.54	113.41
2	B	347	TYR	N-CA-C	6.66	120.66	112.54
2	B	423	LEU	CB-CA-C	6.64	121.71	111.02
2	D	272	PRO	O-C-N	6.62	124.35	121.31
2	B	175	VAL	CA-C-N	6.60	128.09	119.84
2	B	175	VAL	C-N-CA	6.60	128.09	119.84
2	B	180	GLU	CB-CG-CD	6.52	123.69	112.60
2	D	364	LEU	CA-C-N	6.47	128.85	120.44
2	D	364	LEU	C-N-CA	6.47	128.85	120.44
1	C	251	VAL	CB-CA-C	-6.46	103.56	112.02
1	A	220	GLY	CA-C-O	-6.39	116.68	122.24
1	A	126	ARG	N-CA-C	6.25	120.48	112.86
1	A	41	THR	N-CA-CB	6.18	120.94	110.49
1	C	241	PRO	CA-C-O	-6.17	114.51	121.43
1	C	98	GLY	CA-C-N	-6.03	118.50	122.60
1	C	98	GLY	C-N-CA	-6.03	118.50	122.60
1	A	10	ILE	N-CA-CB	-5.91	105.72	111.57
2	D	176	PRO	N-CA-C	5.88	124.59	112.47
1	A	193	PHE	N-CA-C	-5.87	104.79	111.07
1	C	36	ARG	CB-CA-C	5.83	119.34	109.84
2	D	381	GLY	N-CA-C	-5.71	106.28	115.08
2	D	378	ARG	N-CA-C	5.68	117.56	111.36
1	C	39	THR	N-CA-C	-5.66	102.65	110.35
1	A	253	PRO	N-CA-C	5.65	117.59	110.70
1	A	247	ASP	CB-CA-C	5.60	118.63	109.90
2	B	205	ASP	N-CA-C	5.57	120.23	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	GLU	CB-CG-CD	-5.55	103.16	112.60
1	C	84	HIS	CA-CB-CG	-5.54	108.25	113.80
1	A	293	VAL	N-CA-C	-5.50	97.00	108.88
2	D	219	VAL	N-CA-C	-5.50	105.14	110.42
2	D	299	LEU	N-CA-C	5.50	117.27	111.28
2	D	421	VAL	N-CA-C	5.46	118.70	111.17
1	A	247	ASP	N-CA-CB	-5.43	101.37	109.69
2	D	268	GLU	N-CA-C	5.43	119.91	113.12
2	D	365	TYR	N-CA-C	5.43	116.88	111.07
1	A	225	VAL	CB-CA-C	5.41	119.11	112.02
2	B	270	ILE	N-CA-C	-5.40	105.46	110.53
1	A	120	SER	CA-CB-OG	-5.39	100.31	111.10
2	D	250	ARG	NE-CZ-NH1	5.38	126.88	121.50
2	D	247	SER	CB-CA-C	5.34	118.55	109.84
2	B	367	VAL	N-CA-C	5.34	116.00	110.82
2	B	312	ASN	N-CA-C	5.32	117.77	111.33
2	B	285	THR	N-CA-C	-5.29	105.69	111.82
1	C	74	ASN	N-CA-C	5.24	119.58	112.04
1	C	92	ASP	N-CA-C	-5.21	105.51	111.14
1	C	74	ASN	N-CA-CB	-5.19	102.14	110.19
1	A	197	VAL	N-CA-C	5.17	115.39	110.53
1	A	80	PHE	CA-CB-CG	5.17	118.97	113.80
2	D	322	GLN	N-CA-C	5.15	117.50	110.24
2	D	407	GLN	N-CA-C	5.10	121.27	113.61
1	C	49	ILE	N-CA-CB	-5.09	104.86	110.51
2	D	250	ARG	CD-NE-CZ	5.08	131.51	124.40
2	D	279	VAL	N-CA-CB	5.07	117.06	110.57
1	C	246	GLN	CB-CA-C	-5.07	100.84	109.51
1	C	180	TYR	N-CA-C	-5.05	101.68	109.52
1	C	29	VAL	N-CA-C	-5.05	101.18	108.71
1	C	253	PRO	N-CA-C	5.05	116.86	110.70
1	C	12	GLU	N-CA-C	5.02	116.96	108.02
1	A	295	HIS	CA-C-N	-5.02	112.67	121.70
1	A	295	HIS	C-N-CA	-5.02	112.67	121.70
1	A	3	ASN	N-CA-C	5.00	119.01	113.01

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	2388	0	2430	93	1
1	C	2388	0	2430	133	0
2	B	2083	0	2107	69	1
2	D	2083	0	2107	118	0
3	A	28	0	22	5	0
3	C	28	0	22	1	0
4	A	271	0	0	21	0
4	B	182	0	0	13	0
4	C	138	0	0	40	0
4	D	112	0	0	35	0
All	All	9701	0	9118	397	1

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 22.

