



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 PM UTC

PDB ID : 1H25 / pdb_00001h25
Title : CDK2/Cyclin A in complex with an 11-residue recruitment peptide from retinoblastoma-associated protein
Authors : Tews, I.; Cheng, K.Y.; Lowe, E.D.; Noble, M.E.M.; Brown, N.R.; Gul, S.; Gamblin, S.; Johnson, L.N.
Deposited on : 2002-07-31
Resolution : 2.50 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
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

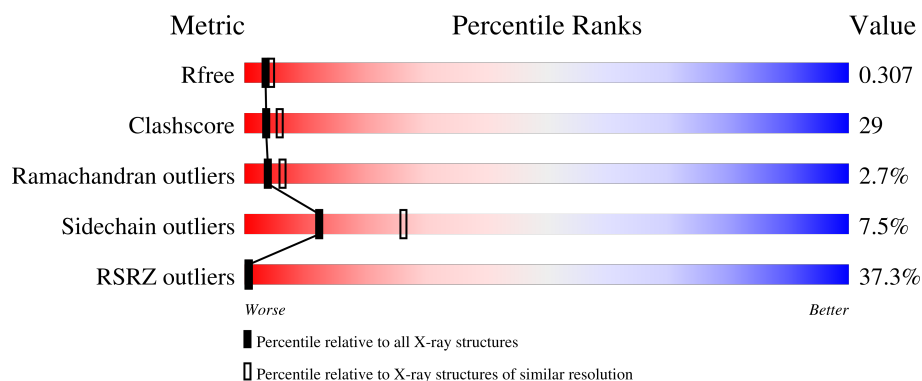
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

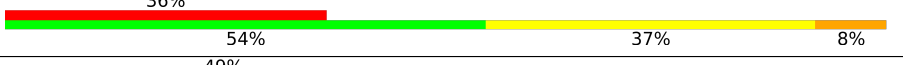
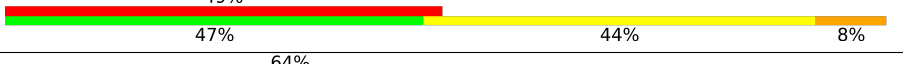
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	259	
2	D	259	
3	E	11	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9037 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	294	Total	C	N	O	P	S	0	0	0
			2363	1533	399	422	1	8			
1	C	279	Total	C	N	O	P	S	0	0	0
			2229	1443	376	401	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 a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			87	59	16	12			

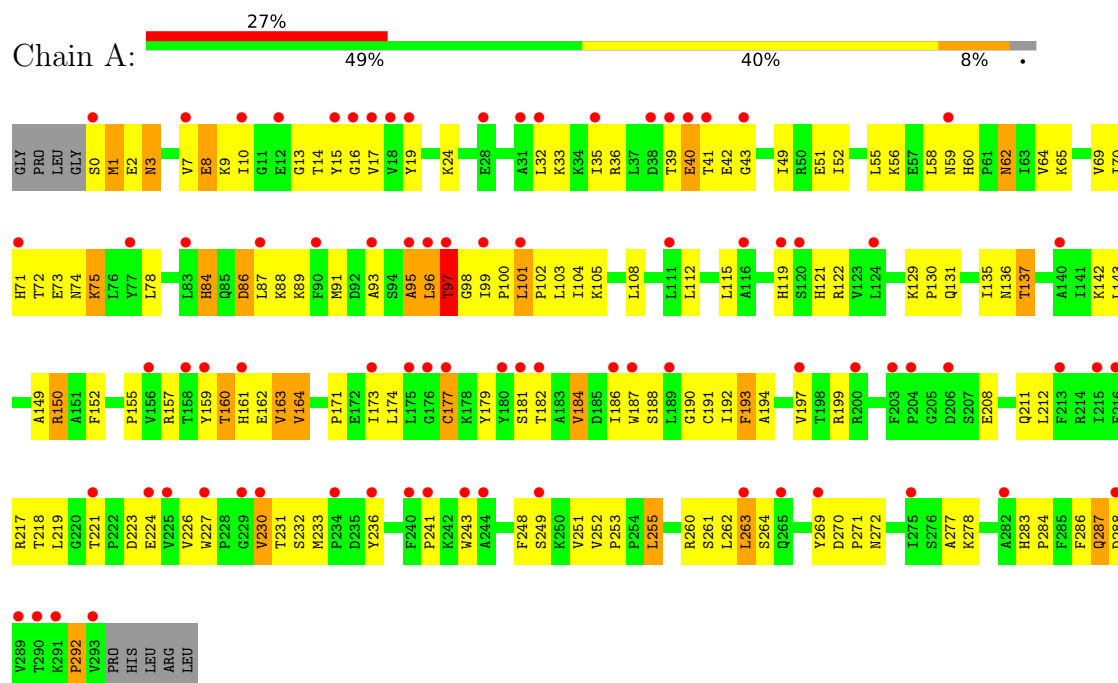
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	61	Total	O	0	0
			61	61		
4	C	47	Total	O	0	0
			47	47		
4	D	21	Total	O	0	0
			21	21		
4	E	1	Total	O	0	0
			1	1		

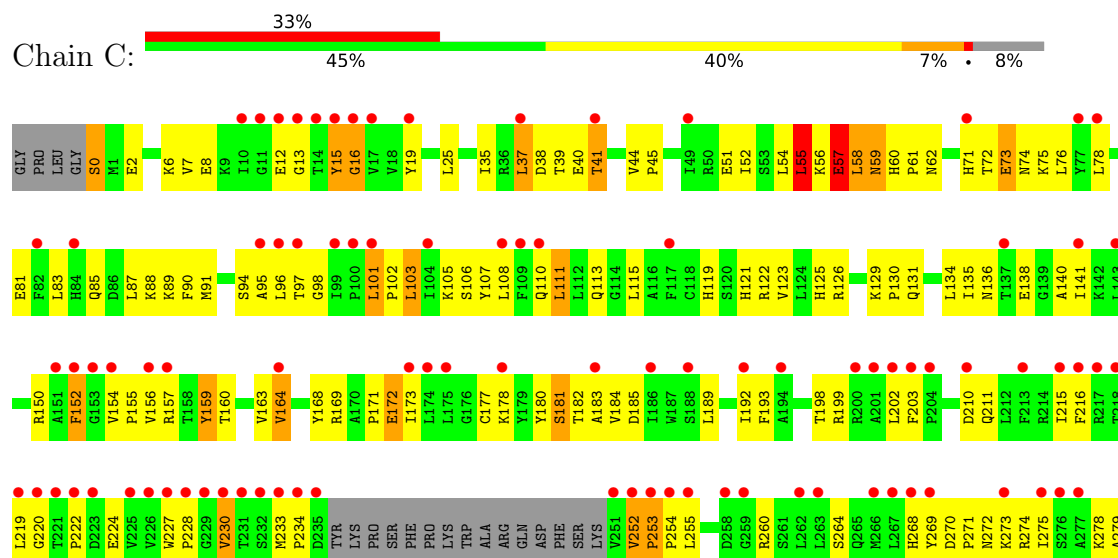
3 Residue-property plots [i](#)

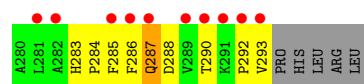
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

