



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H1S
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2/CYCLIN A COM-
PLEXED 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

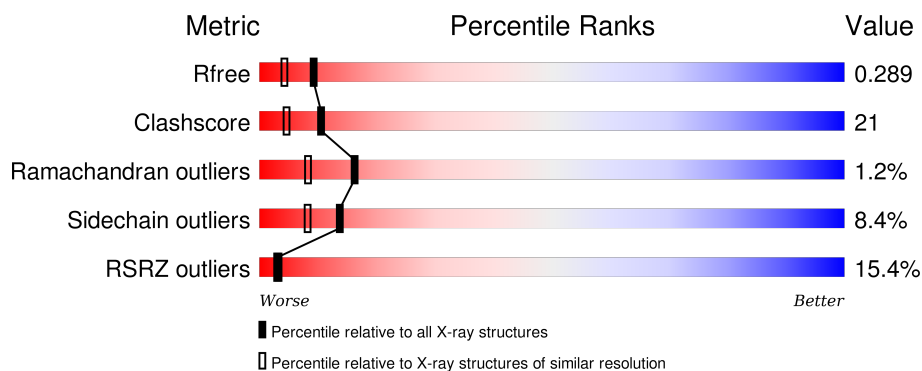
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div>66%</div> <div>25%</div> <div>6%</div> <div>..</div> </div>
1	C	303	<div> <div>19%</div> <div>54%</div> <div>34%</div> <div>9%</div> <div>..</div> </div>
2	B	258	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
2	D	258	<div> <div>28%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>

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.

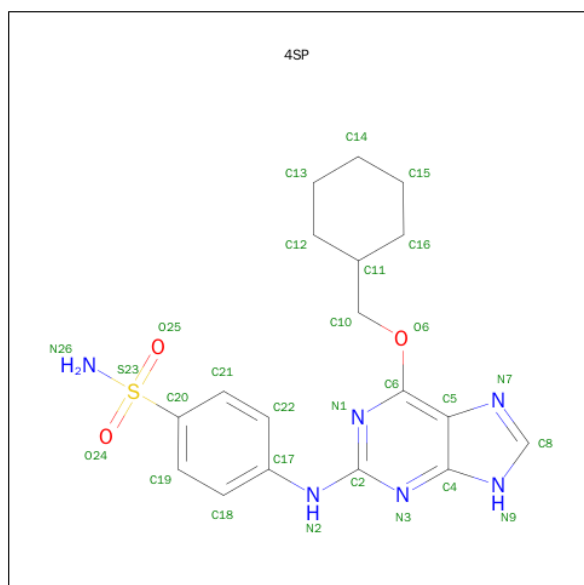
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

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 (three-letter code: 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		

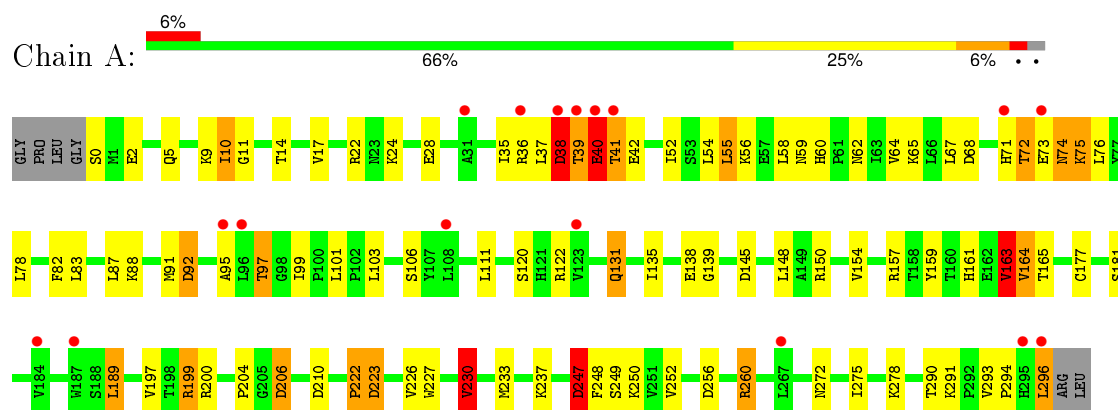
- Molecule 4 is water.

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		

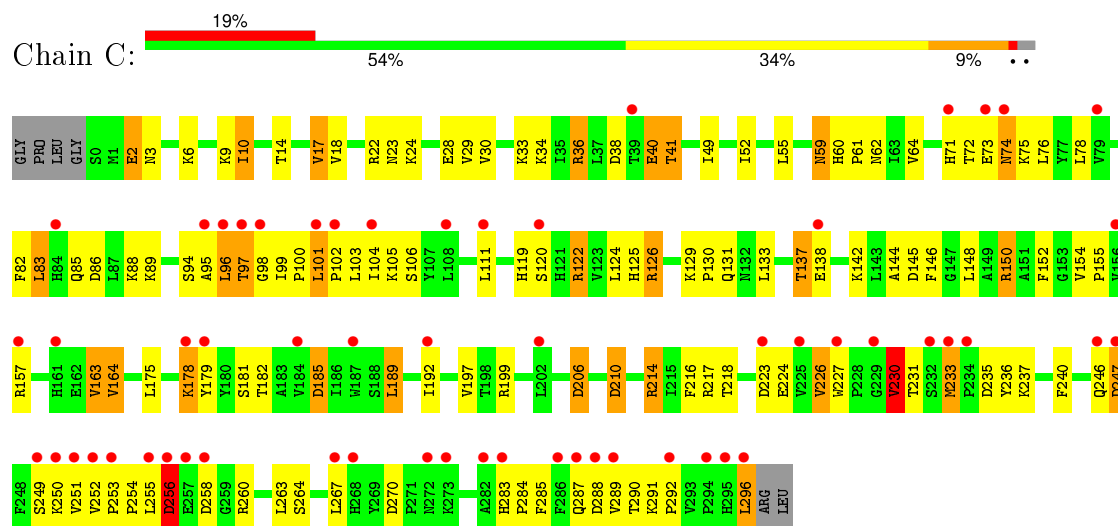
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