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:LEU:HB2	4:B:2176:HOH:O	1.21	1.33
2:B:414:LYS:HG2	2:B:423:LEU:HD11	1.34	1.07
1:A:272:ASN:HB3	4:A:2246:HOH:O	1.56	1.05
2:B:334:MET:HG2	4:B:2107:HOH:O	1.57	1.03
1:A:72:THR:HB	1:A:75:LYS:O	1.60	1.01
1:C:85:GLN:HE21	1:C:296:LEU:HD21	1.20	1.00
1:C:40:GLU:OE1	4:C:2031:HOH:O	1.81	0.97
1:C:88:LYS:HD2	1:C:131:GLN:HG3	1.48	0.95
2:B:423:LEU:CB	4:B:2176:HOH:O	1.88	0.94
2:D:312:ASN:HB2	4:D:2038:HOH:O	1.66	0.93
1:C:88:LYS:HB2	1:C:131:GLN:HE21	1.33	0.93
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.49	0.92
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.35	0.92
2:B:423:LEU:CG	4:B:2176:HOH:O	2.14	0.89
2:D:270:ILE:O	4:D:2048:HOH:O	1.93	0.86
2:B:423:LEU:CD1	4:B:2176:HOH:O	2.22	0.85
1:C:60:HIS:HD2	1:C:62:ASN:H	1.21	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.58	0.84
2:B:423:LEU:HD13	4:B:2176:HOH:O	1.78	0.83
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.60	0.83
2:D:355:ILE:HG21	4:D:2080:HOH:O	1.78	0.81
1:A:88:LYS:CD	1:A:131:GLN:HE21	1.94	0.81
1:A:177:CYS:SG	4:A:2024:HOH:O	2.39	0.80
2:B:334:MET:SD	4:B:2120:HOH:O	2.39	0.80
1:C:175:LEU:HD13	1:C:233:MET:CE	2.11	0.80
1:A:260:ARG:HD3	4:A:2228:HOH:O	1.81	0.79
1:A:60:HIS:CD2	1:A:62:ASN:H	2.01	0.79
2:D:318:TYR:HE1	4:D:2069:HOH:O	1.66	0.78
1:C:287:GLN:HG2	4:C:2132:HOH:O	1.83	0.78
1:A:95:ALA:O	1:A:199:ARG:NH1	2.16	0.77
1:C:38:ASP:HB3	1:C:41:THR:HB	1.66	0.77
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.67	0.77
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.77
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.67	0.77
2:D:374:GLU:HA	2:D:377:ILE:HG13	1.67	0.77
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.66	0.76
1:C:10:ILE:HG23	4:C:2009:HOH:O	1.85	0.76
2:D:402:PRO:HB2	2:D:403:GLN:OE1	1.85	0.76
2:B:283:ASP:HB2	4:B:2086:HOH:O	1.86	0.76
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.20	0.75
1:C:144:ALA:HA	4:C:2071:HOH:O	1.87	0.75
2:D:336:LEU:HD22	4:D:2098:HOH:O	1.87	0.75
2:D:327:CYS:HB2	2:D:419:HIS:NE2	2.01	0.74
4:A:2051:HOH:O	2:B:316:THR:HG21	1.87	0.74
1:C:88:LYS:HB2	1:C:131:GLN:NE2	2.00	0.74
1:C:240:PHE:HB2	4:C:2111:HOH:O	1.87	0.73
1:C:30:VAL:HG13	4:C:2023:HOH:O	1.87	0.73
1:C:146:PHE:CE1	4:C:2071:HOH:O	2.41	0.73
1:A:38:ASP:O	1:A:39:THR:CB	2.37	0.72
1:A:88:LYS:HD2	1:A:131:GLN:HG3	1.71	0.72
1:C:88:LYS:CB	1:C:131:GLN:HE21	2.01	0.72
1:C:256:ASP:O	1:C:260:ARG:HG3	1.89	0.72
1:A:72:THR:OG1	4:A:2083:HOH:O	2.08	0.71
1:C:40:GLU:CD	4:C:2031:HOH:O	2.25	0.71
1:A:72:THR:HG22	1:A:74:ASN:H	1.57	0.69
2:B:289:LYS:HE3	2:B:293:ARG:NE	2.07	0.69
2:B:217:TRP:CH2	2:B:281:ILE:HD12	2.28	0.69
2:B:414:LYS:CG	2:B:423:LEU:HD11	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CD2	1:C:62:ASN:H	2.07	0.69
1:C:85:GLN:NE2	1:C:296:LEU:HD21	2.02	0.69
1:C:130:PRO:HB2	1:C:131:GLN:HE22	1.58	0.69
2:D:358:ALA:HB1	4:D:2096:HOH:O	1.91	0.69
1:A:181:SER:HB3	4:A:2165:HOH:O	1.92	0.68
1:C:85:GLN:OE1	1:C:89:LYS:HB3	1.93	0.68
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.76	0.68
1:C:249:SER:OG	1:C:250:LYS:HE3	1.93	0.68
1:C:94:SER:OG	4:C:2059:HOH:O	2.12	0.67
2:D:394:LEU:HB2	4:D:2096:HOH:O	1.93	0.67
1:A:38:ASP:O	1:A:39:THR:HB	1.95	0.66
2:B:414:LYS:HG2	2:B:423:LEU:CD1	2.20	0.66
1:A:28:GLU:OE2	4:A:2029:HOH:O	2.13	0.66
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.78	0.65
2:D:318:TYR:CE1	4:D:2069:HOH:O	2.44	0.65
2:B:289:LYS:HE3	2:B:293:ARG:HE	1.62	0.65
2:D:362:LEU:HD23	4:D:2098:HOH:O	1.96	0.65
1:C:154:VAL:O	2:D:316:THR:HG22	1.97	0.65
1:C:10:ILE:HD11	1:C:82:PHE:HE1	1.62	0.65
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.77	0.65
1:C:283:HIS:ND1	4:C:2130:HOH:O	2.29	0.64
2:D:346:PRO:O	2:D:349:LYS:HG2	1.97	0.64
2:D:394:LEU:CB	4:D:2096:HOH:O	2.46	0.64
2:D:417:LYS:HA	4:D:2105:HOH:O	1.97	0.64
1:C:130:PRO:HB2	1:C:131:GLN:NE2	2.11	0.64
1:C:292:PRO:HA	4:C:2134:HOH:O	1.98	0.64
1:C:197:VAL:HA	4:C:2098:HOH:O	1.98	0.64
2:B:330:GLU:O	2:B:334:MET:HG3	1.97	0.64
2:D:183:HIS:HE1	4:D:2069:HOH:O	1.80	0.64
2:B:210:MET:HE1	2:B:250:ARG:CB	2.27	0.63
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.81	0.63
1:C:146:PHE:HE1	4:C:2071:HOH:O	1.77	0.62
1:A:247:ASP:OD2	1:A:249:SER:OG	2.09	0.62
1:C:285:PHE:HB2	4:C:2130:HOH:O	1.98	0.62
2:D:210:MET:HE1	2:D:250:ARG:HD3	1.81	0.62
2:D:277:GLU:O	2:D:281:ILE:HG23	1.99	0.62
1:A:71:HIS:ND1	2:B:304:PHE:HZ	1.98	0.62
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.82	0.62
2:D:325:ALA:HB3	4:D:2075:HOH:O	1.99	0.62
1:C:40:GLU:OE2	4:C:2031:HOH:O	2.16	0.62
2:B:293:ARG:HD3	1:C:2:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD13	1:C:189:LEU:HD21	1.81	0.61
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.82	0.61
2:D:418:TYR:O	2:D:421:VAL:HG13	2.01	0.61
1:A:88:LYS:CG	1:A:131:GLN:HE21	2.14	0.61
2:D:210:MET:HE1	2:D:250:ARG:CB	2.31	0.61
1:A:39:THR:HA	2:B:292:LEU:HD23	1.83	0.60
1:A:95:ALA:HA	4:A:2101:HOH:O	2.01	0.60
1:A:161:HIS:HD2	4:A:2055:HOH:O	1.83	0.60
1:C:218:THR:HG23	4:C:2116:HOH:O	2.02	0.60
1:C:223:ASP:H	1:C:226:VAL:CG1	2.14	0.60
1:A:71:HIS:NE2	4:A:2082:HOH:O	2.30	0.60
1:C:283:HIS:CE1	4:C:2130:HOH:O	2.55	0.59
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.03	0.59
1:C:100:PRO:O	1:C:104:ILE:HG13	2.03	0.59
1:C:210:ASP:O	1:C:214:ARG:HG3	2.03	0.59
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.30	0.59
1:A:88:LYS:HD2	1:A:131:GLN:NE2	2.14	0.58
2:D:362:LEU:HD13	2:D:430:LEU:HD21	1.84	0.58
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.85	0.58
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.33	0.58
2:D:183:HIS:CE1	4:D:2069:HOH:O	2.54	0.58
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.84	0.58
1:A:154:VAL:O	2:B:316:THR:HG23	2.03	0.57
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.39	0.57
2:D:211:ARG:O	2:D:215:VAL:HG23	2.03	0.57
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.86	0.57
1:A:237:LYS:HE2	4:A:2200:HOH:O	2.04	0.57
2:B:289:LYS:CE	2:B:293:ARG:HE	2.17	0.57
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.87	0.56
2:B:422:SER:C	2:B:423:LEU:HG	2.30	0.56
1:C:10:ILE:HD11	1:C:82:PHE:CE1	2.39	0.56
