



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:48 PM UTC

PDB ID : 1H26 / pdb_00001h26
Title : CDK2/CyclinA in complex with an 11-residue recruitment peptide from p53
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 : 2.24 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

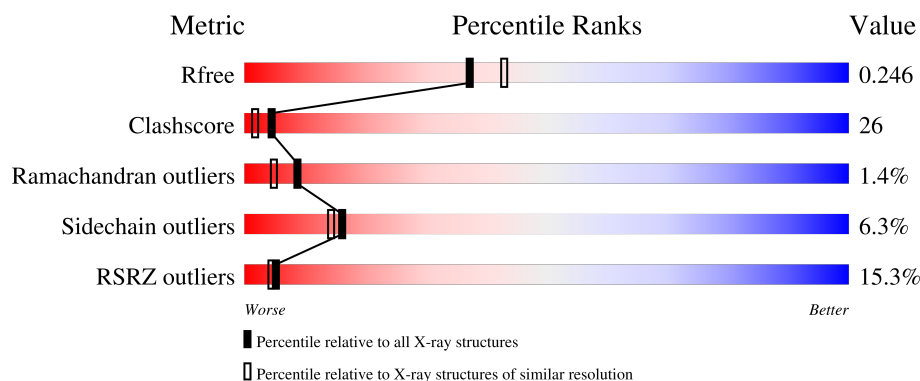
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	9% 59% 31% 7% ..
1	C	303	16% 47% 37% 5% 11%
2	B	259	12% 73% 22% 5%
2	D	259	22% 46% 46% 7%
3	E	11	36% 45% 27% 9% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8981 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	298	Total	C	N	O	P	S	9	0	1
			2389	1550	405	425	1	8			
1	C	269	Total	C	N	O	P	S	0	0	1
			2149	1392	367	382	1	7			

- 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
			2084	1350	339	384	11				
2	D	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				

- Molecule 3 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	S		0	0	0
			82	53	17	11	1				

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	66	Total	O	0	0
			66	66		
4	C	19	Total	O	0	0
			19	19		
4	D	21	Total	O	0	0
			21	21		

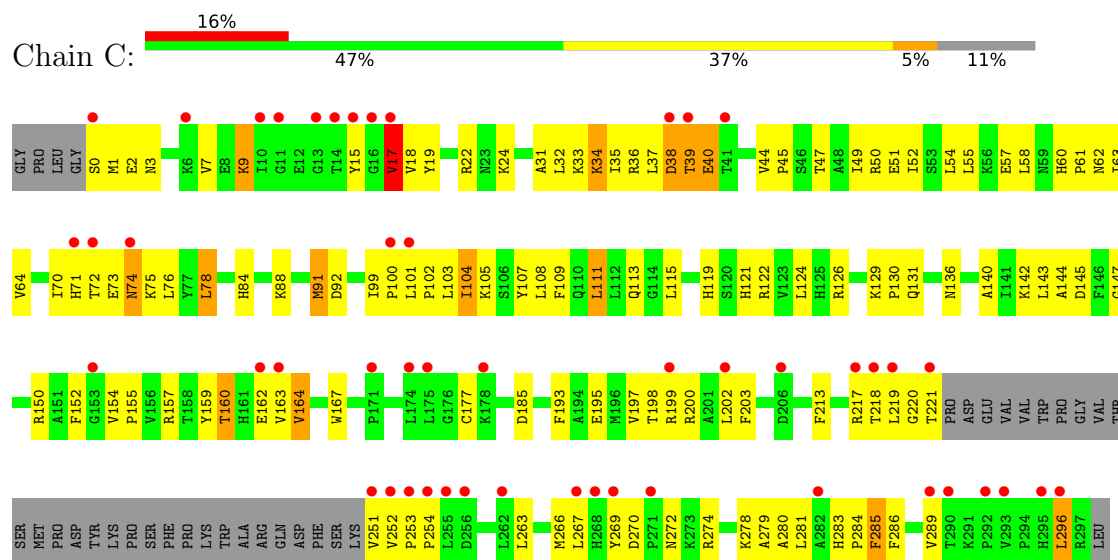
3 Residue-property plots

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.

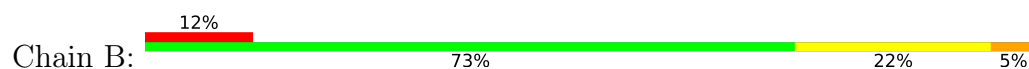
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

