WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H26
Title : CDK2/CYCLIN A 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)

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

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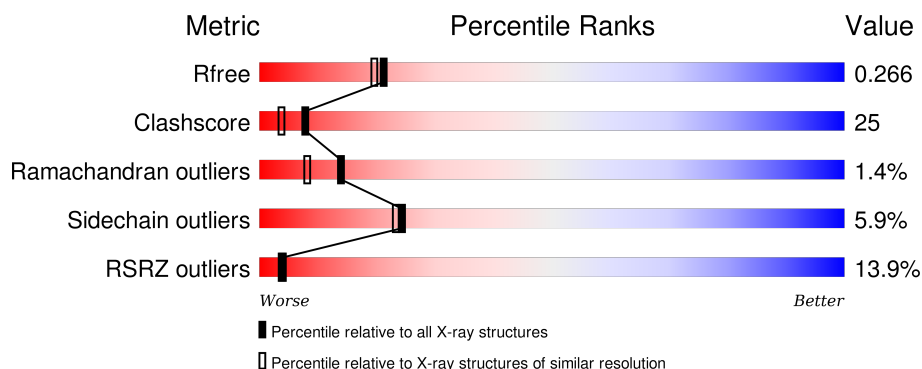Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		25
Ramachandran outliers		1.4%
Sidechain outliers		5.9%
RSRZ outliers		13.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% / 59% 33% 6% ••
1	C	303	14% / 48% 38% • 11%
2	B	259	11% / 75% 21% •
2	D	259	23% / 47% 47% 5%
3	E	11	9% / 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 2389	C 1550	N 405	O 425	P 1	S 8	9	0	1
1	C	269	Total 2149	C 1392	N 367	O 382	P 1	S 7	0	0	1

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total 2084	C 1350	N 339	O 384	S 11	0	0	0
2	D	258	Total 2084	C 1350	N 339	O 384	S 11	0	0	0

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

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

- Molecule 4 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CELL DIVISION PROTEIN KINASE 2
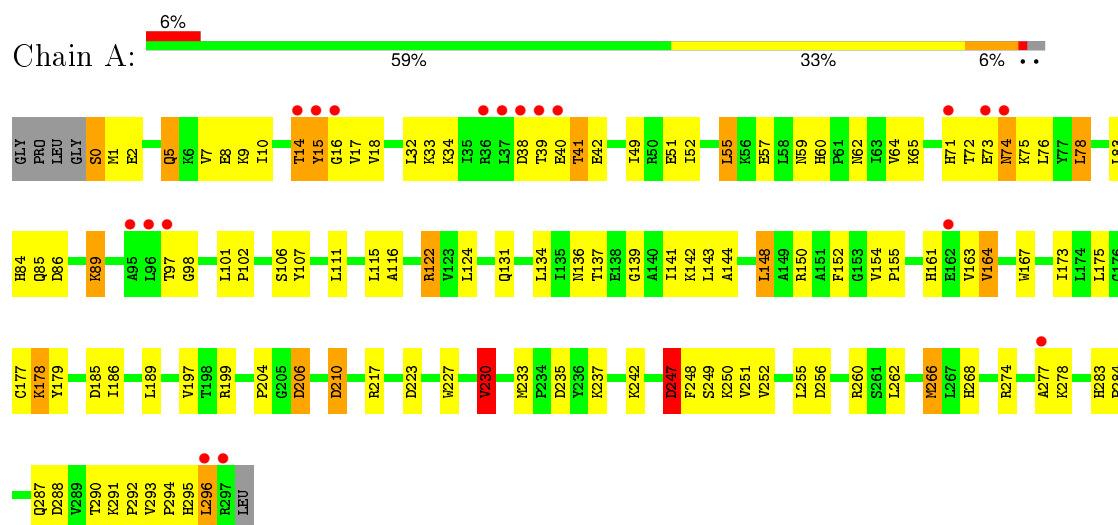
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

• Molecule 2: CYCLIN A2

Chain B:

Chain B residue diagram

• Molecule 2: CYCLIN A2

Chain D:

Chain D residue diagram
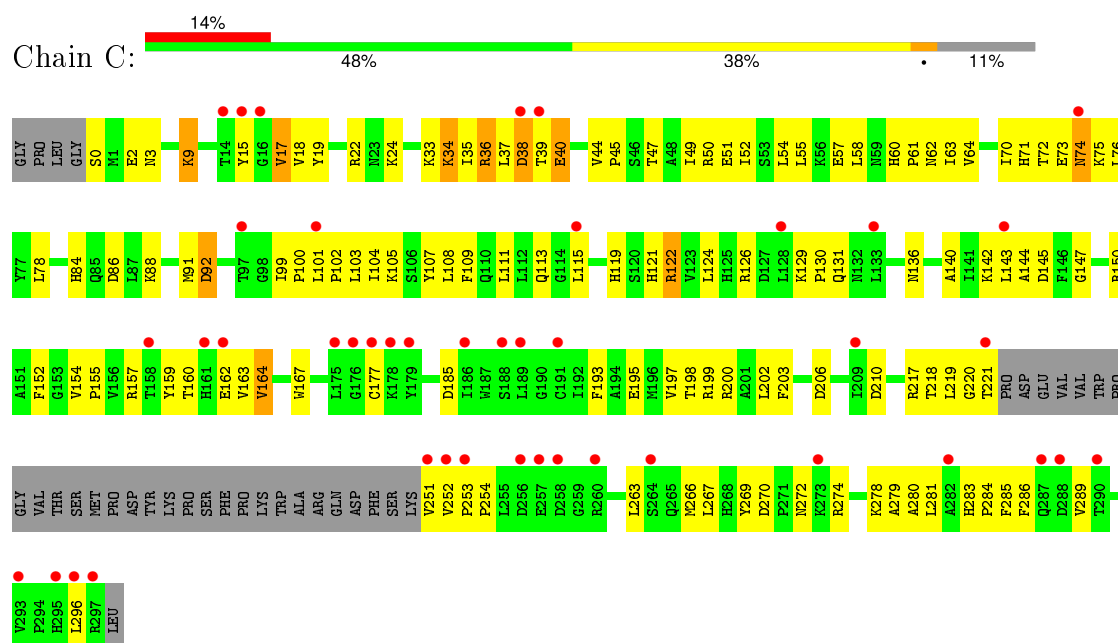
• Molecule 3: CELLULAR TUMOR ANTIGEN P53

Chain E:

Chain E residue diagram

Full wwPDB X-ray Structure Validation Report
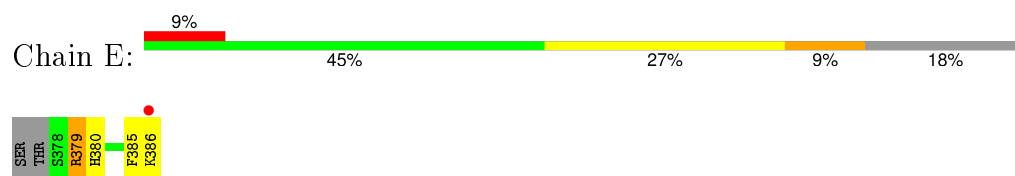
4 Data and refinement statistics (i)