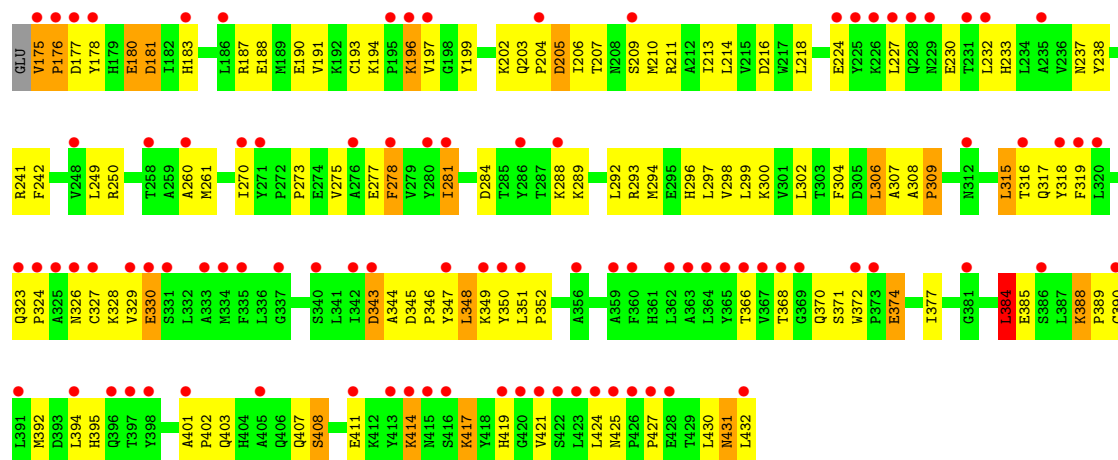


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

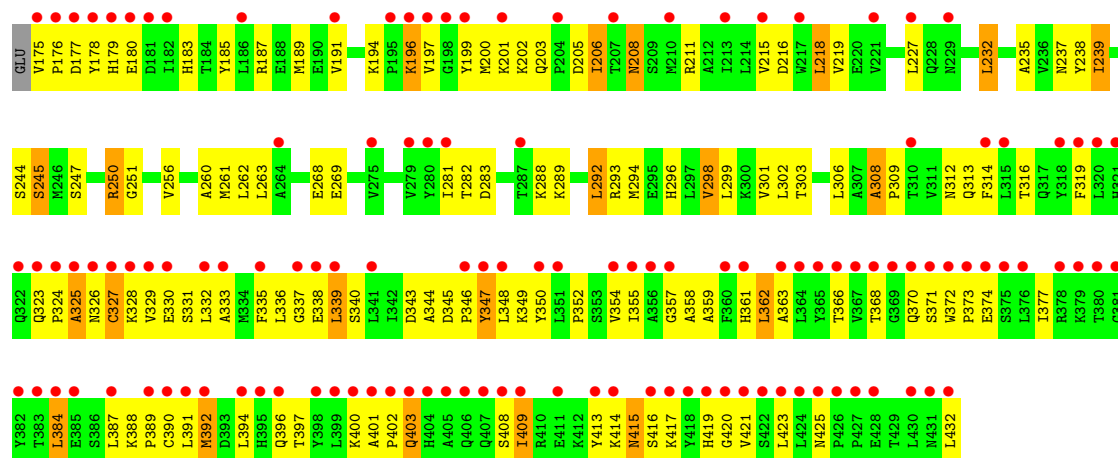




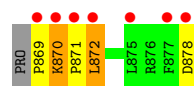
● Molecule 2: CYCLIN A2



● Molecule 2: CYCLIN A2



● Molecule 3: RETINOBLASTOMA-ASSOCIATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.61Å 133.85Å 147.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.50 28.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.00-2.50) 99.8 (28.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.266 0.296 , 0.307	Depositor DCC
R_{free} test set	2656 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9037	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.01	0/2411	1.29	16/3270 (0.5%)
1	C	0.76	0/2269	1.09	6/3077 (0.2%)
2	B	1.03	4/2133 (0.2%)	1.25	16/2897 (0.6%)
2	D	0.70	0/2133	1.08	10/2897 (0.3%)
3	E	0.73	0/89	0.90	0/116
All	All	0.89	4/9035 (0.0%)	1.18	48/12257 (0.4%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	ALA	CA-C	-7.13	1.45	1.53
2	B	260	ALA	CA-CB	-5.93	1.43	1.53
2	B	294	MET	SD-CE	5.76	1.94	1.79
2	B	233	HIS	N-CA	5.49	1.53	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	LEU	N-CA-C	-10.28	98.89	111.33
1	A	193	PHE	N-CA-C	-9.28	101.11	111.14
1	A	230	VAL	CB-CA-C	-7.19	102.67	111.88
1	A	163	VAL	N-CA-C	7.17	119.14	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	GLU	N-CA-C	-7.12	103.59	111.36
1	A	283	HIS	N-CA-C	7.03	118.21	109.57
1	A	58	LEU	CA-C-N	-6.89	113.88	122.84
1	A	58	LEU	C-N-CA	-6.89	113.88	122.84
1	A	221	THR	N-CA-C	-6.63	99.93	109.48
2	B	414	LYS	N-CA-C	-6.58	104.29	112.90
2	B	348	LEU	N-CA-C	-6.53	105.14	113.23
2	B	306	LEU	N-CA-C	6.47	121.26	113.23
2	B	315	LEU	CA-C-N	-6.39	111.71	120.28
2	B	315	LEU	C-N-CA	-6.39	111.71	120.28
2	D	268	GLU	N-CA-C	6.32	119.12	111.40
2	D	256	VAL	N-CA-C	-6.25	104.24	110.62
1	A	65	LYS	N-CA-C	6.17	119.29	109.24
2	B	197	VAL	N-CA-C	5.96	118.50	111.05
1	C	57	GLU	N-CA-C	-5.96	98.11	110.80
2	B	278	PHE	N-CA-C	-5.93	104.89	111.36
1	C	152	PHE	N-CA-C	5.90	118.34	108.96
1	C	16	GLY	N-CA-C	5.89	119.20	110.42
2	B	237	ASN	N-CA-C	-5.81	104.87	111.14
2	D	298	VAL	CB-CA-C	-5.80	104.44	112.04
2	D	201	LYS	N-CA-C	-5.79	105.05	111.71
1	A	253	PRO	N-CA-C	5.62	117.56	110.70
1	A	112	LEU	N-CA-C	-5.59	105.34	111.82
2	B	384	LEU	N-CA-C	-5.58	105.29	111.71
2	D	282	THR	N-CA-C	-5.56	106.82	113.21
2	B	328	LYS	N-CA-C	-5.52	105.16	111.07
2	D	308	ALA	N-CA-C	5.52	116.78	109.93
2	D	245	SER	N-CA-C	5.40	120.53	113.88
2	B	260	ALA	N-CA-C	-5.39	105.48	111.36
2	B	270	ILE	N-CA-C	-5.37	105.37	110.42
2	B	309	PRO	CA-C-O	-5.36	115.13	121.67
1	A	93	ALA	N-CA-C	-5.25	106.92	113.38
1	C	211	GLN	N-CA-C	-5.25	104.99	111.40
2	B	343	ASP	N-CA-C	5.23	118.78	107.49
2	B	205	ASP	N-CA-C	5.22	119.34	112.92
1	C	253	PRO	N-CA-C	5.19	117.03	110.70
2	D	269	GLU	N-CA-C	5.12	117.86	110.28
2	D	384	LEU	N-CA-C	-5.12	106.99	113.18
1	A	149	ALA	N-CA-C	5.07	116.65	110.41
1	C	111	LEU	N-CA-C	-5.07	105.75	111.28
1	A	62	ASN	CA-C-N	-5.05	116.93	123.19
1	A	62	ASN	C-N-CA	-5.05	116.93	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	343	ASP	N-CA-C	5.04	116.63	108.41
1	A	84	HIS	N-CA-C	5.04	117.67	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159	TYR	Mainchain

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	2363	0	2405	140	1
1	C	2229	0	2273	165	0
2	B	2083	0	2107	109	1
2	D	2083	0	2107	132	0
3	E	87	0	101	11	0
4	A	62	0	0	17	1
4	B	61	0	0	16	1
4	C	47	0	0	23	0
4	D	21	0	0	10	0
4	E	1	0	0	0	0
All	All	9037	0	8993	524	2

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 29.