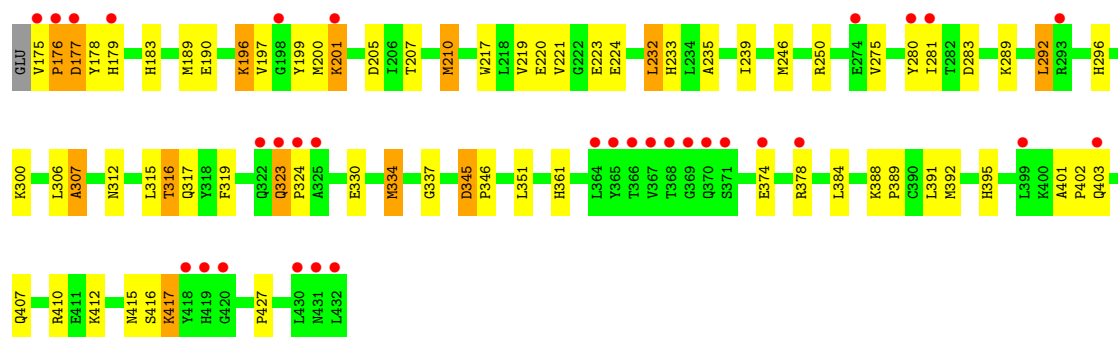


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

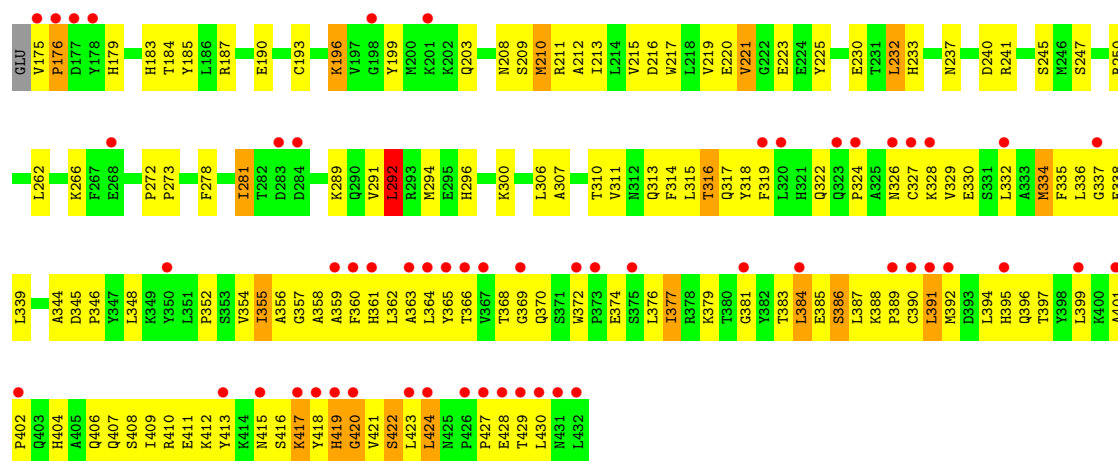


• Molecule 2: CYCLIN A2





• Molecule 2: CYCLIN A2



• Molecule 3: CELLULAR TUMOR ANTIGEN P53



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.67Å 134.03Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.88 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.88-2.24) 96.4 (29.88-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.268 (Not available) , 0.246	Depositor DCC
R_{free} test set	3458 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8981	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.48	10/2439 (0.4%)	1.32	15/3310 (0.5%)
1	C	1.04	3/2186 (0.1%)	1.13	7/2961 (0.2%)
2	B	1.32	6/2134 (0.3%)	1.14	7/2897 (0.2%)
2	D	1.09	5/2134 (0.2%)	1.16	9/2897 (0.3%)
3	E	0.90	0/83	0.99	0/104
All	All	1.25	24/8976 (0.3%)	1.19	38/12169 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	MET	SD-CE	-25.17	1.16	1.79
1	A	89	LYS	C-N	-13.37	1.15	1.33
2	B	210	MET	SD-CE	-13.22	1.46	1.79
2	D	210	MET	SD-CE	-9.37	1.56	1.79
1	C	91	MET	SD-CE	-9.06	1.56	1.79
2	B	246	MET	SD-CE	-8.25	1.58	1.79
2	D	294	MET	SD-CE	-7.47	1.60	1.79
2	B	307	ALA	C-O	-7.31	1.15	1.23
1	A	116	ALA	CA-CB	7.05	1.64	1.53
1	C	31	ALA	CA-CB	-6.89	1.43	1.53
1	A	88	LYS	C-N	-6.36	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	LEU	C-N	-6.35	1.24	1.33
1	C	296	LEU	C-N	-6.34	1.24	1.33
1	A	151	ALA	CA-CB	-6.20	1.43	1.53
2	B	200	MET	SD-CE	-6.07	1.64	1.79
2	B	334	MET	SD-CE	-6.01	1.64	1.79
2	D	272	PRO	C-O	-5.65	1.20	1.25
2	B	345	ASP	C-O	-5.51	1.17	1.24
1	A	266	MET	C-O	-5.16	1.17	1.24
1	A	203	PHE	CA-C	5.16	1.58	1.52
1	A	49	ILE	C-O	-5.14	1.18	1.24
1	A	151	ALA	C-O	-5.07	1.17	1.23
2	D	292	LEU	C-O	-5.04	1.18	1.24
2	D	291	VAL	CA-CB	-5.02	1.48	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	CA-C-N	12.95	146.27	121.54
1	A	89	LYS	C-N-CA	12.95	146.27	121.54
1	A	230	VAL	CB-CA-C	-10.51	98.43	111.88
1	A	89	LYS	O-C-N	-10.27	108.93	122.59
2	B	177	ASP	N-CA-C	-8.35	104.23	114.75
1	A	10	ILE	CB-CA-C	-7.72	104.26	111.06
1	C	39	THR	N-CA-C	7.62	119.23	111.07
1	A	230	VAL	N-CA-CB	7.49	118.82	110.51
2	D	221	VAL	N-CA-C	-7.35	103.12	110.62
1	A	163	VAL	N-CA-C	6.84	117.64	108.27
2	D	334	MET	N-CA-C	-6.65	104.04	111.28
2	B	205	ASP	N-CA-C	6.57	121.44	113.17
2	D	355	ILE	N-CA-C	-6.49	103.55	110.36
1	A	247	ASP	CB-CA-C	6.19	119.55	110.26
1	C	104	ILE	N-CA-C	-6.15	104.51	110.72
1	A	181	SER	N-CA-C	5.98	115.91	108.19
2	D	390	CYS	N-CA-C	-5.94	104.80	111.28
2	D	221	VAL	CB-CA-C	-5.71	104.43	112.14
1	C	111	LEU	N-CA-C	-5.67	105.19	111.71
2	B	337	GLY	N-CA-C	-5.61	106.00	112.73
1	A	296	LEU	O-C-N	-5.55	114.11	123.00
2	B	378	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	A	257	GLU	N-CA-C	5.46	117.66	111.11
1	A	85	GLN	N-CA-C	5.41	115.51	107.88
2	B	197	VAL	CB-CA-C	-5.34	104.93	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	VAL	N-CA-C	-5.32	106.99	111.56
2	D	337	GLY	N-CA-C	-5.28	106.38	112.50
1	A	173	ILE	N-CA-C	-5.28	105.70	110.82
1	A	98	GLY	N-CA-C	-5.25	106.41	112.29
2	D	377	ILE	N-CA-C	-5.25	104.64	110.62
2	B	315	LEU	CA-C-N	5.24	127.30	120.28
2	B	315	LEU	C-N-CA	5.24	127.30	120.28
1	C	285	PHE	N-CA-C	-5.17	105.61	112.34
2	D	211	ARG	N-CA-C	-5.12	105.88	111.82
2	D	422	SER	N-CA-C	-5.11	106.31	112.54
1	A	294	PRO	CA-C-O	-5.10	115.77	121.23
1	C	213	PHE	N-CA-C	-5.10	105.80	111.36
1	C	17	VAL	N-CA-C	5.08	119.91	109.34