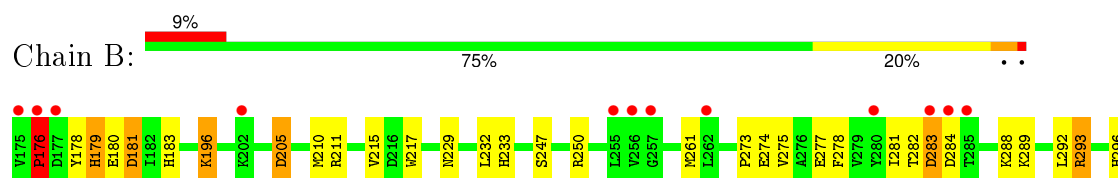
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

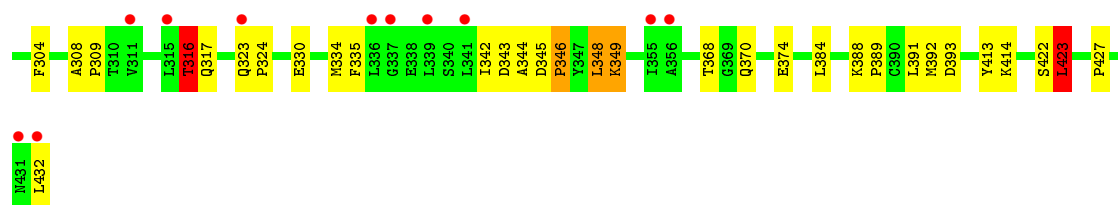


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

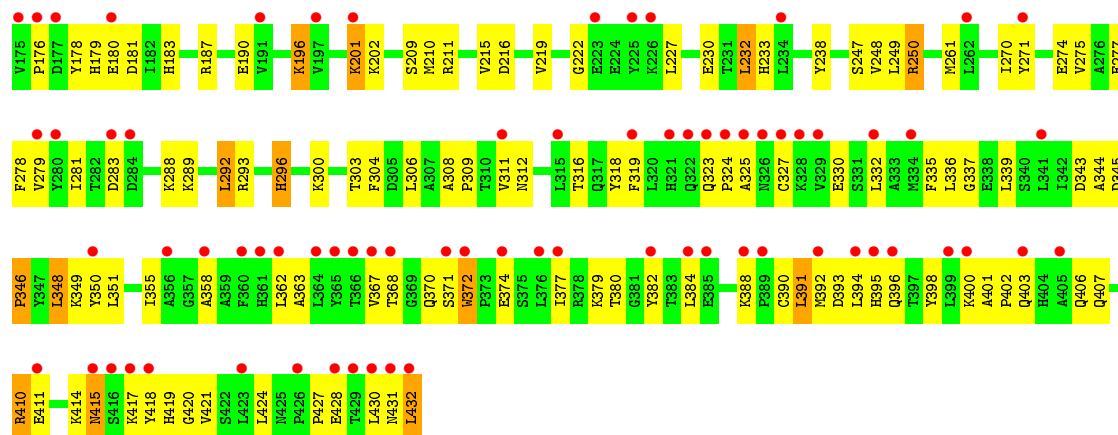


• Molecule 2: CYCLIN A2





• 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 23.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.00) 84.6 (23.70-1.90)	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	4743 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 100118 reflections	Xtriage
F_o, F_c correlation	0.93	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, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, 4SP

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	0.94	2/2438 (0.1%)	1.29	31/3308 (0.9%)
1	C	0.74	0/2438	1.35	24/3308 (0.7%)
2	B	0.88	0/2133	1.16	14/2897 (0.5%)
2	D	0.68	0/2133	1.20	13/2897 (0.4%)
All	All	0.82	2/9142 (0.0%)	1.26	82/12410 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	SER	CB-OG	-6.36	1.33	1.42
1	A	159	TYR	CD1-CE1	5.34	1.47	1.39