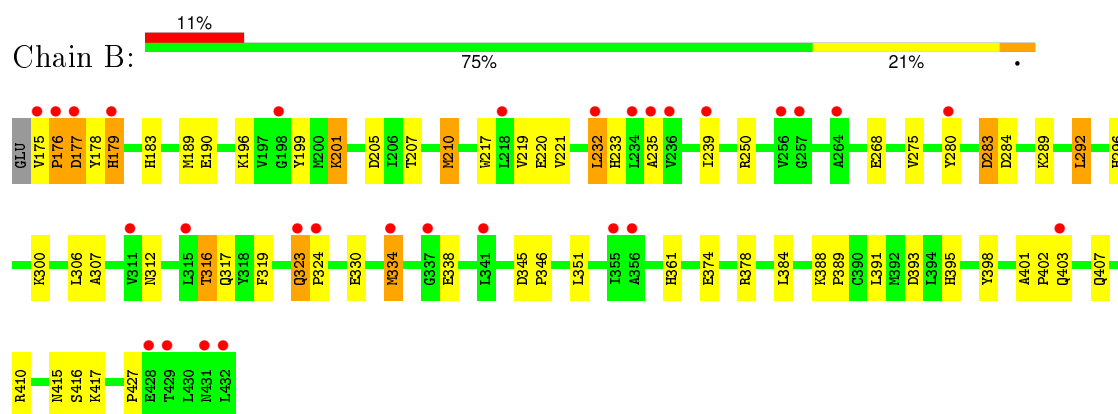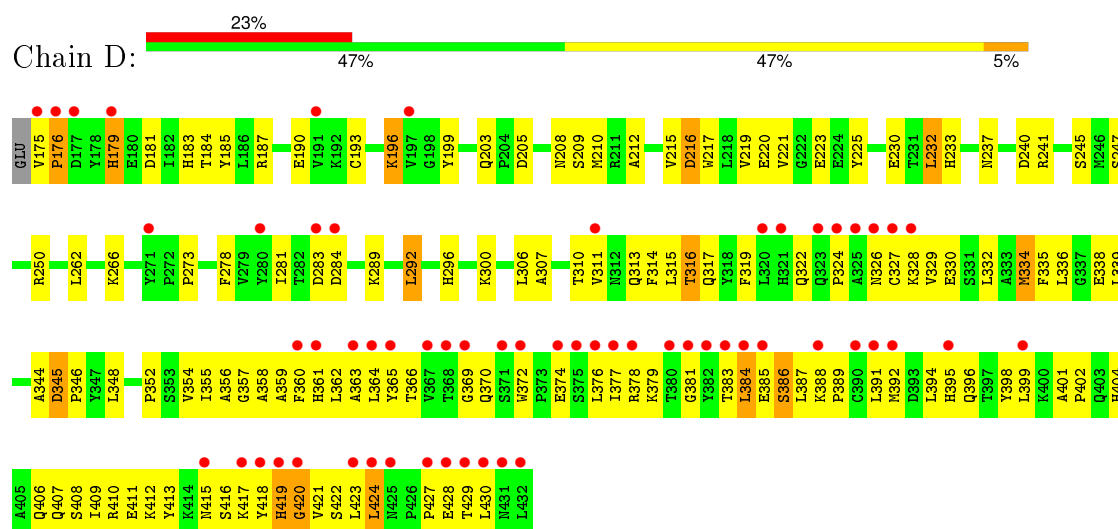| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.67Å 134.03Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.87 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.88-2.24) 96.5 (29.87-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.268 0.233 , 0.266	Depositor DCC
R_{free} test set	3458 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	2 of 68281 reflections (0.003%)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.08	3/2439 (0.1%)	1.06	15/3310 (0.5%)
1	C	0.80	0/2186	0.90	5/2961 (0.2%)
2	B	0.98	4/2134 (0.2%)	0.88	8/2897 (0.3%)
2	D	0.86	0/2134	0.93	8/2897 (0.3%)
3	E	0.78	0/83	0.74	0/104
All	All	0.94	7/8976 (0.1%)	0.95	36/12169 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	MET	SD-CE	-10.93	1.16	1.77
1	A	89	LYS	C-N	-8.29	1.15	1.34
1	A	116	ALA	CA-CB	5.64	1.64	1.52
2	B	210	MET	SD-CE	-5.60	1.46	1.77
2	B	268	GLU	CD-OE2	-5.53	1.19	1.25
2	B	338	GLU	CD-OE2	-5.38	1.19	1.25
2	B	398	TYR	CD2-CE2	-5.16	1.31	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	C-N-CA	9.83	146.27	121.70
1	A	89	LYS	O-C-N	-8.60	108.93	122.70
2	B	378	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	A	122	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	D	181	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	247	ASP	CB-CG-OD2	7.08	124.68	118.30
1	A	274	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	210	ASP	CB-CG-OD2	6.93	124.54	118.30
2	B	177	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	230	VAL	CB-CA-C	-6.83	98.43	111.40
1	C	206	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	223	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	256	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	92	ASP	CB-CG-OD2	6.46	124.11	118.30
2	D	283	ASP	CB-CG-OD2	6.08	123.78	118.30
2	B	205	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	206	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	A	235	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	345	ASP	CB-CG-OD2	5.91	123.62	118.30
2	D	284	ASP	CB-CG-OD2	5.79	123.52	118.30
2	B	378	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	A	288	ASP	CB-CG-OD2	5.67	123.40	118.30
2	D	216	ASP	CB-CG-OD2	5.63	123.37	118.30
2	B	283	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	284	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	210	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	89	LYS	CA-C-N	5.41	129.11	117.20
2	D	205	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	296	LEU	O-C-N	-5.37	114.11	122.70
2	B	393	ASP	CB-CG-OD2	5.35	123.11	118.30
2	D	240	ASP	CB-CG-OD1	5.21	122.99	118.30
2	B	205	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	206	ASP	CB-CG-OD2	5.14	122.93	118.30
2	D	378	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	86	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	38	ASP	CB-CG-OD2	5.00	122.80	118.30

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

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Mol	Chain	Res	Type	Group
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	137	1
1	C	2149	0	2203	150	0
2	B	2084	0	2107	72	1
2	D	2084	0	2107	131	0
3	E	82	0	92	9	0
4	A	87	0	0	10	0
4	B	66	0	0	8	0
4	C	19	0	0	1	0
4	D	21	0	0	2	0
All	All	8981	0	8937	443	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 25.