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Peptide
1	C	160	TPO	Mainchain
1	C	37	LEU	Peptide
1	C	70	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2428	140	1
1	C	2149	0	2203	155	0
2	B	2084	0	2107	76	1
2	D	2084	0	2107	142	0
3	E	82	0	92	9	0
4	A	87	0	0	11	0
4	B	66	0	0	9	0
4	C	19	0	0	1	0
4	D	21	0	0	2	0
All	All	8981	0	8937	465	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 26.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:HE2	1:C:47:THR:OG1	1.16	1.29
1:C:17:VAL:HG11	1:C:19:TYR:CZ	1.70	1.25
1:A:266:MET:SD	1:A:266:MET:CE	1.16	1.25
1:A:266:MET:CE	1:A:266:MET:CG	2.21	1.18
1:C:39:THR:O	2:D:292:LEU:CD2	1.90	1.18
1:C:39:THR:O	2:D:292:LEU:HD23	0.99	1.17
1:A:266:MET:SD	1:A:266:MET:HE3	1.74	1.14
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.29	1.12
1:A:266:MET:SD	1:A:266:MET:HE2	1.74	1.10
1:A:266:MET:SD	1:A:266:MET:HE1	1.74	1.07
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.27	1.03
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.07	1.02
1:C:60:HIS:CD2	1:C:62:ASN:H	1.79	1.01
1:C:64:VAL:HG21	1:C:144:ALA:CB	1.90	1.01
1:C:64:VAL:HG23	1:C:143:LEU:O	1.60	1.01
2:D:193:CYS:SG	4:D:2009:HOH:O	2.18	1.00
2:B:296:HIS:CD2	2:B:300:LYS:HE2	1.99	0.97
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.46	0.96
1:C:64:VAL:CG2	1:C:144:ALA:HB2	1.97	0.95
1:C:121:HIS:O	1:C:122:ARG:HG3	1.67	0.94
1:C:15:TYR:OH	1:C:47:THR:HB	1.69	0.93
1:C:60:HIS:HD2	1:C:62:ASN:H	0.96	0.92
1:A:41:THR:HA	4:A:2008:HOH:O	1.70	0.92
1:A:177:CYS:HB2	4:A:2048:HOH:O	1.67	0.92
1:A:39:THR:HG21	2:B:289:LYS:CD	1.99	0.90
4:A:2010:HOH:O	2:B:189:MET:HE2	1.70	0.90
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.53	0.89
1:A:39:THR:HG21	2:B:289:LYS:CE	2.01	0.89
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.55	0.89
2:B:283:ASP:HB2	3:E:380:HIS:O	1.75	0.87
1:A:210:ASP:OD1	4:A:2062:HOH:O	1.91	0.87
2:B:210:MET:HE3	3:E:385:PHE:HB3	1.57	0.87
1:A:64:VAL:HG21	1:A:144:ALA:HB2	1.57	0.86
1:C:17:VAL:CG1	1:C:19:TYR:CZ	2.58	0.86
1:A:217:ARG:NH2	4:A:2063:HOH:O	2.09	0.85
1:A:177:CYS:SG	1:A:179:TYR:O	2.35	0.85
2:D:216:ASP:OD1	2:D:408:SER:OG	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.59	0.83
1:A:230:VAL:HA	1:A:233:MET:HE2	1.61	0.83
1:A:154:VAL:O	2:B:316:THR:HG22	1.79	0.83
1:C:15:TYR:HE2	1:C:47:THR:CB	1.92	0.83
2:D:387:LEU:O	2:D:391:LEU:HB2	1.79	0.82
2:D:413:TYR:O	2:D:422:SER:OG	1.97	0.81
1:C:15:TYR:HD1	1:C:33:LYS:CE	1.94	0.80
1:C:15:TYR:CE2	1:C:47:THR:CB	2.64	0.80
1:C:60:HIS:HD2	1:C:62:ASN:N	1.78	0.80
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.61	0.80
1:C:71:HIS:HB3	2:D:300:LYS:NZ	1.96	0.80
2:D:175:VAL:N	2:D:179:HIS:CE1	2.51	0.79
1:C:154:VAL:O	2:D:316:THR:HG22	1.83	0.79
2:D:210:MET:HE1	2:D:250:ARG:CB	2.13	0.78
1:A:39:THR:CB	2:B:289:LYS:HZ1	1.97	0.78
1:A:230:VAL:HG12	1:A:233:MET:CE	2.13	0.78
1:A:154:VAL:O	2:B:316:THR:CG2	2.32	0.78
1:C:57:GLU:OE2	2:D:307:ALA:HB3	1.84	0.77
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.15	0.77
1:C:17:VAL:HG11	1:C:19:TYR:CE1	2.21	0.76
1:C:15:TYR:CD1	1:C:33:LYS:CE	2.70	0.75
1:A:85:GLN:HG3	1:A:86:ASP:H	1.52	0.75
2:D:176:PRO:HA	2:D:179:HIS:CG	2.22	0.75
1:A:64:VAL:HG23	1:A:143:LEU:O	1.87	0.74
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.67	0.74
1:A:227:TRP:O	1:A:230:VAL:HG22	1.87	0.74
1:A:230:VAL:CG1	1:A:233:MET:HE2	2.17	0.74
1:C:40:GLU:CD	1:C:40:GLU:H	1.96	0.74
1:A:284:PRO:O	1:A:287:GLN:HG2	1.88	0.73
1:A:42:GLU:OE1	2:B:275:VAL:HG23	1.88	0.73
1:A:39:THR:CB	2:B:289:LYS:NZ	2.52	0.73
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.24	0.73
2:B:175:VAL:N	2:B:179:HIS:CE1	2.56	0.72
1:C:17:VAL:CG1	1:C:19:TYR:CE1	2.72	0.72
1:A:72:THR:HG22	1:A:74:ASN:ND2	2.04	0.72
1:A:148:LEU:HD23	4:A:2041:HOH:O	1.89	0.72
1:A:262:LEU:HG	1:A:266:MET:HE2	1.72	0.72
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.24	0.71
1:C:72:THR:HG22	1:C:73:GLU:N	2.06	0.71
1:A:178:LYS:HE2	1:A:179:TYR:CZ	2.25	0.71
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:HG11	1:C:19:TYR:CE2	2.26	0.71
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.21	0.71
1:A:85:GLN:HG3	1:A:86:ASP:N	2.05	0.71
1:A:39:THR:CG2	2:B:289:LYS:HD2	2.20	0.70
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.26	0.70
1:A:72:THR:CG2	1:A:74:ASN:ND2	2.54	0.70
2:B:175:VAL:HG12	4:B:2008:HOH:O	1.92	0.70
2:D:415:ASN:OD1	2:D:417:LYS:N	2.25	0.70
1:A:101:LEU:N	1:A:102:PRO:CD	2.55	0.70
2:D:413:TYR:C	2:D:422:SER:OG	2.35	0.69
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.60	0.69
1:A:17:VAL:HG12	1:A:18:VAL:N	2.07	0.68
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.75	0.68
1:C:71:HIS:NE2	2:D:296:HIS:CD2	2.60	0.68
1:C:105:LYS:HE2	1:C:285:PHE:CZ	2.29	0.68
1:C:107:TYR:O	1:C:111:LEU:HG	1.93	0.68
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.23	0.68
1:A:39:THR:HG22	1:A:40:GLU:H	1.59	0.67
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.09	0.67
1:C:154:VAL:O	2:D:316:THR:CG2	2.42	0.67
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.75	0.67
2:D:210:MET:CE	2:D:250:ARG:HB2	2.25	0.67
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.60	0.67
1:C:71:HIS:CG	2:D:300:LYS:HZ3	2.12	0.67
2:B:296:HIS:CD2	2:B:300:LYS:CE	2.76	0.67
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.68	0.66
1:A:39:THR:HG21	2:B:289:LYS:NZ	2.10	0.66
1:A:60:HIS:HD2	1:A:62:ASN:H	1.44	0.66
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.77	0.66
1:C:15:TYR:CZ	1:C:47:THR:HB	2.30	0.66
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.30	0.66
2:D:413:TYR:C	2:D:422:SER:HG	2.04	0.65
1:C:15:TYR:OH	1:C:147:GLY:HA2	1.97	0.65
1:C:100:PRO:O	1:C:104:ILE:HG13	1.97	0.65
1:C:51:GLU:O	1:C:55:LEU:HB2	1.96	0.65