All (524) 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:327:CYS:HB3	4:B:2039:HOH:O	1.34	1.23
1:A:163:VAL:HG12	1:A:164:VAL:HG23	1.26	1.11
1:C:154:VAL:O	2:D:316:THR:HG23	1.55	1.06
3:E:869:PRO:HB2	3:E:871:PRO:HD2	1.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:O	1:A:122:ARG:HG3	1.56	1.05
2:B:300:LYS:HE2	4:B:2027:HOH:O	1.53	1.05
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.19	1.01
1:C:121:HIS:O	1:C:122:ARG:HG3	1.62	0.98
1:C:136:ASN:ND2	1:C:140:ALA:HB3	1.79	0.97
3:E:872:LEU:O	3:E:872:LEU:HG	1.68	0.93
2:B:227:LEU:HB2	4:B:2019:HOH:O	1.69	0.91
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.01	0.90
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.54	0.89
2:B:177:ASP:HB3	4:B:2007:HOH:O	1.70	0.89
2:D:235:ALA:O	2:D:239:ILE:HG13	1.73	0.88
1:A:88:LYS:HD2	1:A:131:GLN:NE2	1.87	0.88
1:A:41:THR:HG21	4:A:2011:HOH:O	1.74	0.88
2:B:300:LYS:HE3	4:C:2009:HOH:O	1.74	0.87
3:E:869:PRO:O	3:E:872:LEU:HD23	1.74	0.87
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.39	0.86
1:C:95:ALA:O	1:C:199:ARG:NH1	2.06	0.85
1:C:227:TRP:O	1:C:230:VAL:HG23	1.76	0.85
1:C:181:SER:O	1:C:184:VAL:HG22	1.75	0.85
1:A:181:SER:HB3	4:A:2040:HOH:O	1.77	0.85
1:C:60:HIS:HD2	1:C:62:ASN:H	1.19	0.85
2:B:180:GLU:HB3	4:B:2001:HOH:O	1.75	0.85
2:D:238:TYR:CZ	2:D:306:LEU:HD22	2.11	0.85
1:C:172:GLU:OE2	1:C:274:ARG:NH1	2.09	0.84
2:D:333:ALA:HA	4:D:2015:HOH:O	1.77	0.84
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.12	0.84
2:B:299:LEU:HD22	2:B:304:PHE:CE1	2.13	0.83
2:D:361:HIS:CG	4:D:2016:HOH:O	2.30	0.83
2:B:216:ASP:OD1	2:B:408:SER:OG	1.97	0.83
2:D:319:PHE:HB3	2:D:330:GLU:OE2	1.77	0.83
1:C:71:HIS:HD2	2:D:296:HIS:NE2	1.76	0.83
2:D:313:GLN:O	2:D:316:THR:HG22	1.79	0.82
2:B:417:LYS:HZ3	2:B:417:LYS:HB3	1.45	0.81
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.62	0.81
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.62	0.81
1:C:40:GLU:O	2:D:288:LYS:HE3	1.82	0.80
1:C:88:LYS:HB2	1:C:131:GLN:HE21	1.45	0.80
2:B:194:LYS:HZ2	2:B:351:LEU:HD23	1.44	0.80
1:C:163:VAL:N	4:C:2034:HOH:O	2.16	0.78
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.46	0.78
1:C:233:MET:HG3	1:C:234:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLU:O	1:C:55:LEU:HB2	1.84	0.77
2:B:196:LYS:NZ	2:B:196:LYS:HB3	1.99	0.77
2:B:417:LYS:HB3	2:B:417:LYS:NZ	1.98	0.76
2:B:216:ASP:CG	2:B:408:SER:OG	2.28	0.76
2:D:361:HIS:HE1	2:D:371:SER:HB3	1.50	0.76
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.66	0.75
1:A:40:GLU:C	2:B:288:LYS:HE2	2.12	0.75
2:D:361:HIS:CE1	2:D:384:LEU:HD21	2.22	0.75
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.02	0.74
2:B:175:VAL:HG22	2:B:175:VAL:O	1.88	0.74
1:C:164:VAL:N	4:C:2035:HOH:O	2.19	0.74
2:B:196:LYS:HB3	2:B:196:LYS:HZ2	1.54	0.73
1:C:126:ARG:HD2	1:C:163:VAL:HG11	1.70	0.73
1:A:121:HIS:C	1:A:122:ARG:HG3	2.13	0.73
2:D:361:HIS:ND1	4:D:2016:HOH:O	2.22	0.73
2:D:372:TRP:HB3	2:D:384:LEU:HD11	1.71	0.73
1:A:16:GLY:N	4:A:2007:HOH:O	2.21	0.72
1:C:13:GLY:HA3	4:C:2006:HOH:O	1.88	0.72
2:D:336:LEU:HB3	2:D:394:LEU:HD11	1.70	0.72
3:E:869:PRO:HB2	3:E:871:PRO:CD	2.16	0.72
2:B:417:LYS:NZ	2:B:417:LYS:CB	2.53	0.72
2:B:193:CYS:C	4:B:2015:HOH:O	2.33	0.71
1:C:121:HIS:C	1:C:122:ARG:HG3	2.14	0.71
1:A:87:LEU:HG	1:A:91:MET:HE2	1.73	0.71
1:A:86:ASP:C	1:A:86:ASP:OD1	2.34	0.71
1:A:2:GLU:HB2	1:C:73:GLU:OE1	1.90	0.71
1:C:107:TYR:CE1	4:C:2026:HOH:O	2.44	0.71
2:D:176:PRO:O	4:D:2001:HOH:O	2.08	0.70
2:D:227:LEU:HD12	2:D:261:MET:HE3	1.73	0.70
2:B:299:LEU:HD22	2:B:304:PHE:CD1	2.27	0.70
3:E:869:PRO:C	3:E:871:PRO:HD2	2.17	0.69
1:A:177:CYS:SG	1:A:179:TYR:O	2.50	0.69
2:B:194:LYS:NZ	2:B:351:LEU:HD23	2.07	0.69
1:A:72:THR:HB	1:A:75:LYS:H	1.58	0.69
2:B:430:LEU:O	2:B:431:ASN:HB2	1.93	0.69
1:A:39:THR:C	1:A:41:THR:H	2.02	0.68
2:D:326:ASN:OD1	2:D:329:VAL:HG23	1.93	0.68
2:D:288:LYS:O	2:D:292:LEU:HD22	1.94	0.68
2:D:218:LEU:HD21	2:D:261:MET:HB2	1.76	0.67
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.77	0.67
2:D:368:THR:OG1	2:D:370:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:SER:HA	1:A:260:ARG:HD3	1.77	0.67
2:D:238:TYR:CE1	2:D:306:LEU:HD22	2.29	0.67
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.77	0.67
2:D:359:ALA:O	4:D:2015:HOH:O	2.12	0.66
2:B:181:ASP:OD1	4:B:2010:HOH:O	2.13	0.66
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.75	0.66
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.77	0.66
1:A:223:ASP:H	1:A:226:VAL:HG12	1.61	0.66
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.78	0.66
1:A:7:VAL:O	1:A:8:GLU:HB3	1.96	0.65
1:A:284:PRO:O	1:A:287:GLN:HG2	1.97	0.65
1:C:98:GLY:HA2	1:C:199:ARG:CZ	2.27	0.65
1:C:72:THR:HG22	1:C:74:ASN:H	1.61	0.65
1:C:111:LEU:HD21	1:C:141:ILE:HD13	1.79	0.65
1:A:73:GLU:HA	4:A:2021:HOH:O	1.97	0.65
1:A:227:TRP:CG	1:A:230:VAL:HG13	2.31	0.65
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.32	0.64
1:C:75:LYS:NZ	4:C:2021:HOH:O	2.23	0.64
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.78	0.64
2:D:263:LEU:HD11	2:D:299:LEU:HG	1.78	0.64
2:D:218:LEU:CD2	2:D:261:MET:SD	2.86	0.64
1:A:88:LYS:CD	1:A:131:GLN:HE21	2.02	0.64
2:D:208:ASN:OD1	2:D:344:ALA:HB3	1.98	0.64
2:D:175:VAL:HG22	2:D:177:ASP:HB2	1.80	0.63
1:A:161:HIS:NE2	1:A:173:ILE:O	2.31	0.63
1:C:219:LEU:HB2	1:C:269:TYR:OH	1.98	0.63
2:D:361:HIS:CE1	2:D:371:SER:HB3	2.31	0.63
1:A:136:ASN:C	1:A:136:ASN:OD1	2.41	0.63
1:A:218:THR:HG23	1:A:251:VAL:HG22	1.80	0.63
1:A:39:THR:O	1:A:41:THR:N	2.31	0.63
1:A:39:THR:C	1:A:41:THR:N	2.53	0.63
1:C:215:ILE:HG23	1:C:219:LEU:HD12	1.81	0.63
2:D:361:HIS:HE1	2:D:384:LEU:HD21	1.64	0.63
2:D:176:PRO:HA	2:D:179:HIS:HB2	1.80	0.62
3:E:869:PRO:CB	3:E:871:PRO:HD2	2.21	0.62
1:A:36:ARG:HD3	4:A:2010:HOH:O	1.98	0.62
1:A:41:THR:CG2	4:A:2011:HOH:O	2.40	0.62
2:D:361:HIS:CE1	4:D:2016:HOH:O	2.53	0.62
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.34	0.62
1:C:260:ARG:O	1:C:264:SER:OG	2.14	0.62
1:A:15:TYR:N	4:A:2007:HOH:O	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.35	0.61
1:A:71:HIS:HE2	2:B:304:PHE:HE2	1.47	0.61
2:B:302:LEU:C	4:B:2028:HOH:O	2.43	0.61
1:A:95:ALA:O	1:A:199:ARG:NH1	2.33	0.61
2:B:209:SER:O	2:B:213:ILE:HG13	2.01	0.61
1:A:71:HIS:NE2	2:B:304:PHE:HE2	1.99	0.61
1:C:40:GLU:O	2:D:288:LYS:CE	2.48	0.61
1:A:278:LYS:HD2	4:B:2007:HOH:O	2.00	0.61
1:C:111:LEU:HD21	1:C:141:ILE:CD1	2.31	0.61
2:D:294:MET:O	2:D:294:MET:HG3	2.00	0.61
1:A:60:HIS:CD2	1:A:62:ASN:H	2.19	0.61
4:A:2001:HOH:O	2:D:293:ARG:HD3	2.00	0.61
2:D:349:LYS:HE3	2:D:350:TYR:CZ	2.36	0.61
1:C:13:GLY:CA	4:C:2006:HOH:O	2.48	0.60
1:C:108:LEU:O	1:C:108:LEU:HD12	2.01	0.60
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.82	0.60
1:C:85:GLN:HB3	4:C:2023:HOH:O	2.00	0.60
1:C:15:TYR:CE1	1:C:35:ILE:HG12	2.37	0.60
1:C:60:HIS:CD2	1:C:62:ASN:H	2.10	0.60
1:C:94:SER:O	1:C:199:ARG:HD3	2.00	0.59
1:C:54:LEU:O	1:C:56:LYS:N	2.35	0.59
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.84	0.59
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.85	0.59
1:A:252:VAL:HG11	1:A:255:LEU:HD22	1.82	0.59
2:B:216:ASP:OD2	2:B:408:SER:OG	2.21	0.59
2:B:249:LEU:HD12	4:C:2008:HOH:O	2.02	0.59
1:C:177:CYS:SG	1:C:233:MET:SD	2.94	0.59
2:D:358:ALA:HA	2:D:391:LEU:HD13	1.85	0.59
2:D:392:MET:HB2	4:D:2019:HOH:O	2.02	0.59
2:B:421:VAL:O	4:B:2058:HOH:O	2.17	0.58
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.18	0.58
1:C:107:TYR:HE1	4:C:2026:HOH:O	1.80	0.58
2:D:211:ARG:HG2	2:D:211:ARG:HH11	1.67	0.58
2:D:237:ASN:HA	4:D:2008:HOH:O	2.03	0.58
2:D:339:LEU:HD22	2:D:397:THR:CG2	2.32	0.58
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.33	0.58
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.38	0.58
1:C:189:LEU:HA	1:C:192:ILE:HD12	1.84	0.58
1:C:0:SER:C	4:C:2002:HOH:O	2.47	0.58
2:D:196:LYS:NZ	2:D:196:LYS:HB3	2.18	0.58
1:C:95:ALA:HA	1:C:199:ARG:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:O	1:C:40:GLU:HB2	2.02	0.57
1:C:57:GLU:O	1:C:58:LEU:C	2.46	0.57
1:C:122:ARG:HD3	4:C:2030:HOH:O	2.04	0.57
2:D:298:VAL:HG13	2:D:302:LEU:HD12	1.85	0.57