2:D:196:LYS:HE3	2:D:202:LYS:NZ	2.20	0.56
1:C:146:PHE:CD1	4:C:2071:HOH:O	2.59	0.56
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.86	0.56
2:D:396:GLN:HB3	2:D:400:LYS:HE3	1.88	0.56
1:C:2:GLU:HG2	1:C:3:ASN:N	2.21	0.56
2:D:372:TRP:HD1	4:D:2094:HOH:O	1.87	0.56
1:C:49:ILE:HG23	2:D:306:LEU:CD1	2.35	0.56
2:D:229:ASN:ND2	2:D:334:MET:HE3	2.20	0.56
1:C:10:ILE:HG22	1:C:18:VAL:O	2.06	0.56
2:D:275:VAL:HG11	2:D:292:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:ASP:OD1	4:B:2130:HOH:O	2.18	0.56
2:D:388:LYS:O	2:D:392:MET:HG2	2.05	0.56
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.04	0.55
1:C:101:LEU:HD13	1:C:101:LEU:O	2.06	0.55
1:C:129:LYS:HD2	1:C:131:GLN:OE1	2.07	0.55
1:C:155:PRO:HA	4:C:2077:HOH:O	2.07	0.55
1:A:223:ASP:H	1:A:226:VAL:CG1	2.19	0.55
1:A:9:LYS:HE3	1:A:17:VAL:HG13	1.89	0.55
1:C:125:HIS:NE2	4:C:2064:HOH:O	2.33	0.55
1:C:131:GLN:CD	1:C:131:GLN:H	2.15	0.55
1:A:10:ILE:HG22	1:A:11:GLY:N	2.21	0.55
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.89	0.55
2:D:363:ALA:HB3	4:D:2088:HOH:O	2.06	0.55
1:C:88:LYS:HD2	1:C:131:GLN:CG	2.29	0.55
2:D:394:LEU:HG	4:D:2098:HOH:O	2.07	0.55
1:A:72:THR:HG22	1:A:75:LYS:H	1.71	0.54
1:C:126:ARG:CZ	1:C:150:ARG:HG2	2.37	0.54
1:C:10:ILE:HG21	1:C:18:VAL:HG12	1.89	0.54
2:D:303:THR:O	2:D:304:PHE:HB2	2.07	0.54
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.88	0.54
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.41	0.54
1:C:131:GLN:CD	1:C:131:GLN:N	2.66	0.54
1:A:40:GLU:HA	2:B:288:LYS:HE2	1.90	0.53
1:C:88:LYS:CG	1:C:131:GLN:HE21	2.20	0.53
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.44	0.53
1:C:178:LYS:HE2	1:C:179:TYR:CZ	2.44	0.53
2:B:233:HIS:HD2	4:B:2106:HOH:O	1.90	0.53
2:D:196:LYS:HE3	2:D:202:LYS:HZ2	1.74	0.53
2:D:358:ALA:HA	2:D:391:LEU:HD22	1.90	0.53
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.74	0.52
2:B:281:ILE:HG13	2:B:282:THR:N	2.22	0.52
1:C:237:LYS:HD3	4:C:2109:HOH:O	2.10	0.52
1:C:59:ASN:C	1:C:59:ASN:ND2	2.68	0.52
1:C:285:PHE:N	4:C:2130:HOH:O	2.41	0.52
1:A:10:ILE:HG22	1:A:11:GLY:H	1.75	0.52
2:D:215:VAL:O	2:D:219:VAL:HG23	2.10	0.52
1:C:181:SER:OG	1:C:182:THR:N	2.39	0.52
3:C:1298:4SP:H101	4:C:2009:HOH:O	2.10	0.52
2:D:190:GLU:HG3	2:D:351:LEU:HD22	1.91	0.52
4:A:2082:HOH:O	2:B:296:HIS:CG	2.62	0.52
1:C:249:SER:HB3	4:C:2117:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:O	1:C:199:ARG:NH1	2.43	0.51
1:A:39:THR:HG23	2:B:289:LYS:HD3	1.93	0.51
1:C:88:LYS:HD2	1:C:131:GLN:HE21	1.75	0.51
1:C:99:ILE:O	1:C:104:ILE:HD11	2.11	0.51
2:D:358:ALA:CB	2:D:391:LEU:HD22	2.41	0.51
1:A:39:THR:CG2	2:B:289:LYS:HD3	2.40	0.51
2:D:396:GLN:O	2:D:400:LYS:HG3	2.10	0.51
2:D:428:GLU:HG2	4:D:2111:HOH:O	2.10	0.51
2:D:419:HIS:CE1	4:D:2108:HOH:O	2.63	0.51
2:B:289:LYS:HE3	2:B:293:ARG:NH2	2.26	0.51
1:A:64:VAL:HG21	3:A:1298:4SP:C8	2.41	0.51
2:D:279:VAL:HB	4:D:2052:HOH:O	2.10	0.51
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.46	0.51
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.76	0.50
2:B:323:GLN:OE1	2:B:324:PRO:HA	2.11	0.50
1:C:231:THR:HA	1:C:236:TYR:CD1	2.46	0.50
2:B:289:LYS:NZ	2:B:293:ARG:HE	2.08	0.50
2:D:201:LYS:O	2:D:201:LYS:HD3	2.11	0.50
2:D:279:VAL:HG21	2:D:288:LYS:HA	1.94	0.50
1:C:10:ILE:HG23	1:C:10:ILE:O	2.11	0.50
1:A:222:PRO:HA	1:A:226:VAL:HG11	1.94	0.50
2:D:417:LYS:NZ	2:D:417:LYS:HB3	2.27	0.50
1:A:5:GLN:OE1	1:A:24:LYS:HE2	2.11	0.49
2:B:289:LYS:HE3	2:B:293:ARG:CZ	2.42	0.49
2:B:427:PRO:HA	4:B:2180:HOH:O	2.11	0.49
1:C:28:GLU:HB3	4:C:2023:HOH:O	2.12	0.49
1:C:251:VAL:HG22	4:C:2116:HOH:O	2.13	0.49
1:A:131:GLN:CD	1:A:131:GLN:H	2.20	0.49
2:D:248:VAL:HG12	2:D:249:LEU:O	2.12	0.49
2:D:275:VAL:HG12	4:D:2052:HOH:O	2.11	0.49
1:C:263:LEU:HD11	1:C:267:LEU:HD11	1.95	0.49
2:D:222:GLY:HA2	2:D:227:LEU:HB2	1.94	0.48
1:C:85:GLN:HE21	1:C:296:LEU:CD2	2.10	0.48
2:D:279:VAL:CG2	4:D:2052:HOH:O	2.60	0.48
2:D:414:LYS:O	2:D:415:ASN:C	2.54	0.48
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.95	0.48
1:C:74:ASN:HB2	4:C:2049:HOH:O	2.12	0.48
1:C:23:ASN:HB2	4:C:2023:HOH:O	2.13	0.48
1:C:285:PHE:HA	4:C:2131:HOH:O	2.13	0.48
2:D:380:THR:HB	2:D:382:TYR:CD2	2.49	0.48
1:A:71:HIS:CE1	4:A:2082:HOH:O	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:C	1:C:59:ASN:HD22	2.21	0.48
1:C:206:ASP:HA	4:C:2100:HOH:O	2.14	0.48
1:A:199:ARG:HD2	4:A:2101:HOH:O	2.14	0.47
2:B:323:GLN:OE1	2:B:323:GLN:HA	2.14	0.47
1:C:6:LYS:HE2	4:C:2003:HOH:O	2.14	0.47
1:A:154:VAL:O	2:B:316:THR:CG2	2.62	0.47
2:B:183:HIS:HB2	2:B:317:GLN:NE2	2.29	0.47
1:C:85:GLN:HG2	1:C:296:LEU:HD11	1.96	0.47
2:D:358:ALA:CA	2:D:391:LEU:HD22	2.44	0.47
1:A:39:THR:HG22	1:A:40:GLU:HG3	1.96	0.47
1:C:106:SER:HB2	1:C:290:THR:O	2.14	0.47
2:D:196:LYS:O	2:D:196:LYS:HG3	2.14	0.47
2:D:279:VAL:HG23	4:D:2052:HOH:O	2.14	0.47
1:A:9:LYS:HE3	1:A:17:VAL:CG1	2.44	0.47
1:A:71:HIS:CG	1:A:76:LEU:HD13	2.50	0.47
1:C:142:LYS:NZ	4:C:2070:HOH:O	2.43	0.47
2:D:391:LEU:HA	4:D:2096:HOH:O	2.14	0.47
1:A:92:ASP:O	1:A:95:ALA:HB2	2.14	0.47
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.96	0.47
2:B:278:PHE:O	2:B:281:ILE:HG12	2.14	0.47
2:D:401:ALA:CB	2:D:402:PRO:HD3	2.38	0.47
1:C:38:ASP:HB3	1:C:41:THR:CB	2.41	0.47
1:C:111:LEU:CD1	1:C:189:LEU:HD21	2.44	0.47
2:D:323:GLN:OE1	2:D:324:PRO:HA	2.15	0.47
2:B:229:ASN:HD22	2:B:334:MET:CE	2.28	0.47
1:C:14:THR:HG21	1:C:148:LEU:HD13	1.97	0.47
1:C:95:ALA:O	1:C:199:ARG:NH1	2.45	0.47
1:C:144:ALA:CA	4:C:2071:HOH:O	2.55	0.47
1:C:255:LEU:HB3	1:C:260:ARG:HG2	1.96	0.47
2:D:178:TYR:HE2	4:D:2011:HOH:O	1.97	0.47
2:D:332:LEU:HB3	2:D:363:ALA:HB1	1.97	0.47
1:A:2:GLU:OE2	1:C:73:GLU:HG3	2.15	0.46
2:B:176:PRO:HA	2:B:179:HIS:CG	2.50	0.46
1:C:258:ASP:HB3	4:C:2130:HOH:O	2.14	0.46
2:D:180:GLU:OE1	2:D:379:LYS:NZ	2.47	0.46
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.42	0.46
2:D:371:SER:O	2:D:372:TRP:C	2.58	0.46
2:B:277:GLU:O	2:B:281:ILE:HG23	2.15	0.46
1:A:111:LEU:HD13	1:A:189:LEU:HD21	1.98	0.46
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.45	0.46
2:D:407:GLN:O	2:D:411:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:ND1	2:B:304:PHE:CZ	2.80	0.46
1:C:254:PRO:HB2	4:C:2121:HOH:O	2.15	0.46
1:A:237:LYS:CE	4:A:2200:HOH:O	2.63	0.46