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	ARG	NE-CZ-NH2	18.79	129.69	120.30
1	C	36	ARG	NE-CZ-NH1	-17.56	111.52	120.30
2	D	250	ARG	NE-CZ-NH1	13.15	126.88	120.30
2	D	293	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	C	247	ASP	CB-CG-OD2	10.98	128.19	118.30
2	B	293	ARG	NE-CZ-NH1	10.80	125.70	120.30
2	D	250	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	C	36	ARG	CG-CD-NE	10.36	133.55	111.80
1	C	36	ARG	CD-NE-CZ	10.10	137.74	123.60
1	A	260	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	230	VAL	CB-CA-C	-9.76	92.86	111.40
1	C	145	ASP	CB-CG-OD2	9.55	126.90	118.30
2	B	293	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	C	17	VAL	CB-CA-C	-8.77	94.74	111.40
2	D	293	ARG	NE-CZ-NH1	8.63	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	284	ASP	CB-CG-OD2	8.48	125.94	118.30
1	A	210	ASP	CB-CG-OD1	8.40	125.86	118.30
2	D	181	ASP	CB-CG-OD2	7.83	125.35	118.30
2	D	393	ASP	CB-CG-OD2	7.78	125.30	118.30
2	D	283	ASP	CB-CG-OD2	7.75	125.28	118.30
1	C	122	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	260	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	36	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	C	230	VAL	CB-CA-C	-7.35	97.44	111.40
1	A	256	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	247	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	38	ASP	N-CA-C	7.26	130.59	111.00
1	C	214	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	A	157	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	B	205	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	122	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	270	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	145	ASP	CB-CG-OD2	6.61	124.25	118.30
2	D	343	ASP	CB-CG-OD2	6.55	124.20	118.30
1	C	157	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	163	VAL	CG1-CB-CG2	6.45	121.23	110.90
1	A	163	VAL	N-CA-CB	-6.37	97.48	111.50
1	C	76	LEU	CA-CB-CG	6.29	129.76	115.30
2	D	432	LEU	CA-CB-CG	6.24	129.66	115.30
1	C	126	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	86	ASP	CB-CG-OD2	6.22	123.90	118.30
2	B	176	PRO	N-CA-C	6.20	128.23	112.10
1	C	206	ASP	CB-CG-OD2	6.12	123.81	118.30
2	B	343	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	36	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	92	ASP	CB-CG-OD2	6.07	123.76	118.30
2	B	423	LEU	CB-CA-C	6.06	121.71	110.20
2	B	393	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	296	LEU	CA-CB-CG	5.88	128.82	115.30
2	B	316	THR	N-CA-CB	-5.86	99.17	110.30
1	C	217	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	38	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	210	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	248	PHE	CB-CG-CD1	-5.78	116.76	120.80
2	B	432	LEU	CA-CB-CG	5.75	128.53	115.30
2	D	384	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	235	ASP	CB-CG-OD2	5.75	123.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	MET	CG-SD-CE	5.71	109.34	100.20
2	B	423	LEU	CB-CG-CD1	5.70	120.69	111.00
1	A	199	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	256	ASP	CB-CG-OD2	5.66	123.39	118.30
2	D	250	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	206	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	41	THR	N-CA-CB	5.60	120.94	110.30
1	C	288	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	72	THR	N-CA-CB	-5.56	99.74	110.30
1	A	55	LEU	CB-CG-CD1	5.51	120.36	111.00
1	C	185	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	83	LEU	CA-CB-CG	-5.38	102.92	115.30
1	A	97	THR	CB-CA-C	-5.29	97.33	111.60
2	D	232	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	200	ARG	NE-CZ-NH1	-5.25	117.68	120.30
2	B	181	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	216	PHE	CB-CG-CD2	-5.24	117.13	120.80
2	B	283	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	293	VAL	N-CA-C	-5.19	97.00	111.00
1	A	223	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	410	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	68	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	247	ASP	N-CA-CB	-5.13	101.37	110.60
1	A	157	ARG	CG-CD-NE	-5.07	101.15	111.80
1	A	210	ASP	OD1-CG-OD2	-5.05	113.70	123.30

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	92	1
1	C	2388	0	2430	130	0
2	B	2083	0	2107	67	1
2	D	2083	0	2107	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	22	5	0
3	C	28	0	22	1	0
4	A	271	0	0	22	0
4	B	182	0	0	13	0
4	C	138	0	0	40	0
4	D	112	0	0	36	0
All	All	9701	0	9118	388	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 21.