1:A:219:LEU:CD2	1:A:248:PHE:HE1	2.17	0.57
1:C:54:LEU:O	1:C:55:LEU:C	2.46	0.57
1:C:106:SER:O	1:C:110:GLN:HG3	2.04	0.57
1:C:83:LEU:HD13	1:C:134:LEU:HB2	1.86	0.57
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.85	0.57
2:D:361:HIS:C	2:D:363:ALA:H	2.13	0.57
1:A:86:ASP:OD1	1:A:86:ASP:O	2.22	0.57
1:A:41:THR:O	2:B:288:LYS:NZ	2.34	0.57
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.35	0.57
1:A:227:TRP:CD2	1:A:230:VAL:CG1	2.88	0.57
1:A:190:GLY:O	1:A:191:CYS:C	2.48	0.57
1:C:130:PRO:HB2	1:C:131:GLN:NE2	2.20	0.56
1:C:216:PHE:O	1:C:220:GLY:HA2	2.05	0.56
1:C:270:ASP:HB3	1:C:273:LYS:HB2	1.88	0.56
1:A:64:VAL:HG13	1:A:64:VAL:O	2.05	0.56
2:D:362:LEU:O	2:D:362:LEU:HD12	2.05	0.56
2:D:414:LYS:HE2	2:D:423:LEU:HG	1.88	0.56
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.87	0.56
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.88	0.56
2:B:224:GLU:HB2	3:E:871:PRO:HG2	1.87	0.56
2:B:327:CYS:CB	4:B:2039:HOH:O	2.14	0.56
1:A:39:THR:HG21	2:B:289:LYS:NZ	2.21	0.56
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.71	0.56
1:A:262:LEU:O	1:A:263:LEU:C	2.49	0.55
1:C:37:LEU:HD21	1:C:76:LEU:HD13	1.87	0.55
2:D:361:HIS:O	2:D:363:ALA:N	2.40	0.55
1:C:216:PHE:O	1:C:220:GLY:CA	2.54	0.55
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.41	0.55
1:C:216:PHE:CD1	1:C:222:PRO:HD3	2.42	0.55
3:E:869:PRO:C	3:E:871:PRO:CD	2.78	0.55
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.89	0.55
1:C:94:SER:O	1:C:199:ARG:CD	2.54	0.55
2:D:346:PRO:O	2:D:348:LEU:N	2.39	0.55
2:D:415:ASN:OD1	2:D:416:SER:N	2.40	0.55
1:C:60:HIS:CG	1:C:61:PRO:CD	2.89	0.55
1:A:51:GLU:O	1:A:55:LEU:HB2	2.06	0.55
1:C:129:LYS:HD2	1:C:131:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:TYR:O	2:D:202:LYS:HB2	2.07	0.55
2:D:302:LEU:O	2:D:303:THR:C	2.50	0.55
2:B:175:VAL:C	2:B:177:ASP:H	2.15	0.55
2:D:196:LYS:HG2	2:D:244:SER:HB3	1.89	0.55
1:C:91:MET:CE	1:C:130:PRO:HB3	2.37	0.54
1:A:131:GLN:CD	1:A:131:GLN:H	2.15	0.54
1:A:96:LEU:O	1:A:97:THR:C	2.49	0.54
2:B:350:TYR:CE1	2:B:390:CYS:HB2	2.41	0.54
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.54
1:A:9:LYS:HA	1:A:19:TYR:HD2	1.73	0.54
1:A:100:PRO:C	1:A:102:PRO:HD2	2.33	0.54
2:D:387:LEU:O	2:D:391:LEU:HB2	2.08	0.54
1:A:193:PHE:O	1:A:194:ALA:C	2.47	0.54
2:B:316:THR:O	2:B:319:PHE:HB2	2.08	0.54
2:D:298:VAL:CG1	2:D:302:LEU:HD12	2.38	0.54
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.42	0.54
2:D:323:GLN:HB2	2:D:324:PRO:HD3	1.90	0.53
2:D:281:ILE:C	2:D:283:ASP:H	2.16	0.53
1:A:97:THR:HG23	1:A:98:GLY:H	1.72	0.53
2:B:323:GLN:HB3	4:B:2036:HOH:O	2.08	0.53
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.39	0.53
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.43	0.53
1:C:51:GLU:HG3	4:C:2014:HOH:O	2.08	0.53
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.67	0.53
1:A:84:HIS:CE1	1:A:137:THR:HG23	2.43	0.53
1:A:101:LEU:N	1:A:102:PRO:CD	2.72	0.53
2:D:323:GLN:N	2:D:324:PRO:CD	2.71	0.53
1:C:38:ASP:HA	4:C:2013:HOH:O	2.08	0.53
1:C:95:ALA:C	1:C:199:ARG:HH11	2.16	0.53
2:B:202:LYS:O	2:B:204:PRO:HD3	2.10	0.52
2:D:218:LEU:HD22	2:D:261:MET:SD	2.49	0.52
1:A:269:TYR:O	1:A:271:PRO:HD3	2.08	0.52
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.90	0.52
1:A:252:VAL:CG1	1:A:255:LEU:HD22	2.39	0.52
1:C:286:PHE:O	1:C:288:ASP:N	2.43	0.52
1:A:217:ARG:HD3	1:A:243:TRP:CE2	2.44	0.52
2:B:175:VAL:C	2:B:177:ASP:N	2.66	0.52
1:C:39:THR:HG21	2:D:289:LYS:HZ2	1.75	0.52
2:B:417:LYS:CB	2:B:417:LYS:HZ2	2.23	0.52
1:A:131:GLN:CD	1:A:131:GLN:N	2.68	0.52
2:D:337:GLY:O	2:D:340:SER:OG	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:O	2:B:288:LYS:CE	2.58	0.52
2:D:362:LEU:HD23	2:D:394:LEU:HG	1.91	0.52
1:A:103:LEU:HD13	1:A:292:PRO:HB2	1.92	0.51
1:A:171:PRO:HD3	1:A:187:TRP:CZ2	2.45	0.51
2:B:392:MET:HE3	2:B:432:LEU:HD12	1.92	0.51
2:D:377:ILE:HG22	4:D:2017:HOH:O	2.11	0.51
2:D:301:VAL:O	2:D:301:VAL:CG1	2.58	0.51
2:D:361:HIS:C	2:D:363:ALA:N	2.69	0.51
1:A:150:ARG:NH2	1:A:160:TPO:O1P	2.44	0.51
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.92	0.51
1:C:96:LEU:C	4:C:2025:HOH:O	2.53	0.51
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.34	0.51
1:A:122:ARG:HA	1:A:152:PHE:CZ	2.45	0.51
2:B:343:ASP:O	2:B:344:ALA:C	2.53	0.51
1:C:268:HIS:HD2	1:C:270:ASP:H	1.59	0.51
2:D:388:LYS:O	2:D:392:MET:HG2	2.11	0.51
1:A:119:HIS:CD2	1:A:182:THR:HB	2.46	0.50
1:C:39:THR:HG22	2:D:289:LYS:NZ	2.26	0.50
2:D:203:GLN:HB3	2:D:206:ILE:HG13	1.93	0.50
2:B:194:LYS:NZ	2:B:351:LEU:CD2	2.73	0.50
1:A:184:VAL:O	4:A:2041:HOH:O	2.17	0.50
1:A:218:THR:HG23	1:A:251:VAL:CG2	2.41	0.50
2:B:315:LEU:O	2:B:316:THR:C	2.52	0.50
1:C:39:THR:CG2	2:D:289:LYS:HZ2	2.25	0.50
1:A:162:GLU:HG2	4:A:2035:HOH:O	2.11	0.50
1:C:169:ARG:HD3	1:C:173:ILE:HG22	1.92	0.50
1:C:272:ASN:HB3	4:C:2046:HOH:O	2.12	0.50
2:D:211:ARG:HD3	2:D:344:ALA:HB2	1.92	0.50
1:A:161:HIS:HB3	1:A:162:GLU:OE2	2.12	0.50
1:C:293:VAL:HG12	1:C:293:VAL:O	2.12	0.50
1:A:2:GLU:HG3	1:C:73:GLU:CD	2.37	0.49
1:C:268:HIS:CD2	1:C:270:ASP:H	2.31	0.49
2:D:357:GLY:HA2	2:D:372:TRP:CZ3	2.47	0.49
2:D:216:ASP:OD1	2:D:408:SER:OG	2.26	0.49
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.95	0.49
1:C:228:PRO:HD2	1:C:270:ASP:OD2	2.12	0.49
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.40	0.49
2:B:175:VAL:O	2:B:177:ASP:N	2.46	0.49
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.94	0.49
1:A:13:GLY:C	4:A:2007:HOH:O	2.55	0.49
2:B:281:ILE:O	3:E:872:LEU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.28	0.49
1:A:230:VAL:HG23	1:A:231:THR:N	2.28	0.48
2:B:191:VAL:HG12	2:B:191:VAL:O	2.13	0.48
1:C:101:LEU:N	1:C:102:PRO:CD	2.75	0.48
1:C:203:PHE:N	4:C:2037:HOH:O	2.39	0.48
2:B:187:ARG:HD2	2:B:190:GLU:OE2	2.13	0.48
2:D:183:HIS:O	2:D:187:ARG:HG2	2.13	0.48
1:A:159:TYR:O	1:A:160:TPO:C	2.61	0.48
1:A:3:ASN:O	1:A:24:LYS:HG3	2.12	0.48
1:A:98:GLY:HA2	1:A:199:ARG:CD	2.42	0.48
1:C:157:ARG:NH1	1:C:159:TYR:HE1	2.11	0.48
2:D:298:VAL:HG13	2:D:302:LEU:CD1	2.44	0.48
1:C:87:LEU:HG	1:C:91:MET:HE2	1.95	0.48
2:D:191:VAL:O	2:D:194:LYS:HB3	2.14	0.48
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.49	0.48
3:E:870:LYS:N	3:E:871:PRO:CD	2.76	0.48
1:C:98:GLY:HA2	1:C:199:ARG:NE	2.28	0.48
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.79	0.48
2:D:331:SER:O	2:D:421:VAL:HG21	2.14	0.48
1:A:262:LEU:C	1:A:264:SER:N	2.67	0.48
2:B:346:PRO:O	2:B:349:LYS:HG2	2.14	0.48
1:C:115:LEU:HG	1:C:119:HIS:NE2	2.29	0.47
2:B:288:LYS:O	2:B:292:LEU:HD13	2.14	0.47
2:B:424:LEU:HB2	4:B:2058:HOH:O	2.13	0.47
2:D:196:LYS:HB3	2:D:196:LYS:HZ3	1.79	0.47
1:A:230:VAL:HA	1:A:233:MET:SD	2.54	0.47
1:C:76:LEU:HD12	1:C:76:LEU:HA	1.71	0.47
2:D:314:PHE:HE2	2:D:352:PRO:HB2	1.78	0.47
1:A:10:ILE:HG12	1:A:10:ILE:O	2.15	0.47
2:B:395:HIS:CE1	2:B:427:PRO:O	2.67	0.47
1:C:54:LEU:C	1:C:56:LYS:N	2.71	0.47
1:C:88:LYS:O	1:C:89:LYS:C	2.55	0.47
1:C:171:PRO:O	1:C:173:ILE:N	2.47	0.47
1:C:111:LEU:CD2	1:C:141:ILE:HD13	2.44	0.47
1:C:152:PHE:C	4:C:2030:HOH:O	2.57	0.47
2:D:175:VAL:O	2:D:177:ASP:N	2.48	0.47
1:A:73:GLU:CA	4:A:2021:HOH:O	2.61	0.47
2:B:224:GLU:HB2	3:E:871:PRO:CG	2.44	0.47
2:B:347:TYR:OH	2:B:394:LEU:HA	2.14	0.47
2:B:368:THR:OG1	2:B:370:GLN:HG3	2.14	0.47
1:C:136:ASN:HD21	1:C:140:ALA:CB	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:TYR:C	1:C:180:TYR:CD1	2.93	0.47
1:C:182:THR:O	1:C:183:ALA:C	2.58	0.47
1:C:39:THR:CG2	2:D:289:LYS:NZ	2.77	0.47
1:C:40:GLU:OE2	2:D:289:LYS:NZ	2.48	0.47
2:D:401:ALA:O	2:D:403:GLN:N	2.48	0.47
1:C:12:GLU:HG3	1:C:16:GLY:O	2.14	0.47
1:C:39:THR:C	1:C:41:THR:H	2.23	0.47
1:C:269:TYR:O	1:C:271:PRO:HD3	2.16	0.46
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.96	0.46
2:D:350:TYR:CZ	2:D:390:CYS:HA	2.50	0.46
1:A:88:LYS:HA	1:A:91:MET:HE3	1.97	0.46
2:D:373:PRO:O	2:D:377:ILE:HG13	2.16	0.46
1:A:0:SER:HA	1:A:70:ILE:HD13	1.96	0.46
1:C:57:GLU:HB2	1:C:58:LEU:H	1.36	0.46
1:C:171:PRO:C	1:C:173:ILE:N	2.71	0.46
2:B:323:GLN:CB	4:B:2036:HOH:O	2.63	0.46
1:C:107:TYR:O	1:C:111:LEU:HG	2.16	0.46