2:B:196:LYS:CB	2:B:196:LYS:NZ	2.78	0.46
2:D:201:LYS:HD3	2:D:201:LYS:C	2.41	0.46
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.97	0.46
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.84	0.46
1:A:131:GLN:CD	1:A:131:GLN:N	2.74	0.45
1:A:249:SER:HA	4:A:2228:HOH:O	2.15	0.45
1:C:33:LYS:HB3	1:C:78:LEU:HB2	1.97	0.45
1:A:72:THR:CG2	1:A:74:ASN:OD1	2.64	0.45
2:D:350:TYR:CD1	2:D:390:CYS:HB2	2.52	0.45
1:C:72:THR:HG22	1:C:74:ASN:OD1	2.16	0.45
2:D:275:VAL:HG11	2:D:292:LEU:CD1	2.46	0.45
2:D:401:ALA:CB	2:D:402:PRO:CD	2.94	0.45
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.51	0.45
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.97	0.45
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.51	0.45
1:C:72:THR:HG22	1:C:73:GLU:H	1.81	0.45
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.97	0.45
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.68	0.45
1:A:135:ILE:HD12	1:A:296:LEU:HD21	1.99	0.45
1:C:227:TRP:CH2	1:C:233:MET:HE1	2.52	0.45
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.99	0.45
2:B:215:VAL:HG12	2:B:342:ILE:HD13	1.97	0.45
2:D:261:MET:HE1	4:D:2026:HOH:O	2.17	0.45
2:D:421:VAL:O	2:D:424:LEU:HG	2.17	0.45
1:C:52:ILE:CD1	1:C:78:LEU:HD21	2.47	0.45
2:D:311:VAL:HG21	4:D:2080:HOH:O	2.17	0.45
1:A:65:LYS:NZ	4:A:2073:HOH:O	2.49	0.44
1:A:65:LYS:HG2	1:A:67:LEU:HD23	1.99	0.44
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.99	0.44
2:B:211:ARG:HD3	2:B:344:ALA:HB2	1.97	0.44
2:D:211:ARG:HG2	2:D:211:ARG:HH11	1.81	0.44
2:D:358:ALA:HA	2:D:391:LEU:CD2	2.47	0.44
2:D:368:THR:CB	2:D:370:GLN:HE21	2.29	0.44
2:D:395:HIS:HE1	2:D:427:PRO:O	1.99	0.44
1:C:85:GLN:HB3	4:C:2051:HOH:O	2.17	0.44
2:B:371:SER:O	2:B:372:TRP:C	2.61	0.44
2:D:278:PHE:O	2:D:281:ILE:HG12	2.16	0.44
2:D:274:GLU:HG2	2:D:277:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:363:ALA:O	2:D:364:LEU:C	2.61	0.44
1:A:10:ILE:CG2	1:A:11:GLY:N	2.81	0.44
1:A:223:ASP:OD1	1:A:223:ASP:C	2.60	0.44
1:C:96:LEU:O	1:C:97:THR:C	2.60	0.44
1:A:204:PRO:HG3	4:A:2176:HOH:O	2.18	0.44
1:C:83:LEU:HD21	1:C:142:LYS:HG3	2.00	0.44
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.01	0.44
2:D:230:GLU:HA	2:D:230:GLU:OE1	2.17	0.44
1:A:75:LYS:HZ3	1:A:75:LYS:HG2	1.63	0.43
1:C:105:LYS:HG2	1:C:289:VAL:HG23	1.99	0.43
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.48	0.43
1:A:39:THR:HG22	1:A:40:GLU:N	2.33	0.43
1:A:296:LEU:CB	4:A:2269:HOH:O	2.65	0.43
1:C:103:LEU:HD12	1:C:103:LEU:HA	1.71	0.43
2:D:282:THR:O	2:D:283:ASP:C	2.61	0.43
2:D:350:TYR:CE1	2:D:390:CYS:HB2	2.53	0.43
2:D:279:VAL:CB	4:D:2052:HOH:O	2.65	0.43
2:D:368:THR:HB	2:D:370:GLN:HE21	1.83	0.43
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.87	0.43
1:A:88:LYS:CG	1:A:131:GLN:NE2	2.81	0.43
1:C:291:LYS:O	4:C:2134:HOH:O	2.21	0.43
2:D:388:LYS:HB3	4:D:2095:HOH:O	2.18	0.43
1:C:22:ARG:NH2	1:C:24:LYS:HA	2.34	0.43
1:C:223:ASP:H	1:C:226:VAL:HG13	1.81	0.43
1:C:231:THR:HA	1:C:236:TYR:CG	2.53	0.43
2:D:233:HIS:HE1	4:D:2079:HOH:O	2.01	0.43
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.75	0.43
1:C:29:VAL:HG23	4:C:2022:HOH:O	2.18	0.43
1:C:71:HIS:CD2	2:D:296:HIS:CE1	3.07	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.54	0.42
1:A:250:LYS:HA	1:A:250:LYS:HD3	1.85	0.42
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.54	0.42
2:D:238:TYR:OH	2:D:306:LEU:HB3	2.19	0.42
1:A:10:ILE:CG2	3:A:1298:4SP:H101	2.50	0.42
2:B:430:LEU:O	2:B:431:ASN:C	2.61	0.42
1:C:125:HIS:CE1	4:C:2064:HOH:O	2.73	0.42
2:D:417:LYS:HE2	2:D:418:TYR:CZ	2.54	0.42
1:A:54:LEU:O	1:A:58:LEU:HG	2.18	0.42
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.34	0.42
2:B:205:ASP:OD1	2:B:250:ARG:NH2	2.48	0.42
2:B:346:PRO:O	2:B:349:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.00	0.42
2:D:419:HIS:CG	4:D:2108:HOH:O	2.72	0.42
2:D:421:VAL:HA	2:D:424:LEU:HG	2.02	0.42
1:C:64:VAL:HG12	4:C:2071:HOH:O	2.19	0.42
1:C:99:ILE:CG2	1:C:104:ILE:HG12	2.49	0.42
2:D:223:GLU:O	2:D:224:GLU:C	2.61	0.42
1:A:14:THR:HG21	1:A:148:LEU:HD12	2.02	0.42
3:A:1298:4SP:N1	3:A:1298:4SP:H22	2.35	0.42
2:B:183:HIS:HD2	4:B:2031:HOH:O	2.02	0.42
2:B:414:LYS:HG2	2:B:423:LEU:HD21	2.02	0.42
1:A:165:THR:HG22	4:A:2154:HOH:O	2.20	0.42
1:A:223:ASP:H	1:A:226:VAL:HG12	1.85	0.42
1:C:1:MET:HE2	1:C:77:TYR:CD1	2.55	0.42
1:A:72:THR:CG2	1:A:75:LYS:H	2.33	0.42
2:D:337:GLY:HA3	4:D:2078:HOH:O	2.20	0.42
2:D:370:GLN:HB3	4:D:2091:HOH:O	2.20	0.42
2:B:199:TYR:CD1	2:B:199:TYR:C	2.98	0.42
1:C:88:LYS:CD	1:C:131:GLN:HE21	2.33	0.42
1:C:96:LEU:O	1:C:98:GLY:N	2.53	0.42
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41
2:D:380:THR:HG22	4:D:2069:HOH:O	2.19	0.41
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.84	0.41
1:A:64:VAL:HG21	3:A:1298:4SP:H8	2.02	0.41
1:C:10:ILE:CG2	1:C:18:VAL:HG12	2.49	0.41
1:C:83:LEU:HD11	1:C:142:LYS:HD2	2.01	0.41
2:D:415:ASN:OD1	2:D:417:LYS:N	2.44	0.41
1:A:87:LEU:O	1:A:91:MET:HG3	2.20	0.41
2:D:327:CYS:HB2	2:D:419:HIS:CE1	2.55	0.41
2:D:430:LEU:O	2:D:431:ASN:HB2	2.20	0.41
1:A:72:THR:HG23	1:A:74:ASN:OD1	2.21	0.41
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.41
2:D:187:ARG:HD2	2:D:187:ARG:HA	1.85	0.41
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.93	0.41
1:A:296:LEU:HB3	4:A:2269:HOH:O	2.20	0.41
3:A:1298:4SP:N1	3:A:1298:4SP:C22	2.84	0.41
2:B:414:LYS:HE2	2:B:423:LEU:HD21	2.03	0.41
1:C:10:ILE:HG22	1:C:18:VAL:C	2.45	0.41
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.92	0.41
2:B:178:TYR:N	4:B:2028:HOH:O	2.13	0.41
2:B:368:THR:CB	2:B:370:GLN:HE21	2.34	0.41
1:C:252:VAL:HG12	1:C:255:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.56	0.41
1:C:291:LYS:O	1:C:291:LYS:HG2	2.21	0.40
1:A:37:LEU:HB2	1:A:74:ASN:O	2.20	0.40
1:C:181:SER:O	1:C:182:THR:C	2.63	0.40
2:D:358:ALA:HB1	2:D:391:LEU:HD22	2.02	0.40
1:A:106:SER:HB2	1:A:290:THR:O	2.21	0.40
1:A:236:TYR:CD1	1:A:236:TYR:C	2.99	0.40
1:C:137:THR:O	1:C:137:THR:OG1	2.35	0.40
2:D:407:GLN:HA	4:D:2103:HOH:O	2.21	0.40
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.56	0.40
2:D:345:ASP:HA	2:D:346:PRO:HA	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_456]	2.18	0.02