1:C:197:VAL:HG11	1:C:252:VAL:HG12	1.80	0.64
2:D:190:GLU:OE1	2:D:352:PRO:HD2	1.96	0.64
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.62	0.64
2:D:355:ILE:O	2:D:356:ALA:C	2.40	0.64
1:A:230:VAL:CG1	1:A:233:MET:CE	2.74	0.64
1:C:121:HIS:C	1:C:122:ARG:HG3	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:HIS:NE2	2:B:300:LYS:HE2	2.11	0.64
2:D:327:CYS:SG	2:D:419:HIS:CD2	2.92	0.63
1:A:39:THR:HB	2:B:289:LYS:NZ	2.13	0.63
2:D:416:SER:O	2:D:419:HIS:N	2.30	0.63
1:C:15:TYR:HD1	1:C:33:LYS:HE3	1.63	0.63
1:A:16:GLY:HA3	1:A:34:LYS:O	1.99	0.62
1:A:266:MET:CE	1:A:266:MET:HG3	2.25	0.62
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.82	0.62
2:D:419:HIS:O	2:D:421:VAL:N	2.32	0.62
2:D:336:LEU:HB2	2:D:359:ALA:HB1	1.80	0.62
1:C:101:LEU:N	1:C:102:PRO:CD	2.61	0.62
2:B:233:HIS:HD2	4:B:2041:HOH:O	1.83	0.61
1:A:39:THR:HG22	1:A:40:GLU:N	2.14	0.61
2:D:360:PHE:O	2:D:361:HIS:C	2.42	0.61
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.82	0.61
2:D:418:TYR:O	2:D:419:HIS:C	2.43	0.61
2:D:423:LEU:O	2:D:424:LEU:O	2.19	0.61
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.82	0.61
2:B:178:TYR:N	4:B:2009:HOH:O	1.90	0.61
2:D:329:VAL:O	2:D:332:LEU:N	2.33	0.60
1:A:72:THR:CG2	1:A:74:ASN:HD21	2.14	0.60
1:C:220:GLY:O	1:C:221:THR:C	2.43	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.01	0.60
1:A:97:THR:HG21	1:A:295:HIS:CE1	2.36	0.60
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.84	0.60
2:B:210:MET:HE1	2:B:250:ARG:CB	2.31	0.60
1:A:60:HIS:CD2	1:A:62:ASN:H	2.20	0.59
2:D:208:ASN:OD1	2:D:344:ALA:HB3	2.01	0.59
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.29	0.59
2:D:410:ARG:O	2:D:411:GLU:C	2.43	0.59
2:B:296:HIS:NE2	2:B:300:LYS:NZ	2.50	0.59
1:C:198:THR:O	1:C:199:ARG:HB2	2.02	0.59
2:D:209:SER:O	2:D:212:ALA:HB3	2.02	0.59
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.37	0.59
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.90	0.59
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.70	0.59
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.85	0.59
1:A:249:SER:HA	1:A:260:ARG:HD3	1.84	0.58
1:A:10:ILE:O	1:A:10:ILE:HG22	2.03	0.58
1:A:64:VAL:CG2	1:A:144:ALA:HB2	2.32	0.58
2:B:392:MET:HE2	2:B:392:MET:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:LEU:O	1:C:263:LEU:HD12	2.04	0.58
2:D:361:HIS:O	2:D:362:LEU:C	2.47	0.58
2:D:175:VAL:C	2:D:179:HIS:CE1	2.82	0.58
1:A:230:VAL:HG12	1:A:233:MET:HE2	1.81	0.58
2:B:280:TYR:CE2	3:E:380:HIS:CE1	2.92	0.58
1:C:39:THR:HG21	2:D:289:LYS:HE3	1.85	0.58
1:A:72:THR:HG22	1:A:74:ASN:H	1.69	0.57
2:B:175:VAL:N	2:B:179:HIS:HE1	2.01	0.57
2:D:383:THR:O	2:D:384:LEU:C	2.45	0.57
1:A:39:THR:CG2	2:B:289:LYS:NZ	2.68	0.57
2:B:316:THR:HG21	4:B:2045:HOH:O	2.04	0.57
1:A:85:GLN:CG	1:A:86:ASP:N	2.67	0.57
2:D:383:THR:C	2:D:385:GLU:N	2.60	0.57
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.87	0.56
1:A:17:VAL:CG1	1:A:18:VAL:N	2.69	0.56
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.41	0.56
2:D:233:HIS:ND1	4:D:2008:HOH:O	2.15	0.56
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.86	0.56
2:D:332:LEU:O	2:D:336:LEU:HG	2.06	0.56
1:A:18:VAL:HA	1:A:32:LEU:O	2.06	0.56
1:C:9:LYS:HZ2	1:C:17:VAL:HG22	1.70	0.56
1:C:15:TYR:HD1	1:C:33:LYS:NZ	2.04	0.56
1:A:0:SER:C	1:A:2:GLU:H	2.14	0.56
1:A:148:LEU:CD2	4:A:2041:HOH:O	2.51	0.56
1:C:9:LYS:NZ	1:C:17:VAL:HG22	2.21	0.56
1:A:101:LEU:N	1:A:102:PRO:HD3	2.21	0.56
1:A:291:LYS:HB2	4:A:2019:HOH:O	2.04	0.55
2:D:357:GLY:O	2:D:358:ALA:C	2.49	0.55
1:C:15:TYR:CE2	1:C:47:THR:HB	2.39	0.55
1:C:72:THR:CG2	1:C:73:GLU:N	2.70	0.55
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.87	0.55
2:B:415:ASN:OD1	2:B:417:LYS:N	2.27	0.55
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.88	0.55
2:D:196:LYS:HG2	2:D:199:TYR:HB3	1.89	0.55
2:D:418:TYR:O	2:D:420:GLY:N	2.39	0.55
2:B:296:HIS:NE2	2:B:300:LYS:CE	2.69	0.55
1:C:71:HIS:CE1	2:D:296:HIS:CD2	2.95	0.55
2:D:365:TYR:O	2:D:366:THR:C	2.48	0.55
2:D:387:LEU:O	2:D:391:LEU:CB	2.52	0.55
2:D:175:VAL:N	2:D:179:HIS:HE1	2.01	0.54
2:D:354:VAL:O	2:D:355:ILE:C	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:CB	2:D:300:LYS:NZ	2.69	0.54
1:C:284:PRO:C	1:C:286:PHE:H	2.15	0.54
2:D:273:PRO:HB2	2:D:278:PHE:CE2	2.43	0.54
1:C:17:VAL:HG12	1:C:19:TYR:CE1	2.42	0.54
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.42	0.54
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.42	0.54
2:B:296:HIS:HD2	2:B:300:LYS:HE2	1.61	0.54
1:C:71:HIS:HB3	2:D:300:LYS:HZ3	1.73	0.54
2:D:203:GLN:OE1	2:D:247:SER:HA	2.08	0.54
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.43	0.54
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.43	0.53
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.42	0.53
2:D:423:LEU:C	2:D:424:LEU:O	2.51	0.53
1:C:18:VAL:HG22	1:C:33:LYS:HG3	1.90	0.53
2:D:423:LEU:O	2:D:424:LEU:C	2.50	0.53
2:D:395:HIS:ND1	2:D:430:LEU:HD21	2.23	0.53
1:C:105:LYS:HE2	1:C:285:PHE:CE2	2.43	0.53
2:D:383:THR:O	2:D:385:GLU:N	2.42	0.53
1:A:197:VAL:CG1	1:A:252:VAL:CG1	2.84	0.53
1:C:126:ARG:O	1:C:164:VAL:HG22	2.09	0.53
2:B:210:MET:HE3	3:E:385:PHE:CB	2.36	0.53
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.90	0.53
1:C:15:TYR:CD1	1:C:33:LYS:NZ	2.77	0.53
1:C:39:THR:HB	2:D:289:LYS:HZ2	1.73	0.53
2:D:210:MET:HE1	2:D:250:ARG:HB3	1.88	0.53
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.44	0.53
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.90	0.53
2:D:196:LYS:O	2:D:196:LYS:HG3	2.04	0.53
1:C:15:TYR:OH	1:C:47:THR:CB	2.51	0.52
1:C:71:HIS:CG	2:D:300:LYS:NZ	2.76	0.52
2:D:220:GLU:O	2:D:223:GLU:N	2.42	0.52
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.44	0.52
1:C:99:ILE:O	1:C:104:ILE:HD11	2.09	0.52