All (443) 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:CE	1:A:266:MET:SD	1.16	1.25
1:A:266:MET:CG	1:A:266:MET:CE	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:HE2	1:A:266:MET:SD	1.74	1.16
1:A:266:MET:HE1	1:A:266:MET:SD	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:HE3	1.74	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:2010:HOH:O	2:B:189:MET:HE2	1.64	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
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
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
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.59	0.83
1:C:15:TYR:HE2	1:C:47:THR:CB	1.92	0.83
1:A:154:VAL:O	2:B:316:THR:HG22	1.79	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
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
1:A:39:THR:CB	2:B:289:LYS:HZ1	1.97	0.78
1:A:266:MET:CG	1:A:266:MET:HE3	2.02	0.78
2:D:233:HIS:ND1	4:D:2008:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:176:PRO:HA	2:D:179:HIS:CG	2.22	0.75
1:A:85:GLN:HG3	1:A:86:ASP:H	1.52	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: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:D:327:CYS:HG	2:D:419:HIS:CE1	2.06	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:148:LEU:HD23	4:A:2041:HOH:O	1.89	0.72
1:A:72:THR:HG22	1:A:74:ASN:ND2	2.04	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
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:71:HIS:CD2	1:A:76:LEU:HD13	2.26	0.70
1:A:39:THR:CG2	2:B:289:LYS:HD2	2.20	0.70
1:A:72:THR:CG2	1:A:74:ASN:ND2	2.54	0.70
2:D:210:MET:HE2	2:D:250:ARG:HB2	1.73	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
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.60	0.69
1:C:40:GLU:CD	1:C:40:GLU:H	1.96	0.69
1:A:17:VAL:HG12	1:A:18:VAL:N	2.07	0.69
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:107:TYR:O	1:C:111:LEU:HG	1.93	0.68
1:C:105:LYS:HE2	1:C:285:PHE:CZ	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:VAL:O	2:D:316:THR:CG2	2.42	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
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:C:15:TYR:CZ	1:C:47:THR:HB	2.30	0.66
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.77	0.66
1:C:71:HIS:CG	2:D:300:LYS:HZ3	2.13	0.66
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.30	0.66
1:C:15:TYR:OH	1:C:147:GLY:HA2	1.97	0.65
1:A:230:VAL:HG12	1:A:233:MET:HE3	1.78	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
2:D:413:TYR:C	2:D:422:SER:OG	2.35	0.65
1:A:230:VAL:CG1	1:A:233:MET:CE	2.74	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
1:A:266:MET:HG3	1:A:266:MET:HE3	1.78	0.64
2:B:296:HIS:NE2	2:B:300:LYS:HE2	2.11	0.64
1:A:230:VAL:CG1	1:A:233:MET:HE2	2.28	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
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.84	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
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
1:A:230:VAL:HG13	1:A:233:MET:HE2	1.84	0.59
2:D:355:ILE:O	2:D:356:ALA:C	2.40	0.59
1:C:121:HIS:C	1:C:122:ARG:HG3	2.21	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:NE2	2:D:296:HIS:CE1	2.70	0.59
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.90	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:HG22	1:A:10:ILE:O	2.03	0.58
2:D:334:MET:HE3	2:D:334:MET:HA	1.85	0.58
1:A:64:VAL:CG2	1:A:144:ALA:HB2	2.32	0.58
1:C:263:LEU:HD12	1:C:263:LEU:O	2.04	0.58
1:C:39:THR:HG21	2:D:289:LYS:HE3	1.85	0.58
2:B:280:TYR:CE2	3:E:380:HIS:CE1	2.92	0.58
1:A:72:THR:HG22	1:A:74:ASN:H	1.69	0.57
2:D:196:LYS:O	2:D:196:LYS:HG3	2.04	0.57
2:B:175:VAL:N	2:B:179:HIS:HE1	2.01	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
2:D:360:PHE:O	2:D:361:HIS:C	2.42	0.57
1:A:85:GLN:CG	1:A:86:ASP:N	2.67	0.57
2:D:418:TYR:O	2:D:419:HIS:C	2.43	0.56
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
2:D:332:LEU:O	2:D:336:LEU:HG	2.06	0.56
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.86	0.56
1:A:18:VAL:HA	1:A:32:LEU:O	2.06	0.56
1:C:15:TYR:HD1	1:C:33:LYS:NZ	2.04	0.56
1:C:9:LYS:NZ	1:C:17:VAL:HG22	2.21	0.56
1:A:148:LEU:CD2	4:A:2041:HOH:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:CE2	1:C:47:THR:HB	2.39	0.55
1:C:220:GLY:O	1:C:221:THR:C	2.43	0.55
1:A:175:LEU:HD13	1:A:233:MET:HE1	1.88	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:418:TYR:O	2:D:420:GLY:N	2.39	0.55
2:D:196:LYS:HG2	2:D:199:TYR:HB3	1.89	0.55
1:C:71:HIS:CE1	2:D:296:HIS:CD2	2.95	0.55
2:B:296:HIS:NE2	2:B:300:LYS:CE	2.69	0.55