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	294/303 (97%)	281 (96%)	10 (3%)	3 (1%)	12	8
1	C	294/303 (97%)	283 (96%)	6 (2%)	5 (2%)	7	3
2	B	256/258 (99%)	250 (98%)	5 (2%)	1 (0%)	30	27
2	D	256/258 (99%)	244 (95%)	8 (3%)	4 (2%)	7	3
All	All	1100/1122 (98%)	1058 (96%)	29 (3%)	13 (1%)	10	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	176	PRO
1	C	96	LEU
1	C	97	THR
1	C	256	ASP
2	D	176	PRO
1	A	164	VAL
1	C	164	VAL
1	A	40	GLU
1	C	40	GLU
1	A	39	THR
2	D	415	ASN
2	D	372	TRP
2	D	420	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	261/265 (98%)	238 (91%)	23 (9%)	9	6
1	C	261/265 (98%)	225 (86%)	36 (14%)	3	2
2	B	232/232 (100%)	217 (94%)	15 (6%)	15	12
2	D	232/232 (100%)	211 (91%)	21 (9%)	9	6
All	All	986/994 (99%)	891 (90%)	95 (10%)	8	5

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	10	ILE
1	A	22	ARG
1	A	34	LYS
1	A	40	GLU
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	73	GLU

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Mol	Chain	Res	Type
1	A	75	LYS
1	A	97	THR
1	A	101	LEU
1	A	131	GLN
1	A	138	GLU
1	A	150	ARG
1	A	163	VAL
1	A	189	LEU
1	A	206	ASP
1	A	222	PRO
1	A	226	VAL
1	A	230	VAL
1	A	247	ASP
1	A	278	LYS
2	B	176	PRO
2	B	180	GLU
2	B	196	LYS
2	B	232	LEU
2	B	247	SER
2	B	274	GLU
2	B	292	LEU
2	B	316	THR
2	B	346	PRO
2	B	348	LEU
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	417	LYS
2	B	423	LEU
1	C	2	GLU
1	C	9	LYS
1	C	10	ILE
1	C	17	VAL
1	C	34	LYS
1	C	36	ARG
1	C	41	THR
1	C	55	LEU
1	C	59	ASN
1	C	74	ASN
1	C	75	LYS
1	C	83	LEU
1	C	89	LYS

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Mol	Chain	Res	Type
1	C	97	THR
1	C	101	LEU
1	C	104	ILE
1	C	120	SER
1	C	135	ILE
1	C	137	THR
1	C	138	GLU
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	163	VAL
1	C	178	LYS
1	C	189	LEU
1	C	226	VAL
1	C	230	VAL
1	C	233	MET
1	C	246	GLN
1	C	247	ASP
1	C	255	LEU
1	C	256	ASP
1	C	264	SER
1	C	275	ILE
1	C	296	LEU
2	D	175	VAL
2	D	180	GLU
2	D	196	LYS
2	D	201	LYS
2	D	209	SER
2	D	232	LEU
2	D	247	SER
2	D	279	VAL
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU
2	D	296	HIS
2	D	300	LYS
2	D	316	THR
2	D	346	PRO
2	D	348	LEU
2	D	377	ILE
2	D	391	LEU
2	D	406	GLN