2:D:217:TRP:O	2:D:221:VAL:HG23	2.10	0.52
1:C:15:TYR:HD1	1:C:33:LYS:HZ1	1.55	0.52
2:D:326:ASN:OD1	2:D:328:LYS:N	2.43	0.52
2:D:388:LYS:O	2:D:392:MET:N	2.40	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.92	0.52
1:C:278:LYS:O	1:C:281:LEU:HB2	2.09	0.52
1:C:270:ASP:C	1:C:270:ASP:OD1	2.53	0.52
1:C:121:HIS:HD2	2:D:185:TYR:CE1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PRO:C	1:C:286:PHE:N	2.61	0.52
2:B:176:PRO:HD3	2:B:179:HIS:NE2	2.25	0.51
2:B:296:HIS:O	2:B:300:LYS:HG3	2.10	0.51
2:D:388:LYS:N	2:D:389:PRO:CD	2.73	0.51
1:A:137:THR:O	1:A:293:VAL:HG13	2.11	0.51
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.45	0.51
1:A:71:HIS:ND1	2:B:300:LYS:NZ	2.56	0.51
1:A:72:THR:HG22	1:A:73:GLU:N	2.24	0.51
2:D:404:HIS:CE1	2:D:406:GLN:HB2	2.46	0.51
2:B:178:TYR:CA	4:B:2009:HOH:O	2.49	0.51
1:C:198:THR:O	1:C:199:ARG:CB	2.57	0.51
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.93	0.51
2:D:216:ASP:CG	2:D:408:SER:OG	2.53	0.51
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.92	0.51
2:B:178:TYR:HB2	4:B:2009:HOH:O	2.11	0.50
2:D:217:TRP:CZ2	2:D:281:ILE:HD12	2.46	0.50
1:A:178:LYS:HE2	1:A:179:TYR:CE1	2.46	0.50
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.92	0.50
1:C:61:PRO:O	1:C:142:LYS:HE2	2.11	0.50
1:A:33:LYS:HB3	1:A:78:LEU:HB2	1.94	0.50
2:B:207:THR:OG1	2:B:210:MET:HG3	2.12	0.50
1:C:15:TYR:CD1	1:C:33:LYS:HE3	2.43	0.50
1:C:126:ARG:HB3	1:C:163:VAL:HG22	1.94	0.50
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.75	0.50
2:D:376:LEU:O	2:D:379:LYS:N	2.40	0.50
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.47	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.47	0.49
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.94	0.49
2:D:184:THR:O	2:D:187:ARG:HB2	2.11	0.49
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.47	0.49
1:C:34:LYS:NZ	1:C:36:ARG:HE	2.10	0.49
2:D:358:ALA:O	2:D:359:ALA:C	2.53	0.49
1:A:64:VAL:HG21	1:A:144:ALA:CB	2.35	0.49
1:A:72:THR:CG2	1:A:74:ASN:CG	2.85	0.49
1:C:72:THR:HG22	1:C:73:GLU:H	1.75	0.49
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.12	0.49
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.93	0.49
1:A:247:ASP:OD2	1:A:249:SER:OG	2.29	0.49
1:C:195:GLU:O	1:C:199:ARG:N	2.45	0.49
1:A:0:SER:C	1:A:2:GLU:N	2.71	0.48
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HD23	1:C:203:PHE:CE1	2.47	0.48
1:A:178:LYS:HE2	1:A:179:TYR:OH	2.14	0.48
1:A:57:GLU:OE2	2:B:307:ALA:HB3	2.13	0.48
2:D:326:ASN:CG	2:D:329:VAL:HG23	2.38	0.48
1:A:10:ILE:O	1:A:10:ILE:CG2	2.61	0.48
1:A:84:HIS:HB2	4:A:2016:HOH:O	2.13	0.48
2:B:217:TRP:O	2:B:221:VAL:HG23	2.14	0.48
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.13	0.48
1:C:91:MET:O	1:C:92:ASP:C	2.57	0.48
1:A:230:VAL:CA	1:A:233:MET:HE2	2.37	0.48
1:C:72:THR:HG22	1:C:74:ASN:H	1.78	0.48
2:D:310:THR:O	2:D:311:VAL:C	2.55	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.95	0.48
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.28	0.48
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.44	0.48
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.95	0.48
1:C:126:ARG:HB3	1:C:163:VAL:CG2	2.44	0.48
1:C:40:GLU:OE2	2:D:289:LYS:NZ	2.47	0.47
2:D:319:PHE:CG	2:D:330:GLU:HG2	2.49	0.47
1:A:72:THR:HG21	1:A:74:ASN:OD1	2.14	0.47
1:C:266:MET:O	1:C:274:ARG:HD3	2.14	0.47
1:C:162:GLU:H	1:C:162:GLU:CD	2.22	0.47
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.02	0.47
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.96	0.47
1:A:65:LYS:HA	4:A:2012:HOH:O	2.15	0.47
1:A:294:PRO:C	1:A:296:LEU:H	2.23	0.47
2:B:235:ALA:O	2:B:239:ILE:HG13	2.14	0.47
1:C:74:ASN:HB3	4:C:2011:HOH:O	2.14	0.47
2:D:322:GLN:HB3	2:D:324:PRO:O	2.14	0.47
2:D:329:VAL:O	2:D:330:GLU:C	2.58	0.47
1:A:290:THR:OG1	1:A:292:PRO:HD3	2.15	0.47
2:B:323:GLN:HA	2:B:324:PRO:HA	1.73	0.47
1:A:39:THR:CG2	1:A:40:GLU:H	2.26	0.47
1:A:72:THR:HG22	1:A:74:ASN:CG	2.40	0.46
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.97	0.46
1:C:219:LEU:HB2	1:C:269:TYR:OH	2.15	0.46
1:C:284:PRO:O	1:C:285:PHE:C	2.54	0.46
2:D:384:LEU:HD12	2:D:384:LEU:HA	1.80	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46
1:C:71:HIS:HB3	2:D:300:LYS:HZ1	1.79	0.46
2:D:395:HIS:HE1	2:D:427:PRO:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:415:ASN:OD1	2:D:416:SER:N	2.47	0.46
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.03	0.46
1:A:98:GLY:HA2	1:A:199:ARG:CZ	2.45	0.46
2:D:326:ASN:OD1	2:D:329:VAL:HG23	2.16	0.46
1:C:15:TYR:HH	1:C:47:THR:C	2.23	0.46
2:D:377:ILE:O	2:D:381:GLY:HA2	2.16	0.46
2:D:411:GLU:O	2:D:412:LYS:C	2.57	0.46
1:A:72:THR:HG21	1:A:74:ASN:ND2	2.30	0.46
1:A:163:VAL:O	1:A:164:VAL:HB	2.16	0.46
1:C:157:ARG:HB2	1:C:159:TYR:CE1	2.50	0.46
1:C:279:ALA:O	1:C:280:ALA:C	2.59	0.46
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.48	0.46
2:D:383:THR:H	2:D:386:SER:HG	1.63	0.46
1:A:39:THR:HG23	2:B:292:LEU:HD23	1.97	0.45
2:B:415:ASN:OD1	2:B:416:SER:N	2.49	0.45
3:E:379:ARG:H	3:E:379:ARG:HG2	1.47	0.45
1:C:283:HIS:CD2	1:C:284:PRO:HD2	2.52	0.45
2:D:385:GLU:OE2	2:D:385:GLU:HA	2.15	0.45
1:A:262:LEU:HG	1:A:266:MET:CE	2.45	0.45
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.24	0.45
2:B:178:TYR:CB	4:B:2009:HOH:O	2.65	0.45
2:B:196:LYS:HG2	2:B:199:TYR:HB3	1.99	0.45
2:B:280:TYR:HE2	3:E:380:HIS:HE1	1.65	0.45
2:B:312:ASN:ND2	4:B:2042:HOH:O	2.50	0.45
1:C:195:GLU:HG3	1:C:200:ARG:C	2.41	0.45
1:A:39:THR:C	1:A:41:THR:H	2.25	0.45
1:C:71:HIS:CB	2:D:300:LYS:HZ3	2.28	0.45
2:D:237:ASN:OD1	2:D:241:ARG:HD3	2.17	0.45
2:D:377:ILE:O	2:D:381:GLY:N	2.49	0.45
1:C:218:THR:O	1:C:218:THR:HG22	2.16	0.45
1:C:3:ASN:O	1:C:24:LYS:HG3	2.17	0.44
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.86	0.44