2:D:387:LEU:O	2:D:391:LEU:CB	2.52	0.55
2:D:410:ARG:O	2:D:411:GLU:C	2.43	0.55
2:D:175:VAL:N	2:D:179:HIS:HE1	2.01	0.54
1:C:71:HIS:CB	2:D:300:LYS:NZ	2.69	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
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.42	0.54
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.42	0.54
2:B:296:HIS:HD2	2:B:300:LYS:HE2	1.61	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:71:HIS:ND1	2:B:300:LYS:NZ	2.56	0.54
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.42	0.53
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.43	0.53
1:C:18:VAL:HG22	1:C:33:LYS:HG3	1.90	0.53
1:C:71:HIS:HB3	2:D:300:LYS:HZ3	1.73	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
2:D:361:HIS:O	2:D:362:LEU:C	2.47	0.53
2:D:175:VAL:C	2:D:179:HIS:CE1	2.82	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
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
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
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:383:THR:O	2:D:384:LEU:C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:383:THR:C	2:D:385:GLU:N	2.60	0.52
1:C:278:LYS:O	1:C:281:LEU:HB2	2.09	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.92	0.52
1:C:121:HIS:HD2	2:D:185:TYR:CE1	2.28	0.52
2:B:176:PRO:HD3	2:B:179:HIS:NE2	2.25	0.51
1:C:284:PRO:C	1:C:286:PHE:N	2.61	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
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.45	0.51
1:A:137:THR:O	1:A:293:VAL:HG13	2.11	0.51
1:A:72:THR:HG22	1:A:73:GLU:N	2.24	0.51
1:A:0:SER:C	1:A:2:GLU:H	2.14	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:357:GLY:O	2:D:358:ALA:C	2.49	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
2:D:365:TYR:O	2:D:366:THR:C	2.48	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:136:ASN:HD21	1:C:140:ALA:HB3	1.75	0.50
1:C:126:ARG:HB3	1:C:163:VAL:HG22	1.94	0.50
2:D:376:LEU:O	2:D:379:LYS:N	2.40	0.50
2:D:354:VAL:O	2:D:355:ILE:C	2.48	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:175:LEU:CD1	1:A:233:MET:HE1	2.42	0.49
1:A:64:VAL:HG21	1:A:144:ALA:CB	2.35	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:C:284:PRO:C	1:C:286:PHE:H	2.15	0.49
1:C:195:GLU:O	1:C:199:ARG:N	2.45	0.49
1:A:247:ASP:OD2	1:A:249:SER:OG	2.29	0.49
1:C:15:TYR:HD1	1:C:33:LYS:HZ1	1.56	0.49
2:D:423:LEU:C	2:D:424:LEU:O	2.51	0.49
2:D:423:LEU:O	2:D:424:LEU:C	2.50	0.49
1:C:202:LEU:HD23	1:C:203:PHE:CE1	2.47	0.48
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.48	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
1:A:10:ILE:CG2	1:A:10:ILE:O	2.61	0.48
1:A:84:HIS:HB2	4:A:2016:HOH:O	2.13	0.48
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.13	0.48
2:B:217:TRP:O	2:B:221:VAL:HG23	2.14	0.48
1:C:72:THR:HG22	1:C:74:ASN:H	1.78	0.48
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.28	0.48
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.95	0.48
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.44	0.48
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.95	0.48
1:C:9:LYS:HZ2	1:C:17:VAL:HG22	1.78	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:A:262:LEU:HG	1:A:266:MET:HE2	1.97	0.47
1:C:270:ASP:C	1:C:270:ASP:OD1	2.53	0.47
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.02	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
1:A:65:LYS:HA	4:A:2012:HOH:O	2.15	0.47
2:B:235:ALA:O	2:B:239:ILE:HG13	2.14	0.47
1:C:88:LYS:HA	1:C:91:MET:HE2	1.95	0.47
1:A:290:THR:OG1	1:A:292:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLN:HA	2:B:324:PRO:HA	1.73	0.47
1:C:71:HIS:HB3	2:D:300:LYS:HZ1	1.78	0.47
1:A:39:THR:CG2	1:A:40:GLU:H	2.26	0.47
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
2:D:384:LEU:HA	2:D:384:LEU:HD12	1.80	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46
1:A:262:LEU:HG	1:A:266:MET:CE	2.45	0.46
2:D:216:ASP:CG	2:D:408:SER:OG	2.53	0.46
2:D:415:ASN:OD1	2:D:416:SER:N	2.47	0.46
2:D:395:HIS:HE1	2:D:427:PRO:O	1.98	0.46
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.03	0.46
2:D:326:ASN:OD1	2:D:329:VAL:HG23	2.16	0.46
1:A:98:GLY:HA2	1:A:199:ARG:CZ	2.45	0.46
2:D:358:ALA:O	2:D:359:ALA:C	2.53	0.46
2:B:334:MET:HE3	2:B:334:MET:HA	1.98	0.46
2:D:377:ILE:O	2:D:381:GLY:HA2	2.16	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
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.98	0.46
2:D:230:GLU:OE2	2:D:313:GLN:NE2	2.48	0.46
1:C:157:ARG:HB2	1:C:159:TYR:CE1	2.50	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