All (388) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:GLN:HG2	4:C:2132:HOH:O	1.83	0.78
1:C:38:ASP:HB3	1:C:41:THR:HB	1.66	0.77
1:A:95:ALA:O	1:A:199:ARG:NH1	2.16	0.77
2:D:210:MET:HE1	2:D:250:ARG:HD3	1.67	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
2:D:402:PRO:HB2	2:D:403:GLN:OE1	1.85	0.76
1:C:10:ILE:HG23	4:C:2009:HOH:O	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
2:D:336:LEU:HD22	4:D:2098:HOH:O	1.87	0.75
1:C:144:ALA:HA	4:C:2071: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:146:PHE:CE1	4:C:2071:HOH:O	2.41	0.73
1:C:30:VAL:HG13	4:C:2023:HOH:O	1.87	0.73
1:A:88:LYS:HD2	1:A:131:GLN:HG3	1.71	0.72
1:A:38:ASP:O	1:A:39:THR:CB	2.37	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: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:414:LYS:CG	2:B:423:LEU:HD11	2.18	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.07	0.69
2:B:217:TRP:CH2	2:B:281:ILE:HD12	2.28	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:C:85:GLN:OE1	1:C:89:LYS:HB3	1.93	0.68
1:A:181:SER:HB3	4:A:2165:HOH:O	1.92	0.68
1:C:249:SER:OG	1:C:250:LYS:HE3	1.93	0.68
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.76	0.68
1:C:94:SER:OG	4:C:2059:HOH:O	2.12	0.67
1:C:40:GLU:CD	4:C:2031:HOH:O	2.25	0.67
2:D:394:LEU:HB2	4:D:2096:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:362:LEU:HD23	4:D:2098:HOH:O	1.96	0.65
2:B:289:LYS:HE3	2:B:293:ARG:HE	1.62	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:394:LEU:CB	4:D:2096:HOH:O	2.46	0.64
2:D:346:PRO:O	2:D:349:LYS:HG2	1.97	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
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: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
2:D:325:ALA:HB3	4:D:2075:HOH:O	1.99	0.62
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.82	0.62
2:D:261:MET:HE1	4:D:2026: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.30	0.59
1:C:210:ASP:O	1:C:214:ARG:HG3	2.03	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
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: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
1:C:10:ILE:HD11	1:C:82:PHE:CE1	2.39	0.56
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.87	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
1:C:10:ILE:HG22	1:C:18:VAL:O	2.06	0.56
1:A:10:ILE:HG22	1:A:11:GLY:N	2.21	0.56
2:D:275:VAL:HG11	2:D:292:LEU:HD13	1.88	0.56
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:LYS:CG	1:C:131:GLN:HE21	2.20	0.53
1:A:40:GLU:HA	2:B:288:LYS:HE2	1.90	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:358:ALA:HA	2:D:391:LEU:HD22	1.90	0.53
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.90	0.52
2:B:281:ILE:HG13	2:B:282:THR:N	2.22	0.52
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.74	0.52
1:C:237:LYS:HD3	4:C:2109:HOH:O	2.10	0.52
1:C:285:PHE:N	4:C:2130:HOH:O	2.41	0.52
2:D:215:VAL:O	2:D:219:VAL:HG23	2.10	0.52
1:A:10:ILE:HG22	1:A:11:GLY:H	1.75	0.52
3:C:1298:4SP:H101	4:C:2009:HOH:O	2.10	0.52
1:C:181:SER:OG	1:C:182:THR:N	2.39	0.52
2:B:422:SER:C	2:B:423:LEU:HG	2.30	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
1:C:142:LYS:NZ	4:C:2070:HOH:O	2.43	0.51
2:B:210:MET:CE	2:B:250:ARG:HB2	2.40	0.51
1:C:96:LEU:O	1:C:199:ARG:NH1	2.43	0.51
1:C:88:LYS:HD2	1:C:131:GLN:HE21	1.75	0.51
2:D:358:ALA:CB	2:D:391:LEU:HD22	2.41	0.51
1:A:39:THR:HG23	2:B:289:LYS:HD3	1.93	0.51
1:C:99:ILE:O	1:C:104:ILE:HD11	2.11	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
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.46	0.51
2:D:279:VAL:HB	4:D:2052:HOH:O	2.10	0.51
1:A:64:VAL:HG21	3:A:1298:4SP:C8	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LYS:NZ	2:B:293:ARG:HE	2.08	0.50
2:D:201:LYS:HD3	2:D:201:LYS:O	2.11	0.50
1:C:131:GLN:CD	1:C:131:GLN:H	2.15	0.50
2:D:279:VAL:HG21	2:D:288:LYS:HA	1.94	0.50
1:C:10:ILE:O	1:C:10:ILE:HG23	2.11	0.50
1:A:222:PRO:HA	1:A:226:VAL:HG11	1.94	0.50
2:D:417:LYS:HB3	2:D:417:LYS:NZ	2.27	0.50
2:B:289:LYS:HE3	2:B:293:ARG:CZ	2.42	0.49
1:A:5:GLN:OE1	1:A:24:LYS:HE2	2.11	0.49
1:C:28:GLU:HB3	4:C:2023:HOH:O	2.12	0.49
2:B:427:PRO:HA	4:B:2180:HOH:O	2.11	0.49
1:C:251:VAL:HG22	4:C:2116:HOH:O	2.13	0.49
2:D:248:VAL:HG12	2:D:249:LEU:O	2.12	0.49
1:C:131:GLN:CD	1:C:131:GLN:N	2.66	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
1:C:230:VAL:HG13	1:C:233:MET:HE1	1.95	0.48
1:C:74:ASN:HB2	4:C:2049:HOH:O	2.12	0.48
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.95	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
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:HA	2:B:323:GLN:OE1	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:C:59:ASN:C	1:C:59:ASN:ND2	2.68	0.47
1:A:39:THR:HG22	1:A:40:GLU:HG3	1.96	0.47
2:D:279:VAL:HG23	4:D:2052:HOH:O	2.14	0.47
2:D:196:LYS:O	2:D:196:LYS:HG3	2.14	0.47
1:C:106:SER:HB2	1:C:290:THR:O	2.14	0.47
2:D:391:LEU:HA	4:D:2096:HOH:O	2.14	0.47
1:A:71:HIS:CG	1:A:76:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HE3	1:A:17:VAL:CG1	2.44	0.47
2:D:401:ALA:CB	2:D:402:PRO:HD3	2.38	0.47
1:A:92:ASP:O	1:A:95:ALA:HB2	2.14	0.47
2:B:278:PHE:O	2:B:281:ILE:HG12	2.14	0.47
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.96	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:255:LEU:HB3	1:C:260:ARG:HG2	1.96	0.47
1:C:144:ALA:CA	4:C:2071:HOH:O	2.55	0.47
2:D:332:LEU:HB3	2:D:363:ALA:HB1	1.97	0.47
1:C:95:ALA:O	1:C:199:ARG:NH1	2.45	0.47
1:C:14:THR:HG21	1:C:148:LEU:HD13	1.97	0.47