2:D:278:PHE:O	2:D:281:ILE:HG13	2.17	0.44
1:C:202:LEU:HD21	1:C:203:PHE:CZ	2.52	0.44
1:C:88:LYS:HA	1:C:91:MET:HE2	1.98	0.44
2:B:412:LYS:NZ	4:B:2066:HOH:O	2.50	0.44
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.00	0.44
1:A:230:VAL:HG12	1:A:233:MET:HE3	1.97	0.44
2:B:280:TYR:CE2	3:E:380:HIS:HE1	2.34	0.44
2:B:345:ASP:HA	2:B:346:PRO:HA	1.75	0.44
1:C:72:THR:CG2	1:C:73:GLU:H	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:VAL:O	1:C:289:VAL:HG13	2.18	0.44
1:A:197:VAL:HG11	1:A:252:VAL:HG11	1.95	0.44
1:C:60:HIS:CG	1:C:61:PRO:CD	3.00	0.44
1:C:279:ALA:O	1:C:281:LEU:N	2.51	0.44
2:B:250:ARG:NH1	3:E:386:LYS:OXT	2.51	0.43
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.43
2:D:404:HIS:HE1	2:D:406:GLN:OE1	2.02	0.43
1:C:64:VAL:CG2	1:C:144:ALA:CB	2.72	0.43
2:D:314:PHE:O	2:D:315:LEU:C	2.60	0.43
1:C:15:TYR:CD1	1:C:33:LYS:HE2	2.51	0.43
2:D:219:VAL:O	2:D:220:GLU:C	2.59	0.43
1:A:97:THR:HG21	1:A:295:HIS:HE1	1.80	0.43
1:C:99:ILE:O	1:C:100:PRO:C	2.62	0.43
1:C:202:LEU:CD2	1:C:203:PHE:CE1	3.01	0.43
2:D:395:HIS:HB2	2:D:430:LEU:HD11	1.99	0.43
1:A:278:LYS:NZ	2:B:177:ASP:O	2.33	0.43
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.53	0.43
1:C:15:TYR:OH	1:C:47:THR:C	2.61	0.43
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.83	0.43
2:D:215:VAL:O	2:D:219:VAL:HG23	2.18	0.43
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.84	0.43
1:A:250:LYS:HA	1:A:250:LYS:HD3	1.83	0.43
1:C:109:PHE:CD2	1:C:113:GLN:NE2	2.87	0.43
2:D:396:GLN:O	2:D:399:LEU:N	2.52	0.43
2:B:319:PHE:CG	2:B:330:GLU:HG2	2.53	0.43
2:D:326:ASN:OD1	2:D:326:ASN:C	2.62	0.43
2:D:383:THR:O	2:D:386:SER:N	2.51	0.43
1:A:107:TYR:O	1:A:111:LEU:HG	2.19	0.42
1:A:230:VAL:HG13	1:A:233:MET:HE2	1.97	0.42
2:D:216:ASP:OD2	2:D:408:SER:CB	2.67	0.42
1:A:15:TYR:N	1:A:15:TYR:CD1	2.87	0.42
1:A:72:THR:HG21	1:A:74:ASN:HD21	1.81	0.42
1:C:17:VAL:HG11	1:C:19:TYR:OH	2.09	0.42
1:C:35:ILE:HB	1:C:76:LEU:HB3	2.02	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.54	0.42
2:D:368:THR:C	2:D:370:GLN:H	2.27	0.42
2:D:422:SER:HG	2:D:422:SER:H	1.64	0.42
1:A:7:VAL:O	1:A:8:GLU:HB3	2.18	0.42
1:C:263:LEU:HD12	1:C:263:LEU:C	2.43	0.42
2:D:212:ALA:O	2:D:213:ILE:C	2.59	0.42
2:D:317:GLN:O	2:D:318:TYR:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:GLU:O	2:B:224:GLU:C	2.61	0.42
4:A:2010:HOH:O	2:B:189:MET:CE	2.45	0.42
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.54	0.42
1:A:39:THR:C	1:A:41:THR:N	2.77	0.42
1:C:101:LEU:H	1:C:101:LEU:HG	1.66	0.42
1:C:115:LEU:CD1	1:C:119:HIS:CE1	3.02	0.42
1:C:197:VAL:CG1	1:C:252:VAL:CG1	2.95	0.42
1:A:39:THR:HB	2:B:289:LYS:HZ2	1.81	0.42
1:C:102:PRO:O	1:C:105:LYS:N	2.53	0.42
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.86	0.42
2:D:345:ASP:HA	2:D:346:PRO:HA	1.72	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:A:106:SER:HB2	1:A:290:THR:O	2.20	0.42
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.50	0.42
1:A:39:THR:O	1:A:40:GLU:HB2	2.20	0.41
1:A:83:LEU:HD21	1:A:142:LYS:HE3	2.02	0.41
1:A:186:ILE:HD11	1:A:277:ALA:HB2	2.02	0.41
1:C:109:PHE:CE2	1:C:113:GLN:NE2	2.88	0.41
2:D:392:MET:HE2	2:D:392:MET:HA	2.01	0.41
1:A:71:HIS:CG	2:B:300:LYS:NZ	2.87	0.41
1:C:270:ASP:OD1	1:C:272:ASN:N	2.53	0.41
2:D:314:PHE:O	2:D:317:GLN:N	2.52	0.41
2:D:364:LEU:HG	2:D:370:GLN:HB2	2.03	0.41
1:A:42:GLU:OE1	2:B:275:VAL:N	2.44	0.41
1:A:134:LEU:O	1:A:141:ILE:HA	2.20	0.41
2:B:219:VAL:HG22	2:B:232:LEU:HD11	2.03	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
1:C:167:TRP:N	1:C:167:TRP:CD1	2.87	0.41
1:A:72:THR:CG2	1:A:73:GLU:N	2.84	0.41
1:C:60:HIS:HB3	1:C:63:ILE:HD12	2.02	0.41
2:D:199:TYR:OH	2:D:240:ASP:OD1	2.32	0.41
2:D:388:LYS:O	2:D:389:PRO:C	2.64	0.41
1:C:284:PRO:O	1:C:286:PHE:N	2.54	0.41
2:D:396:GLN:O	2:D:397:THR:C	2.63	0.41
1:C:1:MET:HE1	1:C:32:LEU:HD13	2.03	0.41
1:A:14:THR:HB	1:A:15:TYR:CD1	2.56	0.41
1:A:251:VAL:HG12	1:A:252:VAL:HG23	2.02	0.41
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.79	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.88	0.41
1:C:64:VAL:HG21	1:C:144:ALA:CA	2.50	0.41
1:C:279:ALA:C	1:C:281:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ASP:CG	2:D:408:SER:HG	2.26	0.41
2:D:332:LEU:HB3	2:D:363:ALA:HB1	2.02	0.41
2:B:201:LYS:HB3	2:B:201:LYS:HE3	1.56	0.41
1:C:50:ARG:O	1:C:54:LEU:HG	2.21	0.41
1:C:263:LEU:HD11	1:C:267:LEU:CD1	2.50	0.41
2:D:376:LEU:O	2:D:377:ILE:C	2.62	0.41
1:A:266:MET:CG	1:A:266:MET:HE3	2.30	0.40
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.48	0.40
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.04	0.40
2:D:392:MET:O	2:D:395:HIS:HB3	2.22	0.40
1:A:161:HIS:HE1	1:A:173:ILE:O	2.05	0.40
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.97	0.40
1:A:283:HIS:HA	1:A:284:PRO:HD3	1.92	0.40
2:B:220:GLU:HB3	3:E:379:ARG:HD2	2.03	0.40
1:A:5:GLN:HE21	1:A:5:GLN:CA	2.33	0.40
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.93	0.40
1:C:15:TYR:OH	1:C:147:GLY:CA	2.68	0.40
1:C:57:GLU:O	1:C:58:LEU:HD23	2.22	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_466]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/303 (97%)	273 (92%)	19 (6%)	3 (1%)	12	9
1	C	264/303 (87%)	236 (89%)	23 (9%)	5 (2%)	6	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	256/259 (99%)	252 (98%)	3 (1%)	1 (0%)	30	30
2	D	256/259 (99%)	228 (89%)	22 (9%)	6 (2%)	5	1
3	E	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
All	All	1078/1135 (95%)	995 (92%)	68 (6%)	15 (1%)	9	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	VAL
1	C	38	ASP
2	D	420	GLY
2	D	424	LEU
1	A	1	MET
1	A	164	VAL
1	C	145	ASP
2	D	419	HIS
1	A	89	LYS
2	B	176	PRO
1	C	40	GLU
1	C	164	VAL
2	D	176	PRO
2	D	369	GLY
2	D	372	TRP