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.84	0.46
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.89	0.46
2:D:355:ILE:HA	2:D:390:CYS:SG	2.55	0.46
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.51	0.46
1:A:39:THR:HG22	1:A:40:GLU:H	1.81	0.46
1:A:188:SER:O	1:A:192:ILE:HG13	2.15	0.46
1:A:197:VAL:HG11	1:A:252:VAL:HG13	1.98	0.46
2:B:175:VAL:HG23	2:B:177:ASP:CG	2.40	0.46
2:B:205:ASP:OD1	2:B:250:ARG:NH2	2.37	0.46
1:C:108:LEU:HG	1:C:286:PHE:HZ	1.81	0.46
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.62	0.46
1:A:231:THR:HA	1:A:236:TYR:CD1	2.51	0.46
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.50	0.46
2:B:350:TYR:CD1	2:B:390:CYS:HB2	2.51	0.46
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.98	0.46
1:A:224:GLU:OE2	1:A:231:THR:HG23	2.16	0.46
2:B:317:GLN:O	2:B:318:TYR:C	2.57	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.78	0.46
1:C:105:LYS:HD3	1:C:285:PHE:O	2.16	0.46
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.31	0.46
2:B:293:ARG:HB3	1:C:25:LEU:HD11	1.98	0.46
1:A:286:PHE:O	1:A:288:ASP:N	2.49	0.45
1:C:51:GLU:CD	4:C:2014:HOH:O	2.59	0.45
2:D:261:MET:O	2:D:262:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:O	1:A:278:LYS:C	2.59	0.45
1:A:104:ILE:O	1:A:105:LYS:C	2.60	0.45
2:B:318:TYR:O	2:B:319:PHE:C	2.56	0.45
2:B:371:SER:O	2:B:372:TRP:C	2.60	0.45
1:C:125:HIS:O	1:C:126:ARG:HB2	2.16	0.45
2:D:306:LEU:O	2:D:308:ALA:N	2.46	0.45
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.98	0.45
2:B:176:PRO:HB2	4:B:2005:HOH:O	2.16	0.45
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.15	0.45
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.51	0.45
2:D:396:GLN:HB3	2:D:400:LYS:CE	2.47	0.45
1:A:194:ALA:O	1:A:197:VAL:HB	2.17	0.45
1:C:156:VAL:HG11	1:C:181:SER:HB3	1.98	0.45
1:C:163:VAL:HA	4:C:2035:HOH:O	2.17	0.45
1:A:270:ASP:O	1:A:271:PRO:C	2.58	0.45
1:C:60:HIS:HD2	1:C:62:ASN:N	2.01	0.45
1:C:60:HIS:NE2	1:C:61:PRO:HD2	2.32	0.45
1:C:168:TYR:CD2	1:C:168:TYR:N	2.85	0.45
1:A:223:ASP:HB2	4:A:2047:HOH:O	2.17	0.45
2:B:190:GLU:OE1	2:B:352:PRO:HD2	2.17	0.45
2:B:326:ASN:CG	2:B:329:VAL:HG23	2.42	0.44
2:D:345:ASP:HA	2:D:346:PRO:HA	1.57	0.44
2:B:296:HIS:O	2:B:297:LEU:C	2.59	0.44
2:D:237:ASN:ND2	4:D:2008:HOH:O	2.49	0.44
2:B:326:ASN:C	2:B:326:ASN:OD1	2.59	0.44
2:D:196:LYS:NZ	2:D:196:LYS:CB	2.80	0.44
2:D:263:LEU:HD23	2:D:263:LEU:HA	1.89	0.44
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.31	0.44
2:D:403:GLN:HE21	2:D:403:GLN:HB2	1.57	0.44
2:D:175:VAL:C	2:D:177:ASP:N	2.75	0.44
1:A:186:ILE:O	1:A:187:TRP:C	2.61	0.44
2:B:430:LEU:O	2:B:431:ASN:CB	2.62	0.44
1:C:72:THR:HG22	1:C:73:GLU:N	2.32	0.44
2:B:175:VAL:HG23	2:B:177:ASP:OD2	2.18	0.44
1:A:121:HIS:O	1:A:122:ARG:CG	2.47	0.44
2:B:193:CYS:O	2:B:241:ARG:HD2	2.17	0.44
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.99	0.44
1:A:284:PRO:C	1:A:286:PHE:N	2.76	0.44
1:A:155:PRO:HD2	2:B:316:THR:HB	2.00	0.43
2:B:207:THR:HG23	2:B:210:MET:HE3	2.00	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HD21	1:C:185:ASP:HB3	2.00	0.43
1:A:252:VAL:HG12	1:A:252:VAL:O	2.18	0.43
1:C:286:PHE:O	1:C:287:GLN:C	2.61	0.43
1:A:33:LYS:HE2	4:A:2003:HOH:O	2.18	0.43
2:B:407:GLN:O	2:B:411:GLU:HG2	2.18	0.43
2:B:430:LEU:HD12	2:B:432:LEU:HD11	2.00	0.43
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.99	0.43
1:A:64:VAL:O	1:A:64:VAL:CG1	2.66	0.43
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.50	0.43
1:C:154:VAL:HA	1:C:155:PRO:HA	1.80	0.43
1:C:202:LEU:CD2	1:C:203:PHE:CE2	3.02	0.43
2:D:215:VAL:O	2:D:219:VAL:HG23	2.19	0.43
2:D:324:PRO:O	2:D:325:ALA:HB3	2.18	0.43
1:A:39:THR:O	1:A:40:GLU:C	2.61	0.43
1:A:263:LEU:HA	1:A:263:LEU:HD12	1.73	0.43
2:B:191:VAL:O	2:B:191:VAL:CG1	2.63	0.43
1:C:72:THR:CG2	4:C:2020:HOH:O	2.67	0.43
2:D:326:ASN:ND2	2:D:328:LYS:H	2.17	0.43
1:A:35:ILE:HD11	4:A:2003:HOH:O	2.19	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.88	0.43
2:B:238:TYR:N	2:B:238:TYR:CD1	2.83	0.43
1:C:202:LEU:O	1:C:203:PHE:CD1	2.72	0.43
2:D:200:MET:HE2	2:D:200:MET:HB2	1.87	0.43
2:D:250:ARG:HG3	2:D:251:GLY:N	2.34	0.43
1:A:87:LEU:O	1:A:87:LEU:HD12	2.19	0.42
1:A:135:ILE:O	1:A:135:ILE:HG13	2.18	0.42
1:C:122:ARG:HB2	4:C:2030:HOH:O	2.17	0.42
1:C:198:THR:O	1:C:199:ARG:HB2	2.19	0.42
1:C:260:ARG:HG3	1:C:260:ARG:NH1	2.34	0.42
2:D:203:GLN:OE1	2:D:247:SER:HA	2.17	0.42
2:D:205:ASP:CG	2:D:205:ASP:O	2.61	0.42
1:A:69:VAL:O	1:A:69:VAL:HG12	2.18	0.42
2:B:178:TYR:OH	4:B:2008:HOH:O	2.19	0.42
1:C:60:HIS:CD2	1:C:61:PRO:N	2.88	0.42
1:C:85:GLN:HE21	1:C:135:ILE:HD11	1.83	0.42
1:C:224:GLU:OE2	1:C:230:VAL:HB	2.19	0.42
1:A:223:ASP:H	1:A:226:VAL:CG1	2.31	0.42
1:A:13:GLY:O	1:A:16:GLY:N	2.50	0.42
1:A:73:GLU:C	4:A:2021:HOH:O	2.62	0.42
1:A:223:ASP:O	1:A:226:VAL:HG12	2.20	0.42
2:B:181:ASP:OD1	2:B:181:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:N	4:C:2025:HOH:O	2.53	0.42
1:C:193:PHE:C	1:C:193:PHE:CD1	2.96	0.42
1:C:270:ASP:HA	1:C:271:PRO:HD3	1.87	0.42
2:D:185:TYR:O	2:D:189:MET:HG2	2.19	0.42
2:D:323:GLN:N	2:D:324:PRO:HD3	2.34	0.42
1:A:39:THR:HG21	2:B:289:LYS:HZ3	1.83	0.42
1:A:72:THR:HG21	1:A:74:ASN:OD1	2.19	0.42
2:B:395:HIS:CG	2:B:430:LEU:HD21	2.54	0.42
1:C:135:ILE:HA	1:C:140:ALA:O	2.20	0.42
2:D:208:ASN:HD22	2:D:208:ASN:H	1.68	0.42
2:B:327:CYS:SG	2:B:419:HIS:NE2	2.91	0.42
2:D:372:TRP:HB3	2:D:384:LEU:CD1	2.46	0.42
1:C:121:HIS:O	1:C:123:VAL:HG23	2.20	0.42
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.55	0.42
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.19	0.42
2:B:242:PHE:CD1	2:B:298:VAL:HG22	2.55	0.42
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.01	0.41
2:B:411:GLU:O	2:B:414:LYS:HB2	2.20	0.41
1:C:129:LYS:HB2	1:C:130:PRO:HD2	2.02	0.41
1:C:154:VAL:O	2:D:316:THR:CG2	2.46	0.41
1:C:215:ILE:CG2	1:C:219:LEU:HD12	2.49	0.41
1:A:161:HIS:O	1:A:161:HIS:CG	2.73	0.41
1:C:110:GLN:HA	1:C:113:GLN:HE21	1.85	0.41
1:C:6:LYS:HD3	1:C:19:TYR:CD2	2.55	0.41
1:C:40:GLU:O	2:D:288:LYS:NZ	2.51	0.41
1:C:189:LEU:CA	1:C:192:ILE:HD12	2.50	0.41
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.50	0.41
2:D:260:ALA:O	2:D:263:LEU:N	2.53	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.63	0.41
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.91	0.41
1:A:174:LEU:HD11	1:A:211:GLN:HG2	2.03	0.41
2:B:218:LEU:HB3	2:B:261:MET:HE2	2.01	0.41
2:B:211:ARG:O	2:B:214:LEU:N	2.52	0.41
1:C:39:THR:HG22	2:D:289:LYS:HZ3	1.85	0.41
2:D:312:ASN:O	2:D:316:THR:HB	2.21	0.41
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.56	0.41
1:C:102:PRO:O	1:C:103:LEU:C	2.63	0.41
1:C:275:ILE:CG1	1:C:279:ALA:HB3	2.50	0.41
2:D:208:ASN:HD22	2:D:208:ASN:N	2.18	0.41
1:A:41:THR:HB	1:A:43:GLY:H	1.85	0.41
2:D:354:VAL:O	2:D:355:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.93	0.41
1:C:59:ASN:HD22	1:C:59:ASN:HA	1.54	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.92	0.41
2:B:249:LEU:O	2:B:250:ARG:C	2.62	0.41
2:D:366:THR:O	2:D:366:THR:HG22	2.21	0.41
1:A:40:GLU:CA	2:B:288:LYS:HE2	2.51	0.41
1:A:193:PHE:CD2	1:A:263:LEU:HD13	2.56	0.41
2:B:199:TYR:CD1	2:B:199:TYR:C	2.98	0.41
1:C:136:ASN:OD1	1:C:138:GLU:N	2.53	0.41
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.82	0.41
1:A:2:GLU:CG	1:C:73:GLU:CD	2.94	0.40
1:C:278:LYS:HG3	2:D:178:TYR:CE1	2.56	0.40
1:A:52:ILE:O	1:A:56:LYS:HG3	2.22	0.40
1:A:208:GLU:CD	4:A:2045:HOH:O	2.65	0.40
1:C:7:VAL:O	1:C:8:GLU:HB3	2.20	0.40
1:C:85:GLN:NE2	1:C:90:PHE:HB2	2.37	0.40
1:C:101:LEU:HD13	1:C:101:LEU:O	2.21	0.40
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.51	0.40
1:C:287:GLN:HG3	1:C:288:ASP:N	2.35	0.40
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.86	0.40
1:A:122:ARG:HD2	1:A:122:ARG:O	2.21	0.40
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.93	0.40
1:C:215:ILE:HG23	1:C:219:LEU:CD1	2.50	0.40
2:D:211:ARG:HG2	2:D:211:ARG:NH1	2.35	0.40
2:D:330:GLU:C	2:D:332:LEU:N	2.80	0.40
1:C:286:PHE:C	1:C:288:ASP:N	2.79	0.40
2:D:176:PRO:O	2:D:177:ASP:C	2.64	0.40
2:D:260:ALA:O	2:D:261:MET:C	2.64	0.40