2:D:178:TYR:HE2	4:D:2011:HOH:O	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
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.42	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: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
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
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: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
2:D:401:ALA:CB	2:D:402:PRO:CD	2.94	0.45
2:D:275:VAL:HG11	2:D:292:LEU:CD1	2.46	0.45
1:C:72:THR:HG22	1:C:74:ASN:OD1	2.16	0.45
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.51	0.45
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.51	0.45
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.97	0.45
1:C:72:THR:HG22	1:C:73:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD13	1:A:275:ILE:HG21	1.68	0.45
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.97	0.45
1:A:135:ILE:HD12	1:A:296:LEU:HD21	1.99	0.45
2:D:421:VAL:O	2:D:424:LEU:HG	2.17	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:311:VAL:HG21	4:D:2080:HOH:O	2.17	0.45
1:C:52:ILE:CD1	1:C:78:LEU:HD21	2.47	0.45
2:D:358:ALA:HA	2:D:391:LEU:CD2	2.47	0.44
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.81	0.44
2:B:211:ARG:HD3	2:B:344:ALA:HB2	1.97	0.44
2:D:368:THR:CB	2:D:370:GLN:HE21	2.29	0.44
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
2:D:395:HIS:HE1	2:D:427:PRO:O	1.99	0.44
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.99	0.44
1:C:85:GLN:HB3	4:C:2051:HOH:O	2.17	0.44
1:A:131:GLN:H	1:A:131:GLN:CD	2.20	0.44
2:D:278:PHE:O	2:D:281:ILE:HG12	2.16	0.44
1:A:291:LYS:NZ	4:A:2265:HOH:O	2.50	0.44
2:D:274:GLU:HG2	2:D:277:GLU:HG3	2.00	0.44
1:A:10:ILE:CG2	1:A:11:GLY:N	2.81	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
2:D:230:GLU:OE1	2:D:230:GLU:HA	2.17	0.44
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.01	0.44
2:D:414:LYS:O	2:D:415:ASN:C	2.54	0.43
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.48	0.43
1:C:105:LYS:HG2	1:C:289:VAL:HG23	1.99	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:350:TYR:CE1	2:D:390:CYS:HB2	2.53	0.43
2:B:334:MET:HE2	2:B:334:MET:HB3	1.82	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:196:LYS:HE3	2:D:202:LYS:HZ2	1.84	0.43
2:D:388:LYS:HB3	4:D:2095:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:MET:HE1	2:B:250:ARG:HB2	2.01	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:C:22:ARG:NH2	1:C:24:LYS:HA	2.34	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:59:ASN:C	1:C:59:ASN:HD22	2.21	0.42
1:C:71:HIS:CD2	2:D:296:HIS:CE1	3.07	0.42
2:D:238:TYR:OH	2:D:306:LEU:HB3	2.19	0.42
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.54	0.42
1:A:250:LYS:HD3	1:A:250:LYS:HA	1.85	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.54	0.42
2:D:417:LYS:HE2	2:D:418:TYR:CZ	2.54	0.42
1:A:10:ILE:CG2	3:A:1298:4SP:H101	2.50	0.42
1:C:125:HIS:CE1	4:C:2064:HOH:O	2.73	0.42
2:D:210:MET:HE2	2:D:250:ARG:HB2	2.02	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
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
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.34	0.42
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.00	0.42
1:A:54:LEU:O	1:A:58:LEU:HG	2.18	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:B:414:LYS:HG2	2:B:423:LEU:HD21	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
1:A:14:THR:HG21	1:A:148:LEU:HD12	2.02	0.42
1:A:223:ASP:H	1:A:226:VAL:HG12	1.85	0.42
2:D:271:TYR:OH	4:D:2051:HOH:O	2.21	0.42
1:A:165:THR:HG22	4:A:2154:HOH:O	2.20	0.42
1:A:72:THR:CG2	1:A:75:LYS:H	2.33	0.42
2:D:370:GLN:HB3	4:D:2091:HOH:O	2.20	0.42
2:D:337:GLY:HA3	4:D:2078:HOH:O	2.20	0.42
1:C:88:LYS:CD	1:C:131:GLN:HE21	2.33	0.42
2:B:210:MET:HE3	2:B:250:ARG:HD3	2.02	0.42
1:C:96:LEU:O	1:C:98:GLY:N	2.53	0.42
2:D:380:THR:HG22	4:D:2069:HOH:O	2.19	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:CG2	1:C:18:VAL:HG12	2.49	0.41
2:D:415:ASN:OD1	2:D:417:LYS:N	2.44	0.41
2:D:371:SER:O	2:D:372:TRP:C	2.58	0.41
1:A:64:VAL:HG21	3:A:1298:4SP:H8	2.02	0.41
1:C:83:LEU:HD11	1:C:142:LYS:HD2	2.01	0.41
2:D:327:CYS:HB2	2:D:419:HIS:CE1	2.55	0.41
1:A:87:LEU:O	1:A:91:MET:HG3	2.20	0.41
2:D:430:LEU:O	2:D:431:ASN:HB2	2.20	0.41
2:D:201:LYS:C	2:D:201:LYS:HD3	2.41	0.41
1:A:72:THR:HG23	1:A:74:ASN:OD1	2.21	0.41
2:D:187:ARG:HA	2:D:187:ARG:HD2	1.85	0.41
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.56	0.41
2:B:414:LYS:HE2	2:B:423:LEU:HD21	2.03	0.41
1:A:131:GLN:N	1:A:131:GLN:CD	2.74	0.41
3:A:1298:4SP:C22	3:A:1298:4SP:N1	2.84	0.41
1:A:296:LEU:HB3	4:A:2269:HOH:O	2.20	0.41
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.92	0.41
1:A:56:LYS:HB3	1:A:56:LYS:HE2	1.93	0.41
1:C:252:VAL:HG12	1:C:255:LEU:HB2	2.03	0.41
2:D:196:LYS:HE3	2:D:202:LYS:HZ3	1.84	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
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.56	0.41
1:C:291:LYS:HG2	1:C:291:LYS:O	2.21	0.40
1:A:37:LEU:HB2	1:A:74:ASN:O	2.20	0.40
2:D:358:ALA:HB1	2:D:391:LEU:HD22	2.02	0.40
1:A:75:LYS:HZ3	1:A:75:LYS:HG2	1.67	0.40
1:A:106:SER:HB2	1:A:290:THR:O	2.21	0.40
1:C:224:GLU:OE2	1:C:231:THR:OG1	2.31	0.40
2:D:407:GLN:HA	4:D:2103:HOH:O	2.21	0.40
1:C:137:THR:O	1:C:137:THR:OG1	2.35	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%)	19	11
1	C	294/303 (97%)	283 (96%)	6 (2%)	5 (2%)	11	4
2	B	256/258 (99%)	250 (98%)	5 (2%)	1 (0%)	39	33
2	D	256/258 (99%)	244 (95%)	8 (3%)	4 (2%)	12	5
All	All	1100/1122 (98%)	1058 (96%)	29 (3%)	13 (1%)	16	8