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Mol	Chain	Res	Type
2	D	417	LYS
2	D	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	119	HIS
1	A	131	GLN
1	A	161	HIS
1	A	268	HIS
2	B	179	HIS
2	B	183	HIS
2	B	228	GLN
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
2	B	425	ASN
1	C	59	ASN
1	C	60	HIS
1	C	131	GLN
1	C	268	HIS
2	D	183	HIS
2	D	254	GLN
2	D	296	HIS
2	D	313	GLN
2	D	317	GLN
2	D	370	GLN
2	D	395	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	160	1	8,10,11	1.29	0	10,14,16	1.37	2 (20%)
1	TPO	C	160	1	8,10,11	1.05	1 (12%)	10,14,16	1.12	2 (20%)

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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.10	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	CG2-CB-CA	-2.43	108.54	113.26
1	C	160	TPO	O3P-P-O1P	2.20	119.41	110.83
1	A	160	TPO	OG1-P-O1P	-2.12	101.77	109.33
1	C	160	TPO	P-OG1-CB	-2.01	117.86	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	C-CA-CB-CG2
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	4SP	A	1298	-	31,31,31	1.93	9 (29%)	43,44,44	2.76	17 (39%)
3	4SP	C	1298	-	31,31,31	2.11	9 (29%)	43,44,44	3.21	28 (65%)

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	4SP	A	1298	-	-	5/15/23/23	0/4/4/4
3	4SP	C	1298	-	-	0/15/23/23	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	4SP	C4-N3	6.06	1.45	1.34
3	A	1298	4SP	C5-C4	-3.85	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	C21-C20	3.84	1.44	1.38
3	A	1298	4SP	C2-N1	3.69	1.45	1.34
3	C	1298	4SP	C2-N1	3.59	1.44	1.34
3	A	1298	4SP	C4-N9	-3.52	1.31	1.36
3	A	1298	4SP	C4-N3	3.47	1.40	1.34
3	C	1298	4SP	C20-S23	3.42	1.82	1.77
3	C	1298	4SP	C4-N9	-3.12	1.31	1.36
3	C	1298	4SP	C5-N7	2.95	1.44	1.39
3	C	1298	4SP	C5-C6	2.80	1.46	1.41
3	C	1298	4SP	C5-C4	-2.66	1.35	1.39
3	A	1298	4SP	C14-C13	2.62	1.61	1.51
3	A	1298	4SP	C2-N2	-2.55	1.31	1.36
3	A	1298	4SP	C2-N3	-2.52	1.27	1.34
3	C	1298	4SP	C6-N1	-2.37	1.29	1.32
3	C	1298	4SP	C2-N2	-2.11	1.32	1.36
3	A	1298	4SP	C5-N7	2.04	1.42	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	4SP	C5-C4-N3	-9.82	116.92	126.55
3	C	1298	4SP	C5-C4-N3	-6.33	120.34	126.55
3	C	1298	4SP	C2-N1-C6	5.78	125.33	115.38
3	C	1298	4SP	C4-C5-N7	-5.48	103.06	110.67
3	C	1298	4SP	C5-C6-N1	-5.48	116.16	123.49
3	A	1298	4SP	C5-C4-N9	5.31	112.76	105.67
3	C	1298	4SP	C18-C17-C22	-5.12	112.24	119.04
3	A	1298	4SP	N3-C2-N1	-4.86	118.30	126.26
3	C	1298	4SP	N3-C2-N1	-4.84	118.33	126.26
3	A	1298	4SP	O25-S23-C20	4.73	112.69	107.35
3	A	1298	4SP	C4-C5-N7	-4.67	104.18	110.67
3	C	1298	4SP	C4-C5-C6	4.67	119.99	115.38
3	C	1298	4SP	C21-C20-C19	-4.59	114.48	120.47
3	C	1298	4SP	O25-S23-N26	4.39	113.68	107.35
3	C	1298	4SP	C5-N7-C8	4.14	108.15	103.48
3	A	1298	4SP	C21-C22-C17	4.00	124.90	120.30
3	A	1298	4SP	C18-C17-C22	-3.83	113.97	119.04
3	A	1298	4SP	C4-C5-C6	3.77	119.10	115.38
3	C	1298	4SP	O25-S23-O24	3.72	124.51	118.80
3	C	1298	4SP	C22-C21-C20	3.71	123.05	119.44
3	C	1298	4SP	O24-S23-N26	-3.71	102.01	107.35
3	A	1298	4SP	C2-N3-C4	3.68	125.39	116.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	4SP	C4-N9-C8	3.57	109.76	106.43
3	C	1298	4SP	C19-C18-C17	3.56	124.39	120.30
3	C	1298	4SP	C5-C4-N9	3.18	109.92	105.67
3	C	1298	4SP	N9-C8-N7	-3.12	109.11	113.87
3	C	1298	4SP	N2-C2-N3	3.05	127.39	116.90
3	C	1298	4SP	C20-S23-N26	-2.99	104.24	108.40
3	C	1298	4SP	C21-C22-C17	2.97	123.72	120.30
3	C	1298	4SP	C18-C19-C20	2.67	122.04	119.44
3	A	1298	4SP	C19-C18-C17	2.64	123.34	120.30
3	C	1298	4SP	O6-C6-C5	2.61	120.18	116.73
3	C	1298	4SP	C6-C5-N7	2.58	136.85	133.82
3	C	1298	4SP	O6-C6-N1	2.58	123.46	120.02
3	C	1298	4SP	O25-S23-C20	-2.57	104.45	107.35
3	C	1298	4SP	C21-C20-S23	2.51	123.13	119.72
3	C	1298	4SP	C12-C11-C10	-2.48	104.80	111.42
3	A	1298	4SP	C14-C15-C16	2.46	116.48	111.42
3	A	1298	4SP	C22-C17-N2	2.40	128.74	120.61
3	A	1298	4SP	C6-C5-N7	2.26	136.48	133.82
3	A	1298	4SP	C17-N2-C2	-2.20	123.44	129.38
3	C	1298	4SP	C16-C11-C12	2.20	114.67	109.29
3	A	1298	4SP	C21-C20-C19	-2.19	117.61	120.47
3	A	1298	4SP	C13-C12-C11	2.08	116.46	112.08
3	A	1298	4SP	O6-C6-N1	2.01	122.71	120.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