All (2) 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)
4:A:2054:HOH:O	4:B:2013:HOH:O[4_456]	1.64	0.56
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_456]	1.82	0.38

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	291/303 (96%)	265 (91%)	16 (6%)	10 (3%)	3	4
1	C	274/303 (90%)	240 (88%)	25 (9%)	9 (3%)	3	4
2	B	256/259 (99%)	245 (96%)	7 (3%)	4 (2%)	7	14
2	D	256/259 (99%)	225 (88%)	26 (10%)	5 (2%)	6	10
3	E	8/11 (73%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	1085/1135 (96%)	980 (90%)	76 (7%)	29 (3%)	4	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	96	LEU
2	D	347	TYR
1	A	164	VAL
1	C	57	GLU
1	C	58	LEU
1	C	230	VAL
1	C	287	GLN
2	D	197	VAL
1	A	14	THR
1	A	97	THR
1	A	287	GLN
1	C	55	LEU
1	C	172	GLU
1	C	181	SER
1	C	292	PRO
2	D	362	LEU
1	A	1	MET
1	A	8	GLU
1	A	95	ALA
2	B	176	PRO

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Mol	Chain	Res	Type
2	B	284	ASP
2	B	431	ASN
1	C	164	VAL
1	A	292	PRO
2	B	330	GLU
2	D	325	ALA
2	D	415	ASN
3	E	870	LYS