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%)	12	7
1	C	261/265 (98%)	231 (88%)	30 (12%)	7	4
2	B	232/232 (100%)	217 (94%)	15 (6%)	21	15
2	D	232/232 (100%)	217 (94%)	15 (6%)	21	15
All	All	986/994 (99%)	903 (92%)	83 (8%)	14	8

All (83) 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	38	ASP
1	A	40	GLU
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	97	THR
1	A	101	LEU
1	A	122	ARG
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	230	VAL
1	A	247	ASP
2	B	176	PRO
2	B	179	HIS
2	B	180	GLU
2	B	196	LYS
2	B	232	LEU
2	B	247	SER
2	B	274	GLU
2	B	316	THR
2	B	346	PRO
2	B	348	LEU

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Mol	Chain	Res	Type
2	B	349	LYS
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
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	97	THR
1	C	101	LEU
1	C	120	SER
1	C	122	ARG
1	C	137	THR
1	C	138	GLU
1	C	150	ARG
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	256	ASP
1	C	264	SER
1	C	296	LEU
2	D	179	HIS
2	D	196	LYS
2	D	201	LYS
2	D	209	SER
2	D	232	LEU
2	D	247	SER
2	D	289	LYS

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Mol	Chain	Res	Type
2	D	292	LEU
2	D	296	HIS
2	D	300	LYS
2	D	346	PRO
2	D	348	LEU
2	D	391	LEU
2	D	398	TYR
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	183	HIS
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
2	B	431	ASN
1	C	59	ASN
1	C	60	HIS
1	C	113	GLN
1	C	131	GLN
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	1.11	0	7,14,16	1.63	2 (28%)
1	TPO	C	160	1	8,10,11	0.78	0	7,14,16	1.14	1 (14%)

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	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	CG2-CB-CA	-2.28	108.54	113.17
1	A	160	TPO	OG1-P-O1P	-2.14	101.77	107.11
1	C	160	TPO	O3P-P-O1P	2.74	119.41	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	28,31,31	1.82	8 (28%)	35,44,44	3.31	15 (42%)
3	4SP	C	1298	-	28,31,31	1.99	6 (21%)	35,44,44	3.28	23 (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	-	-	0/15/23/23	0/4/4/4
3	4SP	C	1298	-	-	0/15/23/23	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	4SP	O6-C6	-4.65	1.32	1.35
3	A	1298	4SP	C5-C4	-3.24	1.33	1.40
3	A	1298	4SP	O6-C6	-3.23	1.33	1.35
3	A	1298	4SP	C2-N2	-2.90	1.31	1.36
3	C	1298	4SP	C5-C4	-2.41	1.35	1.40
3	C	1298	4SP	C2-N2	-2.37	1.32	1.36
3	A	1298	4SP	C2-N3	-2.07	1.27	1.34
3	A	1298	4SP	C4-N3	2.32	1.40	1.36
3	A	1298	4SP	C14-C13	2.39	1.61	1.51
3	C	1298	4SP	C2-N1	2.85	1.44	1.34
3	A	1298	4SP	C2-N1	2.93	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	4SP	C20-S23	3.56	1.82	1.77
3	A	1298	4SP	C21-C20	3.70	1.44	1.38
3	C	1298	4SP	C4-N3	4.86	1.45	1.36