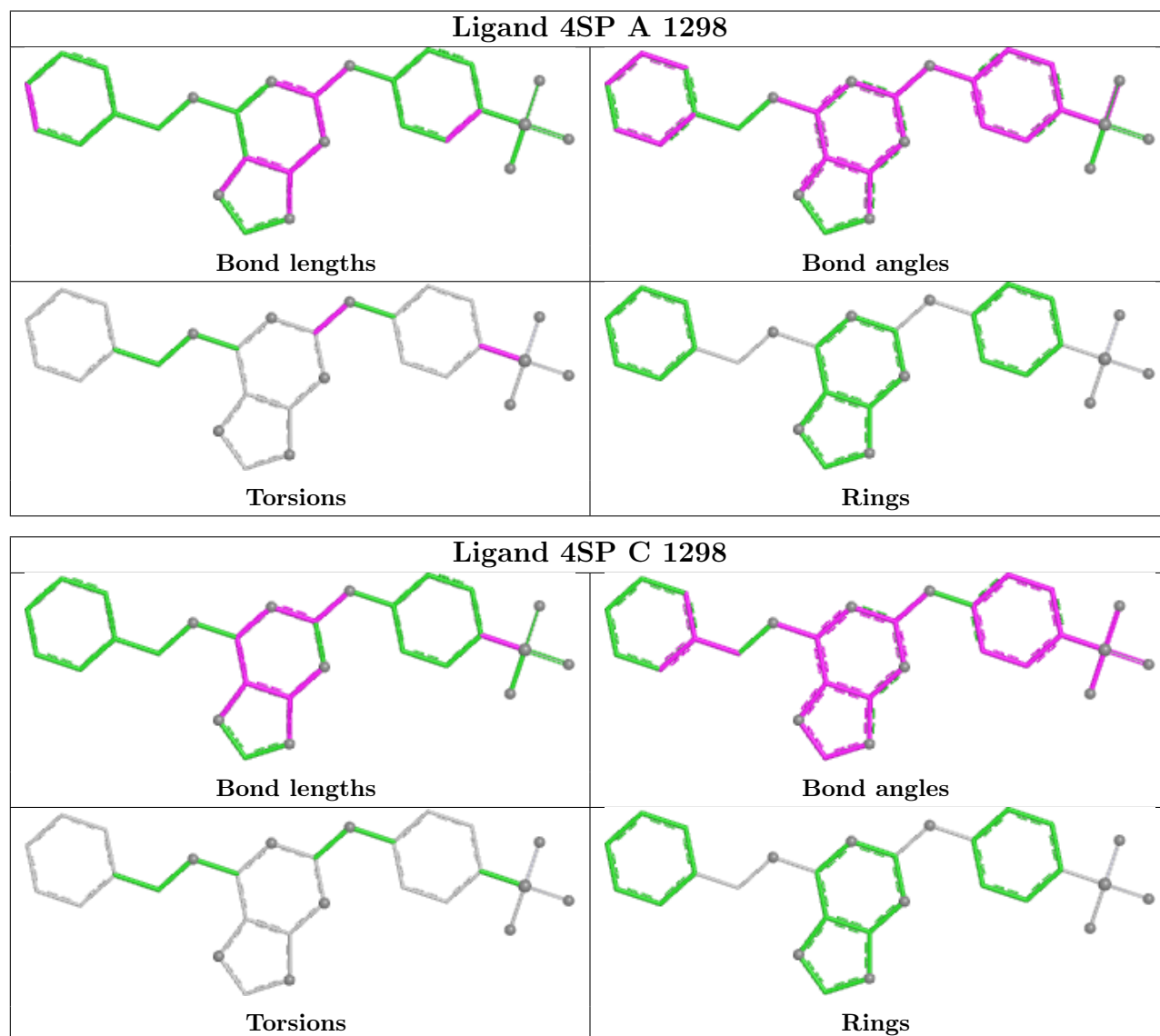
Mol	Chain	Res	Type	Atoms
3	A	1298	4SP	C19-C20-S23-O24
3	A	1298	4SP	C21-C20-S23-O24
3	A	1298	4SP	C19-C20-S23-N26
3	A	1298	4SP	C21-C20-S23-N26
3	A	1298	4SP	N3-C2-N2-C17

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	4SP	5	0
3	C	1298	4SP	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 ⓘ

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	296/303 (97%)	0.25	23 (7%) 19 18	17, 29, 52, 70	0
1	C	296/303 (97%)	1.58	79 (26%) 1 1	32, 45, 62, 80	0
2	B	258/258 (100%)	0.37	16 (6%) 26 25	20, 31, 50, 63	0
2	D	258/258 (100%)	1.68	79 (30%) 1 1	29, 48, 65, 75	0
All	All	1108/1122 (98%)	0.97	197 (17%) 4 3	17, 39, 62, 80	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	8.7
1	C	97	THR	7.4
1	C	98	GLY	7.0
2	B	175	VAL	6.5
1	C	296	LEU	6.1
1	A	295	HIS	6.1
1	A	38	ASP	5.6
1	A	71	HIS	5.6
1	A	39	THR	5.3
2	D	429	THR	5.1
1	C	10	ILE	4.9
2	D	364	LEU	4.8
1	C	120	SER	4.8
2	D	281	ILE	4.7
1	C	295	HIS	4.7
1	C	104	ILE	4.5
2	D	432	LEU	4.5
2	D	372	TRP	4.4
1	A	72	THR	4.3
1	C	256	ASP	4.3
2	B	176	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	280	ALA	4.1
2	D	365	TYR	4.1
2	D	394	LEU	4.0
1	C	294	PRO	4.0
2	D	359	ALA	3.9
2	B	432	LEU	3.9
2	B	327	CYS	3.9
2	D	336	LEU	3.9
1	C	225	VAL	3.9
2	D	325	ALA	3.9
1	C	39	THR	3.9
1	C	282	ALA	3.8
1	C	223	ASP	3.8
1	C	215	ILE	3.8
1	A	40	GLU	3.8
1	C	100	PRO	3.8
2	D	319	PHE	3.8
1	C	190	GLY	3.8
2	D	403	GLN	3.8
1	A	73	GLU	3.7
2	D	279	VAL	3.7
2	D	327	CYS	3.6
1	A	97	THR	3.6
2	D	405	ALA	3.6
2	D	374	GLU	3.6
2	D	381	GLY	3.6
1	C	74	ASN	3.5
1	A	296	LEU	3.5
2	D	320	LEU	3.5
2	D	382	TYR	3.4
2	D	395	HIS	3.4
2	D	176	PRO	3.4
2	D	350	TYR	3.4
1	C	84	HIS	3.4
2	D	418	TYR	3.4
2	D	180	GLU	3.4
2	D	389	PRO	3.4
1	C	250	LYS	3.4
1	C	268	HIS	3.3
2	B	423	LEU	3.3
2	D	341	LEU	3.3
2	D	424	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	284	ASP	3.3
1	C	72	THR	3.2
1	C	139	GLY	3.2
2	B	285	THR	3.2
2	D	366	THR	3.2
2	D	431	ASN	3.2
1	A	96	LEU	3.2
1	C	103	LEU	3.2
2	D	316	THR	3.2
1	C	95	ALA	3.1
1	C	96	LEU	3.1
1	A	36	ARG	3.1
2	D	280	TYR	3.1
1	C	290	THR	3.1
1	C	287	GLN	3.1
2	D	317	GLN	3.1
2	D	401	ALA	3.0
2	D	430	LEU	3.0
1	C	93	ALA	3.0
1	C	252	VAL	3.0
2	D	326	ASN	2.9
2	B	283	ASP	2.9
1	C	227	TRP	2.9
2	B	431	ASN	2.9
1	C	234	PRO	2.9
2	B	280	TYR	2.9
2	B	323	GLN	2.8
2	D	334	MET	2.8
1	C	105	LYS	2.8
1	C	11	GLY	2.8
1	C	71	HIS	2.8
1	A	95	ALA	2.8
1	C	267	LEU	2.8
2	D	188	GLU	2.7
2	D	371	SER	2.7
2	D	177	ASP	2.7
2	D	387	LEU	2.7
1	C	89	LYS	2.7
1	C	255	LEU	2.7
2	D	315	LEU	2.7
2	D	362	LEU	2.7
2	D	329	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	328	LYS	2.7
1	C	183	ALA	2.6
1	C	14	THR	2.6
2	D	391	LEU	2.6
1	C	293	VAL	2.6
1	C	138	GLU	2.6
1	C	253	PRO	2.6
1	A	293	VAL	2.6
2	D	376	LEU	2.6
2	D	396	GLN	2.6
2	D	206	ILE	2.5
1	C	46	SER	2.5
1	C	102	PRO	2.5
1	A	59	ASN	2.5
1	A	41	THR	2.5
2	D	427	PRO	2.5
1	C	2	GLU	2.5
2	D	386	SER	2.5
2	B	296	HIS	2.5
1	C	192	ILE	2.5
1	C	198	THR	2.4
2	D	392	MET	2.4
1	A	5	GLN	2.4
2	B	224	GLU	2.4
1	C	124	LEU	2.4
2	D	420	GLY	2.4
1	C	240	PHE	2.4
2	D	179	HIS	2.4
2	D	324	PRO	2.4
2	D	323	GLN	2.3
1	C	199	ARG	2.3
2	D	191	VAL	2.3
1	C	161	HIS	2.3
2	B	282	THR	2.3
2	B	277	GLU	2.3
1	C	286	PHE	2.3
1	A	226	VAL	2.3
2	D	428	GLU	2.3
1	A	294	PRO	2.3
2	D	222	GLY	2.3
2	D	335	PHE	2.3
1	C	156	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	62	ASN	2.3
1	C	194	ALA	2.3
1	A	37	LEU	2.3
2	D	377	ILE	2.2
1	C	41	THR	2.2
2	D	282	THR	2.2
1	C	111	LEU	2.2
1	C	202	LEU	2.2
1	C	262	LEU	2.2
2	D	185	TYR	2.2
2	D	340	SER	2.2
2	D	360	PHE	2.2
2	D	221	VAL	2.2
1	C	233	MET	2.2
2	D	318	TYR	2.2
1	C	167	TRP	2.2
2	D	400	LYS	2.2
1	C	289	VAL	2.2
2	B	180	GLU	2.2
1	C	201	ALA	2.2
2	D	361	HIS	2.2
1	A	2	GLU	2.1
1	C	230	VAL	2.1
1	C	283	HIS	2.1
1	C	83	LEU	2.1
2	D	375	SER	2.1
1	C	237	LYS	2.1
1	C	203	PHE	2.1
1	C	285	PHE	2.1
2	D	201	LYS	2.1
1	C	13	GLY	2.1
1	A	88	LYS	2.1
1	C	115	LEU	2.1
1	C	59	ASN	2.1
2	D	378	ARG	2.1
2	D	369	GLY	2.1
1	C	275	ILE	2.1
1	C	90	PHE	2.1
1	C	164	VAL	2.1
2	D	354	VAL	2.1
1	C	196	MET	2.0
2	D	189	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	234	LEU	2.0
1	C	238	PRO	2.0
1	C	15	TYR	2.0
2	D	413	TYR	2.0
1	A	35	ILE	2.0
1	A	247	ASP	2.0
2	D	390	CYS	2.0
2	D	426	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	160	11/12	0.89	0.14	34,38,40,41	0
1	TPO	A	160	11/12	0.98	0.05	22,24,24,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