2:B:178:TYR:CB	4:B:2009:HOH:O	2.65	0.45
2:B:280:TYR:HE2	3:E:380:HIS:HE1	1.65	0.45
2:B:196:LYS:HG2	2:B:199:TYR:HB3	1.99	0.45
2:B:312:ASN:ND2	4:B:2042:HOH:O	2.50	0.45
2:B:210:MET:CE	3:E:385:PHE:HB3	2.47	0.45
2:D:377:ILE:O	2:D:381:GLY:N	2.49	0.45
2:D:237:ASN:OD1	2:D:241:ARG:HD3	2.17	0.45
1:C:218:THR:O	1:C:218:THR:HG22	2.16	0.45
1:A:72:THR:CG2	1:A:74:ASN:CG	2.85	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:3:ASN:O	1:C:24:LYS:HG3	2.17	0.44
1:C:202:LEU:HD21	1:C:203:PHE:CZ	2.52	0.44
2:D:383:THR:H	2:D:386:SER:HG	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:SER:C	1:A:2:GLU:N	2.71	0.44
1:C:71:HIS:CB	2:D:300:LYS:HZ3	2.28	0.44
2:B:280:TYR:CE2	3:E:380:HIS:HE1	2.34	0.44
1:C:72:THR:CG2	1:C:73:GLU:H	2.28	0.44
1:A:115:LEU:HD21	1:A:185:ASP:HB3	2.00	0.44
2:B:345:ASP:HA	2:B:346:PRO:HA	1.75	0.44
1:C:289:VAL:HG13	1:C:289:VAL:O	2.18	0.44
1:C:60:HIS:CG	1:C:61:PRO:CD	3.00	0.44
1:A:197:VAL:HG11	1:A:252:VAL:HG11	1.95	0.44
2:D:326:ASN:CG	2:D:329:VAL:HG23	2.38	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:404:HIS:HE1	2:D:406:GLN:OE1	2.02	0.43
1:C:91:MET:O	1:C:92:ASP:C	2.57	0.43
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.43
1:C:64:VAL:CG2	1:C:144:ALA:CB	2.72	0.43
1:C:15:TYR:CD1	1:C:33:LYS:HE2	2.51	0.43
2:D:310:THR:O	2:D:311:VAL:C	2.55	0.43
1:A:97:THR:HG21	1:A:295:HIS:HE1	1.80	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
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
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.83	0.43
2:B:210:MET:HE3	3:E:385:PHE:HB3	2.00	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
1:C:9:LYS:HZ3	1:C:17:VAL:CG2	2.32	0.43
2:D:383:THR:O	2:D:386:SER:N	2.51	0.43
2:B:319:PHE:CG	2:B:330:GLU:HG2	2.53	0.43
2:D:216:ASP:OD2	2:D:408:SER:CB	2.67	0.42
1:A:107:TYR:O	1:A:111:LEU:HG	2.19	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
2:D:422:SER:HG	2:D:422:SER:H	1.64	0.42
1:A:72:THR:HG21	1:A:74:ASN:HD21	1.81	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.54	0.42
1:C:162:GLU:CD	1:C:162:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:TYR:N	1:A:15:TYR:CD1	2.87	0.42
1:A:7:VAL:O	1:A:8:GLU:HB3	2.18	0.42
1:A:294:PRO:C	1:A:296:LEU:H	2.23	0.42
2:D:329:VAL:O	2:D:330:GLU:C	2.58	0.42
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.54	0.42
1:C:197:VAL:CG1	1:C:252:VAL:CG1	2.95	0.42
1:C:101:LEU:H	1:C:101:LEU:HG	1.66	0.42
2:D:411:GLU:O	2:D:412:LYS:C	2.57	0.42
1:C:115:LEU:CD1	1:C:119:HIS:CE1	3.02	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:A:72:THR:HG22	1:A:74:ASN:CG	2.40	0.42
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.02	0.42
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.50	0.42
1:A:106:SER:HB2	1:A:290:THR:O	2.20	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:C:109:PHE:CE2	1:C:113:GLN:NE2	2.88	0.41
1:A:186:ILE:HD11	1:A:277:ALA:HB2	2.02	0.41
1:A:71:HIS:CG	2:B:300:LYS:NZ	2.87	0.41
1:C:284:PRO:O	1:C:285:PHE:C	2.54	0.41
2:D:327:CYS:HG	2:D:419:HIS:CD2	2.34	0.41
1:C:193:PHE:CD1	1:C:266:MET:HE1	2.55	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:C:167:TRP:CD1	1:C:167:TRP:N	2.87	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
1:C:60:HIS:HB3	1:C:63:ILE:HD12	2.02	0.41
1:A:72:THR:CG2	1:A:73:GLU:N	2.84	0.41
2:D:210:MET:CE	2:D:250:ARG:CB	2.97	0.41
1:C:284:PRO:O	1:C:286:PHE:N	2.54	0.41
1:C:64:VAL:HG21	1:C:144:ALA:CA	2.50	0.41
1:A:251:VAL:HG12	1:A:252:VAL:HG23	2.02	0.41
2:D:332:LEU:HB3	2:D:363:ALA:HB1	2.02	0.41
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:O	1:C:280:ALA:C	2.59	0.41
1:A:14:THR:HB	1:A:15:TYR:CD1	2.56	0.41
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.88	0.41
1:C:263:LEU:HD11	1:C:267:LEU:CD1	2.50	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:A:39:THR:CG2	1:A:40:GLU:N	2.81	0.40
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.48	0.40
2:D:314:PHE:O	2:D:315:LEU:C	2.60	0.40
2:D:392:MET:O	2:D:395:HIS:HB3	2.22	0.40
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.04	0.40
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.24	0.40
1:A:161:HIS:HE1	1:A:173:ILE:O	2.05	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:189:LEU:HD23	1:A:189:LEU:HA	1.97	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
1:A:5:GLN:HE21	1:A:5:GLN:CA	2.33	0.40
1:C:195:GLU:HG3	1:C:200:ARG:C	2.41	0.40
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.93	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_466]	1.97	0.23