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	4SP	C10-O6-C6	-11.86	104.83	117.23
3	C	1298	4SP	C4-C5-N7	-6.98	103.06	109.48
3	A	1298	4SP	C4-C5-N7	-5.76	104.18	109.48
3	A	1298	4SP	N3-C2-N1	-5.16	118.30	126.22
3	C	1298	4SP	N3-C2-N1	-5.14	118.33	126.22
3	C	1298	4SP	C18-C17-C22	-4.91	112.24	119.06
3	C	1298	4SP	C21-C20-C19	-4.44	114.48	120.42
3	C	1298	4SP	C5-C6-N1	-4.33	116.16	123.81
3	C	1298	4SP	O24-S23-N26	-4.07	102.01	107.28
3	A	1298	4SP	C18-C17-C22	-3.67	113.97	119.06
3	C	1298	4SP	C20-S23-N26	-3.18	104.24	108.45
3	C	1298	4SP	C12-C11-C10	-3.16	104.80	111.47
3	C	1298	4SP	C10-O6-C6	-2.69	114.41	117.23
3	C	1298	4SP	O25-S23-C20	-2.39	104.45	107.39
3	A	1298	4SP	C17-N2-C2	-2.17	123.44	129.19
3	A	1298	4SP	C21-C20-C19	-2.10	117.61	120.42
3	A	1298	4SP	O25-S23-O24	-2.10	115.85	118.80
3	C	1298	4SP	C21-C20-S23	2.08	123.13	119.74
3	C	1298	4SP	O6-C10-C11	2.12	112.86	107.97
3	A	1298	4SP	C12-C11-C10	2.14	115.97	111.47
3	C	1298	4SP	C16-C11-C12	2.15	114.67	109.26
3	C	1298	4SP	C18-C19-C20	2.32	122.04	119.48
3	A	1298	4SP	C14-C15-C16	2.40	116.48	111.44
3	A	1298	4SP	C22-C17-N2	2.48	128.74	120.66
3	A	1298	4SP	C13-C12-C11	2.63	116.46	112.22
3	A	1298	4SP	C19-C18-C17	2.72	123.34	120.28
3	C	1298	4SP	C21-C22-C17	3.06	123.72	120.28
3	C	1298	4SP	C22-C21-C20	3.23	123.05	119.48
3	C	1298	4SP	O6-C6-C5	3.27	120.18	115.07
3	C	1298	4SP	N2-C2-N3	3.43	127.39	116.93
3	C	1298	4SP	C2-N3-C4	3.65	119.49	115.09
3	C	1298	4SP	C19-C18-C17	3.66	124.39	120.28
3	C	1298	4SP	O25-S23-O24	4.07	124.51	118.80
3	A	1298	4SP	C21-C22-C17	4.11	124.90	120.28
3	A	1298	4SP	O25-S23-C20	4.30	112.69	107.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	4SP	O25-S23-N26	4.94	113.68	107.28
3	C	1298	4SP	C2-N1-C6	7.02	125.33	115.32
3	A	1298	4SP	C2-N3-C4	8.56	125.39	115.09

There are no chirality outliers.

There are no torsion outliers.