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%)	237 (91%)	24 (9%)	8	5
1	C	234/265 (88%)	221 (94%)	13 (6%)	19	18
2	B	232/233 (100%)	221 (95%)	11 (5%)	23	24
2	D	232/233 (100%)	220 (95%)	12 (5%)	21	20
3	E	9/11 (82%)	8 (89%)	1 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	968/1007 (96%)	907 (94%)	61 (6%)	16	14

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	9	LYS
1	A	14	THR
1	A	15	TYR
1	A	34	LYS
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	64	VAL
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	178	LYS
1	A	184	VAL
1	A	206	ASP
1	A	230	VAL
1	A	242	LYS
1	A	247	ASP
1	A	255	LEU
1	A	268	HIS
2	B	196	LYS
2	B	201	LYS
2	B	232	LEU
2	B	281	ILE
2	B	292	LEU
2	B	316	THR
2	B	323	GLN
2	B	334	MET
2	B	384	LEU
2	B	403	GLN
2	B	417	LYS
1	C	0	SER
1	C	2	GLU

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Mol	Chain	Res	Type
1	C	9	LYS
1	C	22	ARG
1	C	34	LYS
1	C	38	ASP
1	C	74	ASN
1	C	75	LYS
1	C	78	LEU
1	C	131	GLN
1	C	150	ARG
1	C	177	CYS
1	C	217	ARG
2	D	196	LYS
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	292	LEU
2	D	316	THR
2	D	334	MET
2	D	348	LEU
2	D	384	LEU
2	D	386	SER
2	D	391	LEU
2	D	417	LYS
3	E	379	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	GLN
1	A	60	HIS
1	A	62	ASN
1	A	161	HIS
1	A	295	HIS
2	B	179	HIS
2	B	233	HIS
2	B	317	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	84	HIS