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	295/303 (97%)	273 (92%)	19 (6%)	3 (1%)	19	14
1	C	264/303 (87%)	236 (89%)	23 (9%)	5 (2%)	10	4
2	B	256/259 (99%)	252 (98%)	3 (1%)	1 (0%)	39	42
2	D	256/259 (99%)	228 (89%)	22 (9%)	6 (2%)	8	3
3	E	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
All	All	1078/1135 (95%)	995 (92%)	68 (6%)	15 (1%)	14	8

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 (i)

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%)	239 (92%)	22 (8%)	14	10
1	C	234/265 (88%)	220 (94%)	14 (6%)	24	22
2	B	232/233 (100%)	223 (96%)	9 (4%)	39	45
2	D	232/233 (100%)	221 (95%)	11 (5%)	32	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	9/11 (82%)	8 (89%)	1 (11%)	8	4
All	All	968/1007 (96%)	911 (94%)	57 (6%)	24	23

All (57) 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	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	178	LYS
1	A	206	ASP
1	A	230	VAL
1	A	242	LYS
1	A	247	ASP
1	A	248	PHE
1	A	255	LEU
1	A	268	HIS
2	B	179	HIS
2	B	201	LYS
2	B	232	LEU
2	B	292	LEU
2	B	316	THR
2	B	323	GLN
2	B	334	MET
2	B	384	LEU
2	B	403	GLN
1	C	0	SER
1	C	2	GLU
1	C	9	LYS
1	C	22	ARG
1	C	34	LYS

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Mol	Chain	Res	Type
1	C	36	ARG
1	C	38	ASP
1	C	74	ASN
1	C	75	LYS
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	177	CYS
1	C	217	ARG
2	D	179	HIS
2	D	196	LYS
2	D	232	LEU
2	D	245	SER
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	398	TYR
3	E	379	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
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	425	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	119	HIS
1	C	121	HIS
2	D	179	HIS
2	D	254	GLN

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Mol	Chain	Res	Type
2	D	317	GLN
2	D	361	HIS
2	D	370	GLN
2	D	395	HIS
2	D	419	HIS
2	D	431	ASN
3	E	380	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2.94	4 (50%)	7,14,16	2.80	2 (28%)
1	TPO	C	160	1	8,10,11	3.39	4 (50%)	7,14,16	3.74	5 (71%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