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	258/265 (97%)	238 (92%)	20 (8%)	11	24
1	C	244/265 (92%)	227 (93%)	17 (7%)	14	29
2	B	232/233 (100%)	216 (93%)	16 (7%)	14	30
2	D	232/233 (100%)	214 (92%)	18 (8%)	11	24
3	E	10/11 (91%)	8 (80%)	2 (20%)	1	2
All	All	976/1007 (97%)	903 (92%)	73 (8%)	12	26

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	17	VAL
1	A	59	ASN
1	A	75	LYS
1	A	78	LEU
1	A	86	ASP
1	A	89	LYS
1	A	97	THR
1	A	99	ILE
1	A	101	LEU
1	A	137	THR

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	150	ARG
1	A	157	ARG
1	A	177	CYS
1	A	184	VAL
1	A	232	SER
1	A	255	LEU
1	A	261	SER
1	A	272	ASN
2	B	175	VAL
2	B	180	GLU
2	B	181	ASP
2	B	196	LYS
2	B	232	LEU
2	B	277	GLU
2	B	281	ILE
2	B	366	THR
2	B	374	GLU
2	B	384	LEU
2	B	385	GLU
2	B	388	LYS
2	B	403	GLN
2	B	408	SER
2	B	417	LYS
2	B	425	ASN
1	C	0	SER
1	C	2	GLU
1	C	15	TYR
1	C	37	LEU
1	C	41	THR
1	C	55	LEU
1	C	57	GLU
1	C	59	ASN
1	C	73	GLU
1	C	81	GLU
1	C	101	LEU
1	C	103	LEU
1	C	150	ARG
1	C	178	LYS
1	C	210	ASP
1	C	252	VAL
1	C	290	THR

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Mol	Chain	Res	Type
2	D	180	GLU
2	D	196	LYS
2	D	206	ILE
2	D	208	ASN
2	D	218	LEU
2	D	232	LEU
2	D	239	ILE
2	D	245	SER
2	D	250	ARG
2	D	292	LEU
2	D	327	CYS
2	D	339	LEU
2	D	392	MET
2	D	403	GLN
2	D	409	ILE
2	D	417	LYS
2	D	425	ASN
2	D	432	LEU
3	E	872	LEU
3	E	878	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	84	HIS
1	A	85	GLN
1	A	119	HIS
1	A	131	GLN
1	A	246	GLN
1	A	265	GLN
1	A	272	ASN
2	B	296	HIS
2	B	317	GLN
2	B	395	HIS
2	B	431	ASN
1	C	59	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN

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Mol	Chain	Res	Type
1	C	113	GLN
1	C	131	GLN
1	C	265	GLN
1	C	268	HIS
2	D	254	GLN
2	D	312	ASN
2	D	313	GLN
2	D	317	GLN
2	D	361	HIS
2	D	396	GLN
2	D	403	GLN

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	3.82	4 (50%)	10,14,16	2.70	2 (20%)
1	TPO	C	160	1	8,10,11	3.73	4 (50%)	10,14,16	2.11	1 (10%)

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	-	3/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	6.61	1.45	1.20
1	A	160	TPO	P-O1P	6.48	1.70	1.50
1	C	160	TPO	P-O1P	6.35	1.70	1.50
1	C	160	TPO	O-C	6.16	1.43	1.20
1	C	160	TPO	P-O3P	4.24	1.70	1.54
1	A	160	TPO	P-O2P	3.87	1.69	1.54
1	A	160	TPO	P-O3P	3.86	1.69	1.54
1	C	160	TPO	P-O2P	3.80	1.68	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-7.97	104.26	124.77
1	C	160	TPO	O-C-CA	-6.27	108.66	124.77
1	A	160	TPO	O3P-P-OG1	2.01	113.69	105.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	O-C-CA-CB
1	A	160	TPO	CB-OG1-P-O3P
1	C	160	TPO	CB-OG1-P-O2P
1	A	160	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	293/303 (96%)	1.59	81 (27%) 1 1	28, 40, 70, 79	0
1	C	278/303 (91%)	1.80	101 (36%) 1 1	38, 60, 99, 109	0
2	B	258/259 (99%)	1.83	94 (36%) 1 1	27, 42, 57, 76	0
2	D	258/259 (99%)	2.11	126 (48%) 0 0	36, 71, 106, 114	0
3	E	10/11 (90%)	2.38	7 (70%) 0 0	58, 65, 72, 73	0
All	All	1097/1135 (96%)	1.83	409 (37%) 1 1	27, 51, 98, 114	0