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	119	HIS
1	C	121	HIS
1	C	211	GLN
1	C	265	GLN
2	D	179	HIS
2	D	254	GLN
2	D	317	GLN
2	D	395	HIS
2	D	419	HIS
2	D	431	ASN
3	E	380	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	3.26	5 (62%)	10,14,16	3.08	4 (40%)
1	TPO	C	160	1	8,10,11	3.71	4 (50%)	10,14,16	3.63	7 (70%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	6.05	1.42	1.20
1	A	160	TPO	O-C	6.05	1.42	1.20
1	C	160	TPO	P-O1P	6.01	1.69	1.50
1	A	160	TPO	P-O1P	4.62	1.64	1.50
1	C	160	TPO	P-O2P	4.11	1.70	1.54
1	C	160	TPO	P-O3P	3.79	1.68	1.54
1	A	160	TPO	P-O3P	3.52	1.67	1.54
1	A	160	TPO	P-O2P	2.87	1.65	1.54
1	A	160	TPO	CA-N	-2.02	1.41	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-6.84	107.17	124.77
1	C	160	TPO	O2P-P-OG1	-5.90	82.87	105.85
1	A	160	TPO	O-C-CA	-5.66	110.21	124.77
1	A	160	TPO	O2P-P-OG1	5.64	127.83	105.85
1	A	160	TPO	O3P-P-O2P	-4.05	92.63	107.80
1	C	160	TPO	CG2-CB-CA	-3.90	105.67	113.26
1	C	160	TPO	O2P-P-O1P	3.14	123.06	110.83
1	C	160	TPO	O3P-P-O2P	2.87	118.55	107.80
1	A	160	TPO	P-OG1-CB	-2.80	115.71	123.33
1	C	160	TPO	OG1-P-O1P	-2.75	99.52	109.33
1	C	160	TPO	P-OG1-CB	2.48	130.06	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:LYS	C	90:PHE	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/303 (97%)	0.25	26 (8%) 15 14	20, 29, 74, 105	0
1	C	268/303 (88%)	1.07	49 (18%) 3 2	27, 49, 86, 103	0
2	B	258/259 (99%)	0.68	32 (12%) 8 7	25, 40, 67, 96	0
2	D	258/259 (99%)	1.08	56 (21%) 2 2	26, 43, 73, 103	0
3	E	9/11 (81%)	1.75	4 (44%) 0 0	42, 55, 86, 87	0
All	All	1089/1135 (95%)	0.76	167 (15%) 5 4	20, 41, 79, 105	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	7.1
2	D	175	VAL	7.1
2	B	176	PRO	7.0
2	B	175	VAL	6.6
1	C	251	VAL	6.6
1	C	15	TYR	6.3
1	A	16	GLY	6.3
1	A	296	LEU	5.8
1	A	277	ALA	5.5
2	D	432	LEU	5.4
2	D	430	LEU	5.3
2	D	176	PRO	5.1
1	A	297	ARG	5.1
1	C	16	GLY	5.1
1	C	101	LEU	5.1
1	C	253	PRO	5.0
1	A	14	THR	4.7
1	A	96	LEU	4.7
1	A	15	TYR	4.6
1	C	252	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	14	THR	4.2
2	B	177	ASP	4.2
1	A	41	THR	4.1
1	C	71	HIS	4.1
3	E	386	LYS	4.1
1	C	17	VAL	4.1
1	C	282	ALA	4.0
2	B	325	ALA	4.0
2	B	198	GLY	4.0
2	B	324	PRO	4.0
3	E	380	HIS	3.9
1	C	293	VAL	3.9
2	B	432	LEU	3.8
2	B	179	HIS	3.8
1	A	97	THR	3.8
1	C	221	THR	3.8
1	A	39	THR	3.7
2	B	378	ARG	3.7
2	D	177	ASP	3.6
2	D	324	PRO	3.6
1	A	71	HIS	3.6
1	C	38	ASP	3.6
2	D	363	ALA	3.5
2	B	280	TYR	3.5
1	C	295	HIS	3.4
1	A	40	GLU	3.4
2	D	360	PHE	3.4
2	B	367	VAL	3.4
1	A	13	GLY	3.2
1	A	73	GLU	3.2
2	D	372	TRP	3.2
2	D	284	ASP	3.1
2	D	418	TYR	3.1
2	D	367	VAL	3.1
1	A	95	ALA	3.0
1	A	37	LEU	3.0
2	D	332	LEU	3.0
1	C	296	LEU	2.8
2	B	369	GLY	2.8
2	D	365	TYR	2.8
1	C	199	ARG	2.8
2	D	423	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.8
1	C	175	LEU	2.8
2	B	430	LEU	2.8
2	D	429	THR	2.7
1	C	0	SER	2.7
2	D	417	LYS	2.7
2	D	364	LEU	2.7
1	C	289	VAL	2.7
2	D	427	PRO	2.7
1	C	162	GLU	2.7
2	D	327	CYS	2.7
1	A	38	ASP	2.7
1	C	11	GLY	2.7
2	B	374	GLU	2.7
2	D	426	PRO	2.7
1	C	269	TYR	2.6
1	C	255	LEU	2.6
2	D	390	CYS	2.6
2	D	323	GLN	2.6
2	B	403	GLN	2.6
2	B	201	LYS	2.6
2	D	431	ASN	2.6
1	A	17	VAL	2.6
2	D	359	ALA	2.6
2	B	431	ASN	2.6
1	A	72	THR	2.6
2	D	399	LEU	2.5
1	C	217	ARG	2.5
2	D	369	GLY	2.5
2	D	395	HIS	2.5
3	E	378	SER	2.5
2	D	361	HIS	2.5
2	D	375	SER	2.5
2	D	328	LYS	2.5
1	C	13	GLY	2.5
1	C	271	PRO	2.5
2	D	389	PRO	2.4
1	C	72	THR	2.4
2	D	384	LEU	2.4
1	A	19	TYR	2.4
2	D	350	TYR	2.4
2	D	283	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	420	GLY	2.4
1	A	84	HIS	2.4
2	B	419	HIS	2.4
2	D	178	TYR	2.4
2	D	415	ASN	2.4
2	D	201	LYS	2.4
2	D	424	LEU	2.4
2	B	274	GLU	2.4
2	D	401	ALA	2.3
2	B	371	SER	2.3
1	C	10	ILE	2.3
2	D	419	HIS	2.3
1	A	265	GLN	2.3
2	B	370	GLN	2.3
2	D	320	LEU	2.3
1	C	74	ASN	2.3
1	A	0	SER	2.3
1	C	267	LEU	2.3
2	B	420	GLY	2.3
1	C	268	HIS	2.3
2	D	319	PHE	2.2
2	B	323	GLN	2.2
3	E	381	LYS	2.2
1	A	293	VAL	2.2
1	C	206	ASP	2.2
2	D	402	PRO	2.2
1	C	163	VAL	2.2
1	C	6	LYS	2.2
2	D	428	GLU	2.2
2	D	198	GLY	2.2
2	B	418	TYR	2.1
2	B	364	LEU	2.1
2	D	392	MET	2.1
1	C	292	PRO	2.1
2	D	373	PRO	2.1
2	B	293	ARG	2.1
2	B	365	TYR	2.1
1	C	174	LEU	2.1
1	C	262	LEU	2.1
2	B	399	LEU	2.1
2	D	391	LEU	2.1
2	D	381	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	12	GLU	2.1
1	C	256	ASP	2.1
2	D	326	ASN	2.1
1	C	254	PRO	2.1
1	C	153	GLY	2.1
2	D	337	GLY	2.1
1	C	218	THR	2.1
1	C	178	LYS	2.1
2	D	268	GLU	2.1
1	C	290	THR	2.0
1	C	219	LEU	2.0
1	C	100	PRO	2.0
1	C	171	PRO	2.0
2	D	413	TYR	2.0
1	C	41	THR	2.0
2	B	366	THR	2.0
2	B	368	THR	2.0
2	D	366	THR	2.0
2	B	322	GLN	2.0
1	C	202	LEU	2.0
2	B	281	ILE	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	0.94	0.08	39,43,44,47	0
1	TPO	A	160	11/12	0.97	0.07	21,30,35,38	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.