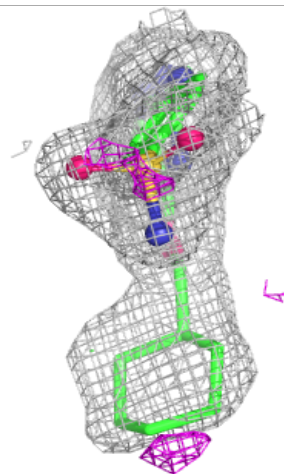
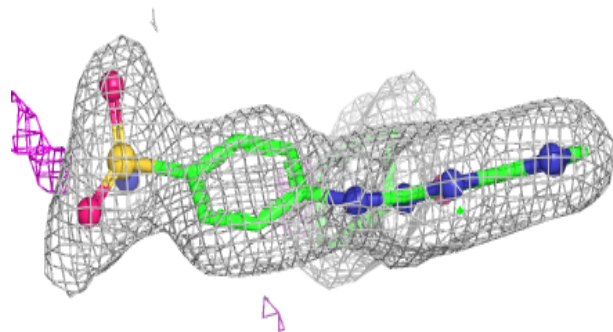
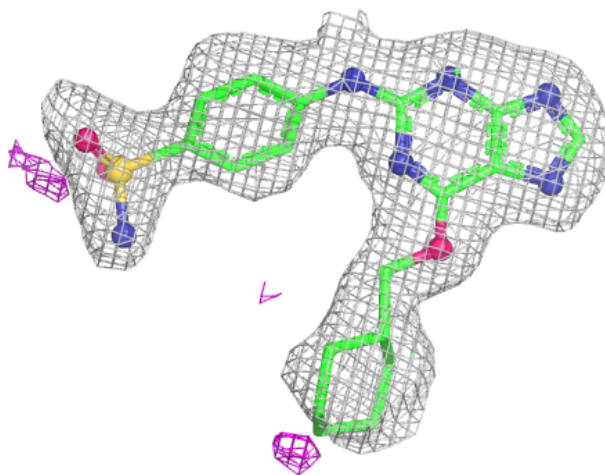
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	4SP	C	1298	28/28	0.88	0.13	38,47,59,62	0
3	4SP	A	1298	28/28	0.97	0.07	25,33,38,44	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.

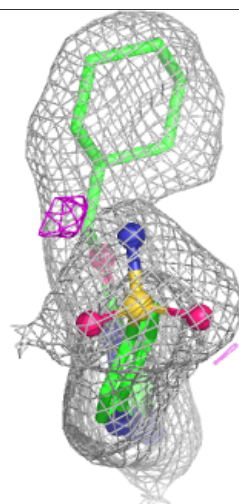
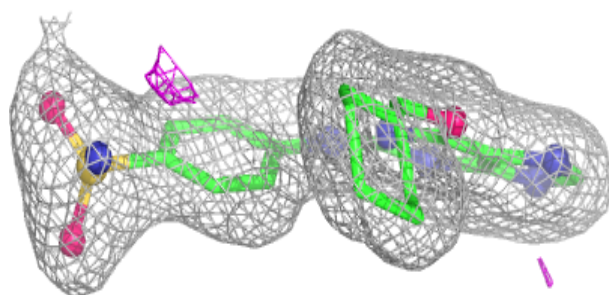
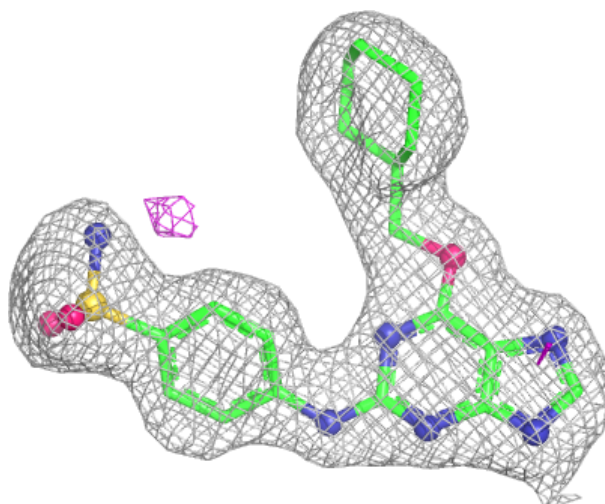
Electron density around 4SP C 1298:

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



Electron density around 4SP A 1298:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.