All (409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	6.8
2	D	372	TRP	6.2
1	C	251	VAL	5.7
1	C	226	VAL	5.7
1	A	96	LEU	5.5
2	D	399	LEU	5.4
2	D	432	LEU	5.4
2	D	357	GLY	5.2
2	B	424	LEU	5.2
1	C	14	THR	4.8
2	D	423	LEU	4.8
2	D	323	GLN	4.7
2	B	325	ALA	4.7
2	D	391	LEU	4.5
2	D	430	LEU	4.5
2	D	176	PRO	4.5
1	C	221	THR	4.5
1	C	227	TRP	4.5
1	C	230	VAL	4.5
2	B	175	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	327	CYS	4.4
1	C	225	VAL	4.4
2	B	421	VAL	4.4
2	B	426	PRO	4.3
3	E	869	PRO	4.3
1	C	15	TYR	4.2
1	A	0	SER	4.2
1	A	15	TYR	4.2
2	D	421	VAL	4.2
2	B	425	ASN	4.2
2	D	409	ILE	4.1
2	D	178	TYR	4.1
2	D	339	LEU	4.1
2	D	351	LEU	4.1
2	B	232	LEU	4.1
2	B	319	PHE	4.1
2	D	365	TYR	4.0
2	D	398	TYR	4.0
2	D	346	PRO	3.9
2	D	321	HIS	3.9
1	C	293	VAL	3.9
2	D	364	LEU	3.9
1	C	291	LYS	3.8
2	B	428	GLU	3.8
1	C	11	GLY	3.8
1	C	259	GLY	3.8
2	D	319	PHE	3.8
2	B	432	LEU	3.8
1	A	39	THR	3.7
2	D	368	THR	3.7
2	B	335	PHE	3.7
1	C	219	LEU	3.7
2	D	367	VAL	3.7
2	D	280	TYR	3.7
2	B	366	THR	3.6
2	B	419	HIS	3.6
2	D	384	LEU	3.6
2	B	342	ILE	3.6
2	D	382	TYR	3.6
2	B	423	LEU	3.6
1	C	273	LYS	3.5
2	D	403	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	364	LEU	3.5
2	D	324	PRO	3.5
2	D	392	MET	3.5
2	D	328	LYS	3.5
2	D	395	HIS	3.5
2	D	431	ASN	3.5
1	C	231	THR	3.5
2	D	366	THR	3.5
2	B	427	PRO	3.4
2	B	398	TYR	3.4
1	C	255	LEU	3.4
2	B	195	PRO	3.4
2	B	312	ASN	3.4
1	A	229	GLY	3.4
2	B	318	TYR	3.4
1	C	285	PHE	3.4
2	D	191	VAL	3.4
2	D	426	PRO	3.4
1	A	244	ALA	3.4
1	A	40	GLU	3.4
2	D	413	TYR	3.3
2	D	177	ASP	3.3
1	C	228	PRO	3.3
1	C	286	PHE	3.3
1	C	223	ASP	3.3
2	D	424	LEU	3.3
1	C	194	ALA	3.3
2	B	362	LEU	3.3
1	C	290	THR	3.3
2	B	372	TRP	3.3
2	D	378	ARG	3.3
2	D	427	PRO	3.3
1	A	181	SER	3.2
1	C	234	PRO	3.2
1	A	161	HIS	3.2
2	D	329	VAL	3.2
1	A	290	THR	3.2
2	B	258	THR	3.2
2	D	337	GLY	3.2
2	D	335	PHE	3.2
1	A	234	PRO	3.2
2	B	368	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	380	THR	3.2
2	B	405	ALA	3.2
1	C	232	SER	3.2
2	D	360	PHE	3.2
2	B	391	LEU	3.2
2	D	199	TYR	3.2
1	C	153	GLY	3.2
2	D	325	ALA	3.1
1	A	230	VAL	3.1
2	D	320	LEU	3.1
1	C	156	VAL	3.1
1	A	173	ILE	3.1
1	C	252	VAL	3.1
2	B	281	ILE	3.1
1	A	269	TYR	3.1
2	B	397	THR	3.1
2	D	333	ALA	3.1
2	B	327	CYS	3.1
2	B	373	PRO	3.1
2	B	197	VAL	3.1
2	B	333	ALA	3.0
2	D	419	HIS	3.0
1	C	263	LEU	3.0
1	C	174	LEU	3.0
3	E	878	ASP	3.0
2	D	371	SER	3.0
2	D	425	ASN	3.0
1	C	220	GLY	3.0
1	A	289	VAL	3.0
1	C	233	MET	3.0
2	B	363	ALA	3.0
2	B	350	TYR	3.0
1	C	229	GLY	3.0
1	C	143	LEU	3.0
2	D	422	SER	3.0
1	C	10	ILE	2.9
2	D	197	VAL	2.9
1	C	222	PRO	2.9
1	C	267	LEU	2.9
1	C	269	TYR	2.9
2	D	348	LEU	2.9
1	C	289	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	324	PRO	2.9
1	C	96	LEU	2.9
1	C	202	LEU	2.9
1	A	236	TYR	2.9
1	A	38	ASP	2.9
1	C	117	PHE	2.9
2	D	182	ILE	2.9
1	A	97	THR	2.9
1	A	116	ALA	2.9
1	C	175	LEU	2.9
1	A	187	TRP	2.9
1	A	227	TRP	2.9
1	A	19	TYR	2.9
2	B	416	SER	2.8
1	A	225	VAL	2.8
2	B	411	GLU	2.8
2	B	196	LYS	2.8
1	A	35	ILE	2.8
1	C	215	ILE	2.8
2	B	326	ASN	2.8
2	D	416	SER	2.8
2	D	204	PRO	2.8
1	C	218	THR	2.8
2	D	363	ALA	2.8
2	D	376	LEU	2.8
1	A	206	ASP	2.8
1	C	109	PHE	2.8
2	B	360	PHE	2.8
2	D	347	TYR	2.8
2	D	381	GLY	2.8
2	B	248	VAL	2.8
2	B	367	VAL	2.8
2	B	276	ALA	2.8
3	E	872	LEU	2.8
2	D	198	GLY	2.8
2	D	420	GLY	2.8
2	D	389	PRO	2.8
1	C	101	LEU	2.8
2	D	400	LYS	2.8
2	B	278	PHE	2.8
2	D	375	SER	2.7
1	C	164	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.7
2	B	369	GLY	2.7
2	B	176	PRO	2.7
2	D	186	LEU	2.7
2	B	356	ALA	2.7
2	B	390	CYS	2.7
2	D	402	PRO	2.7
1	A	293	VAL	2.7
2	D	387	LEU	2.7
2	D	418	TYR	2.7
1	A	200	ARG	2.7
1	C	97	THR	2.7
1	A	43	GLY	2.7
2	D	390	CYS	2.7
1	A	240	PHE	2.7
1	C	275	ILE	2.7
1	C	37	LEU	2.7
1	A	41	THR	2.7
1	A	93	ALA	2.7
1	A	140	ALA	2.7
1	A	243	TRP	2.7
2	D	264	ALA	2.7
1	C	258	ASP	2.6
1	C	104	ILE	2.6
1	A	175	LEU	2.6
1	A	159	TYR	2.6
1	C	77	TYR	2.6
1	C	210	ASP	2.6
2	B	177	ASP	2.6
1	A	71	HIS	2.6
1	C	71	HIS	2.6
1	A	213	PHE	2.6
1	C	216	PHE	2.6
2	D	332	LEU	2.6
1	A	17	VAL	2.6
2	B	228	GLN	2.6
1	A	31	ALA	2.6
2	D	383	THR	2.6
2	B	365	TYR	2.6
2	D	417	LYS	2.6
2	D	210	MET	2.6
1	C	213	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	101	LEU	2.6
1	C	17	VAL	2.6
1	A	282	ALA	2.6
2	B	386	SER	2.6
2	B	420	GLY	2.5
2	D	181	ASP	2.5
3	E	877	PHE	2.5
2	B	323	GLN	2.5
2	B	415	ASN	2.5
1	C	276	SER	2.5
1	C	217	ARG	2.5
2	D	350	TYR	2.5
1	A	59	ASN	2.5
2	B	288	LYS	2.5
2	D	401	ALA	2.5
1	C	204	PRO	2.5
2	B	280	TYR	2.5
1	A	176	GLY	2.5
1	A	32	LEU	2.5
1	A	203	PHE	2.5
1	C	203	PHE	2.5
1	C	287	GLN	2.5
2	B	226	LYS	2.5
1	C	200	ARG	2.5
1	C	137	THR	2.5
1	C	19	TYR	2.5
2	D	201	LYS	2.5
2	D	322	GLN	2.5
1	C	154	VAL	2.5
2	D	221	VAL	2.5
2	D	275	VAL	2.5
2	B	231	THR	2.5
1	C	13	GLY	2.4
2	B	381	GLY	2.4
2	D	369	GLY	2.4
1	A	99	ILE	2.4
1	A	186	ILE	2.4
2	B	414	LYS	2.4
2	D	414	LYS	2.4
1	C	108	LEU	2.4
2	D	370	GLN	2.4
2	D	406	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	207	THR	2.4
2	D	281	ILE	2.4
1	A	265	GLN	2.4
2	B	186	LEU	2.4
2	B	413	TYR	2.4
1	A	18	VAL	2.4
2	B	329	VAL	2.4
2	D	310	THR	2.4
1	A	204	PRO	2.4
1	C	235	ASP	2.4
2	D	213	ILE	2.4
2	B	320	LEU	2.4
2	B	271	TYR	2.4
1	C	277	ALA	2.4
1	A	221	THR	2.4
1	A	224	GLU	2.4
2	B	209	SER	2.4
2	B	270	ILE	2.4
1	A	83	LEU	2.4
1	A	189	LEU	2.4
1	A	288	ASP	2.4
1	A	177	CYS	2.4
1	A	156	VAL	2.4
2	B	229	ASN	2.4
1	A	95	ALA	2.4
2	D	356	ALA	2.4
2	D	385	GLU	2.4
2	D	195	PRO	2.3
2	D	408	SER	2.3
1	A	215	ILE	2.3
1	C	192	ILE	2.3
2	D	326	ASN	2.3
2	B	260	ALA	2.3
2	D	330	GLU	2.3
1	A	241	PRO	2.3
1	C	253	PRO	2.3
2	B	331	SER	2.3
1	A	124	LEU	2.3
1	A	275	ILE	2.3
1	C	268	HIS	2.3
1	C	281	LEU	2.3
2	D	394	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	2.3
1	C	292	PRO	2.3
2	B	359	ALA	2.3
2	D	373	PRO	2.3
1	C	188	SER	2.3
2	B	337	GLY	2.3
2	D	179	HIS	2.3
1	A	263	LEU	2.3
3	E	870	LYS	2.3
2	B	178	TYR	2.3
2	B	286	TYR	2.3
1	C	151	ALA	2.3
1	A	182	THR	2.3
1	C	84	HIS	2.3
1	C	49	ILE	2.3
1	C	262	LEU	2.3
2	B	394	LEU	2.3
1	C	254	PRO	2.3
1	A	180	TYR	2.3
2	B	225	TYR	2.3
2	D	405	ALA	2.2
2	B	316	THR	2.2
2	B	183	HIS	2.2
1	C	173	ILE	2.2
1	C	266	MET	2.2
2	D	355	ILE	2.2
1	A	28	GLU	2.2
2	B	330	GLU	2.2
2	D	374	GLU	2.2
1	A	90	PHE	2.2
1	A	216	PHE	2.2
3	E	871	PRO	2.2
1	C	95	ALA	2.2
2	D	229	ASN	2.2
2	B	349	LYS	2.2
2	D	318	TYR	2.2
2	D	315	LEU	2.2
2	D	180	GLU	2.2
2	D	428	GLU	2.2
2	D	314	PHE	2.2
1	A	7	VAL	2.2
1	A	119	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	201	ALA	2.2
2	D	404	HIS	2.2
2	D	407	GLN	2.2
2	B	347	TYR	2.2
2	D	287	THR	2.2
1	C	16	GLY	2.2
2	B	351	LEU	2.2
2	D	215	VAL	2.1
2	B	334	MET	2.1
2	B	396	GLN	2.1
2	D	396	GLN	2.1
1	C	41	THR	2.1
2	B	343	ASP	2.1
2	B	422	SER	2.1
2	D	379	LYS	2.1
1	C	82	PHE	2.1
2	D	279	VAL	2.1
2	D	361	HIS	2.1
2	D	411	GLU	2.1
1	A	120	SER	2.1
1	A	249	SER	2.1
1	C	178	LYS	2.1
2	D	196	LYS	2.1
1	C	183	ALA	2.1
1	A	158	THR	2.1
1	A	10	ILE	2.1
1	C	141	ILE	2.1
1	C	78	LEU	2.1
2	D	341	LEU	2.1
3	E	875	LEU	2.1
1	A	16	GLY	2.1
1	C	99	ILE	2.1
1	A	291	LYS	2.1
1	A	77	TYR	2.1
2	B	204	PRO	2.1
1	A	197	VAL	2.0
2	B	401	ALA	2.0
1	A	12	GLU	2.0
1	C	110	GLN	2.0
1	C	152	PHE	2.0
1	C	157	ARG	2.0
2	D	354	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	2.0
2	B	235	ALA	2.0
1	C	12	GLU	2.0
2	B	224	GLU	2.0
2	B	227	LEU	2.0
2	D	227	LEU	2.0
2	D	338	GLU	2.0
1	C	186	ILE	2.0
2	D	217	TRP	2.0
1	C	100	PRO	2.0
2	B	340	SER	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	57,62,66,66	0
1	TPO	A	160	11/12	0.92	0.12	39,41,43,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.