All (8) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O2P	2.99	1.65	1.54
1	A	160	TPO	P-O3P	3.66	1.67	1.54
1	C	160	TPO	P-O3P	3.95	1.68	1.54
1	A	160	TPO	P-O1P	4.16	1.64	1.51
1	C	160	TPO	P-O2P	4.27	1.70	1.54
1	A	160	TPO	O-C	5.00	1.42	1.19
1	C	160	TPO	O-C	5.01	1.42	1.19
1	C	160	TPO	P-O1P	5.47	1.69	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-6.92	107.17	125.44
1	A	160	TPO	O-C-CA	-5.77	110.21	125.44
1	A	160	TPO	O3P-P-O2P	-3.87	92.63	107.38
1	C	160	TPO	CG2-CB-CA	-3.69	105.67	113.17
1	C	160	TPO	OG1-P-O1P	-3.04	99.52	107.11
1	C	160	TPO	O3P-P-O2P	2.93	118.55	107.38
1	C	160	TPO	O2P-P-O1P	3.88	123.06	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.19	18 (6%)	25	25	20, 29, 74, 105	0
1	C	268/303 (88%)	0.74	43 (16%)	3	3	27, 49, 86, 103	0
2	B	258/259 (99%)	0.61	29 (11%)	7	7	25, 40, 67, 96	0
2	D	258/259 (99%)	1.00	60 (23%)	1	1	26, 43, 73, 103	0
3	E	9/11 (81%)	1.44	1 (11%)	7	7	42, 55, 86, 87	0
All	All	1089/1135 (95%)	0.63	151 (13%)	4	4	20, 41, 79, 105	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	10.7
2	D	432	LEU	9.4
2	D	176	PRO	8.3
1	A	16	GLY	6.2
3	E	386	LYS	6.1
1	C	253	PRO	5.9
1	C	15	TYR	5.7
2	D	428	GLU	5.6
1	A	96	LEU	5.5
1	A	39	THR	5.5
2	D	381	GLY	5.4
2	D	430	LEU	5.4
1	C	39	THR	5.4
1	C	297	ARG	5.4
1	A	95	ALA	5.3
2	D	325	ALA	5.3
2	D	175	VAL	5.2
1	C	175	LEU	5.1
2	B	175	VAL	5.1
2	D	419	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	176	PRO	5.0
1	A	36	ARG	5.0
1	A	15	TYR	4.8
2	D	384	LEU	4.8
2	D	284	ASP	4.8
1	C	189	LEU	4.7
2	D	327	CYS	4.6
1	A	73	GLU	4.5
1	C	128	LEU	4.4
1	C	295	HIS	4.4
2	D	378	ARG	4.3
2	D	324	PRO	4.2
2	D	431	ASN	4.1
1	A	277	ALA	4.1
1	A	14	THR	4.1
1	A	40	GLU	4.0
1	C	296	LEU	4.0
1	C	282	ALA	4.0
2	D	177	ASP	4.0
2	D	423	LEU	3.9
1	A	97	THR	3.9
1	C	221	THR	3.9
2	B	341	LEU	3.7
2	D	372	TRP	3.7
2	D	392	MET	3.6
2	B	355	ILE	3.6
2	D	283	ASP	3.6
2	D	377	ILE	3.5
2	B	234	LEU	3.5
2	D	323	GLN	3.5
2	D	390	CYS	3.5
2	D	395	HIS	3.5
2	D	420	GLY	3.5
2	D	369	GLY	3.5
2	D	385	GLU	3.4
1	C	273	LYS	3.4
2	D	328	LYS	3.3
2	D	429	THR	3.3
1	C	38	ASP	3.3
2	D	424	LEU	3.3
2	D	326	ASN	3.2
2	D	363	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	251	VAL	3.2
1	C	179	TYR	3.2
1	C	293	VAL	3.2
1	C	178	LYS	3.2
2	B	324	PRO	3.2
2	B	432	LEU	3.2
2	B	235	ALA	3.1
1	C	287	GLN	3.1
2	B	315	LEU	3.1
2	D	365	TYR	3.1
1	C	288	ASP	3.1
2	B	323	GLN	3.0
2	B	256	VAL	3.0
2	B	311	VAL	3.0
1	C	256	ASP	3.0
1	A	296	LEU	3.0
2	D	367	VAL	3.0
1	C	14	THR	2.9
2	B	431	ASN	2.9
2	D	391	LEU	2.9
2	D	179	HIS	2.9
2	B	280	TYR	2.9
1	C	133	LEU	2.8
1	C	252	VAL	2.8
2	D	383	THR	2.8
1	C	143	LEU	2.8
2	D	376	LEU	2.8
2	D	427	PRO	2.8
1	C	257	GLU	2.8
2	B	177	ASP	2.8
2	B	428	GLU	2.8
1	C	258	ASP	2.7
2	B	236	VAL	2.7
2	D	361	HIS	2.7
1	C	176	GLY	2.7
2	D	280	TYR	2.6
2	D	418	TYR	2.6
1	C	16	GLY	2.6
2	D	380	THR	2.6
2	D	374	GLU	2.6
1	C	97	THR	2.6
2	D	368	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	388	LYS	2.5
2	D	360	PHE	2.5
2	B	239	ILE	2.5
1	C	101	LEU	2.5
1	A	71	HIS	2.5
2	B	179	HIS	2.5
1	C	74	ASN	2.5
2	D	375	SER	2.5
2	D	197	VAL	2.5
1	C	161	HIS	2.4
2	B	232	LEU	2.4
2	B	337	GLY	2.4
2	D	425	ASN	2.4
2	D	321	HIS	2.4
1	C	162	GLU	2.4
1	A	37	LEU	2.4
2	D	382	TYR	2.4
2	D	399	LEU	2.3
2	B	403	GLN	2.3
2	B	264	ALA	2.3
1	C	264	SER	2.3
1	C	177	CYS	2.2
2	D	364	LEU	2.2
2	B	429	THR	2.2
1	A	38	ASP	2.2
2	D	271	TYR	2.2
2	D	371	SER	2.2
1	A	162	GLU	2.2
2	B	356	ALA	2.2
2	D	415	ASN	2.2
1	C	115	LEU	2.2
2	B	218	LEU	2.2
2	D	417	LYS	2.2
1	C	209	ILE	2.2
2	B	334	MET	2.2
1	C	158	THR	2.1
2	B	198	GLY	2.1
1	C	290	THR	2.1
1	A	74	ASN	2.1
2	D	191	VAL	2.1
2	D	311	VAL	2.1
1	C	191	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	186	ILE	2.1
2	B	257	GLY	2.0
2	D	320	LEU	2.0
1	C	188	SER	2.0
1	C	260	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	A	160	11/12	0.97	0.12	-	21,30,35,38	0
1	TPO	C	160	11/12	0.97	0.11	-	39,43,44,47	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.