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

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	296/303 (97%)	0.40	17 (5%) 27 29	17, 29, 52, 70	0
1	C	296/303 (97%)	1.20	58 (19%) 1 2	32, 45, 62, 80	0
2	B	258/258 (100%)	0.47	23 (8%) 12 13	20, 31, 50, 63	0
2	D	258/258 (100%)	1.49	73 (28%) 1 1	29, 48, 65, 75	0
All	All	1108/1122 (98%)	0.88	171 (15%) 3 3	17, 39, 62, 80	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	10.9
2	D	432	LEU	8.8
2	D	175	VAL	8.6
2	B	175	VAL	8.3
1	C	295	HIS	7.5
1	A	38	ASP	6.7
1	A	39	THR	6.7
1	C	282	ALA	6.5
2	D	429	THR	6.5
2	D	431	ASN	6.2
1	C	225	VAL	6.1
1	A	73	GLU	5.7
2	D	418	TYR	5.5
2	D	176	PRO	5.4
1	A	40	GLU	5.4
1	C	98	GLY	5.4
1	A	96	LEU	5.3
1	A	95	ALA	5.0
1	C	287	GLN	4.9
2	D	191	VAL	4.9
2	D	365	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	295	HIS	4.8
2	D	374	GLU	4.7
1	C	289	VAL	4.7
2	D	430	LEU	4.7
1	C	252	VAL	4.6
2	D	394	LEU	4.6
1	C	97	THR	4.6
2	D	328	LYS	4.6
2	D	323	GLN	4.6
1	C	247	ASP	4.5
2	D	324	PRO	4.5
2	D	280	TYR	4.5
2	D	197	VAL	4.5
1	C	95	ALA	4.4
2	D	405	ALA	4.4
2	D	372	TRP	4.3
2	B	323	GLN	4.3
2	D	319	PHE	4.2
2	D	283	ASP	4.1
2	D	271	TYR	4.1
2	D	428	GLU	4.0
2	D	403	GLN	4.0
1	C	250	LYS	4.0
2	B	256	VAL	4.0
2	D	177	ASP	4.0
2	D	364	LEU	3.9
2	D	382	TYR	3.8
1	C	255	LEU	3.8
1	C	246	GLN	3.8
1	A	36	ARG	3.7
2	D	326	ASN	3.7
1	C	161	HIS	3.6
2	D	366	THR	3.6
2	B	283	ASP	3.6
2	D	325	ALA	3.6
1	C	267	LEU	3.5
1	A	71	HIS	3.5
1	C	227	TRP	3.5
2	B	284	ASP	3.5
2	D	367	VAL	3.5
2	D	377	ILE	3.5
1	C	229	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	385	GLU	3.4
1	C	249	SER	3.4
1	C	223	ASP	3.3
2	D	201	LYS	3.3
1	C	184	VAL	3.3
2	D	376	LEU	3.3
2	D	350	TYR	3.3
2	D	399	LEU	3.2
2	D	356	ALA	3.2
2	D	284	ASP	3.2
1	A	41	THR	3.1
1	C	84	HIS	3.1
2	D	332	LEU	3.1
2	D	327	CYS	3.0
1	C	156	VAL	3.0
2	D	223	GLU	2.9
2	D	426	PRO	2.9
2	D	321	HIS	2.9
1	C	74	ASN	2.9
2	D	389	PRO	2.9
1	C	256	ASP	2.9
2	B	431	ASN	2.9
2	B	356	ALA	2.9
1	C	273	LYS	2.9
2	D	341	LEU	2.9
1	C	108	LEU	2.8
2	D	417	LYS	2.8
2	D	416	SER	2.8
1	C	73	GLU	2.8
2	D	411	GLU	2.8
2	B	176	PRO	2.8
2	D	388	LYS	2.8
1	A	123	VAL	2.7
1	C	257	GLU	2.7
1	C	234	PRO	2.7
1	C	294	PRO	2.7
2	D	362	LEU	2.7
1	C	258	ASP	2.7
2	D	371	SER	2.7
1	C	283	HIS	2.6
2	D	400	LYS	2.6
2	D	334	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	157	ARG	2.6
2	D	180	GLU	2.6
2	D	279	VAL	2.6
2	B	257	GLY	2.6
2	B	341	LEU	2.6
2	D	415	ASN	2.6
2	D	311	VAL	2.5
1	C	178	LYS	2.5
1	C	286	PHE	2.5
1	C	104	ILE	2.5
1	C	71	HIS	2.5
1	C	268	HIS	2.5
2	D	395	HIS	2.5
2	D	368	THR	2.5
1	C	96	LEU	2.5
2	B	336	LEU	2.5
1	C	101	LEU	2.4
2	D	361	HIS	2.4
1	C	111	LEU	2.4
2	D	315	LEU	2.4
1	C	120	SER	2.4
1	C	192	ILE	2.4
1	A	108	LEU	2.4
2	B	280	TYR	2.4
2	D	384	LEU	2.4
1	C	272	ASN	2.4
2	D	329	VAL	2.3
2	B	202	LYS	2.3
1	A	31	ALA	2.3
2	D	262	LEU	2.3
1	C	138	GLU	2.3
2	B	355	ILE	2.3
2	D	392	MET	2.3
1	C	39	THR	2.3
2	D	423	LEU	2.3
1	C	179	TYR	2.3
1	A	187	TRP	2.3
2	B	337	GLY	2.2
2	D	396	GLN	2.2
1	A	296	LEU	2.2
2	B	315	LEU	2.2
2	D	322	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	288	ASP	2.2
1	C	232	SER	2.2
2	B	177	ASP	2.2
1	C	253	PRO	2.2
1	C	292	PRO	2.2
1	C	233	MET	2.2
2	D	226	LYS	2.2
2	B	285	THR	2.1
1	C	187	TRP	2.1
2	B	262	LEU	2.1
2	B	432	LEU	2.1
2	D	234	LEU	2.1
2	D	360	PHE	2.1
1	C	79	VAL	2.1
2	D	225	TYR	2.1
1	C	251	VAL	2.1
1	C	202	LEU	2.1
1	C	102	PRO	2.1
2	D	358	ALA	2.0
2	B	311	VAL	2.0
1	A	267	LEU	2.0
2	B	255	LEU	2.0
2	B	339	LEU	2.0
1	A	184	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.89	0.19	-	34,38,40,41	0
1	TPO	A	160	11/12	0.99	0.08	-	22,24,24,25	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	4SP	A	1298	28/28	0.96	0.13	-0.24	25,33,38,44	0
3	4SP	C	1298	28/28	0.87	0.15	-0.39	38,47,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.