



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H25
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

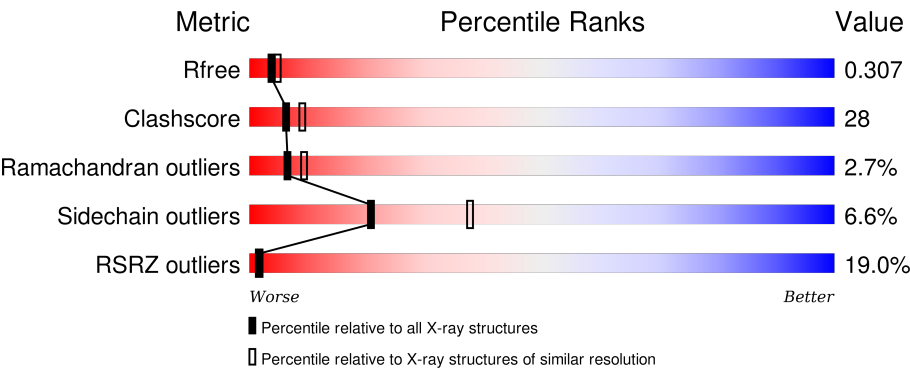
1 Overall quality at a glance i

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	259	
2	D	259	
3	E	11	

2 Entry composition

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.

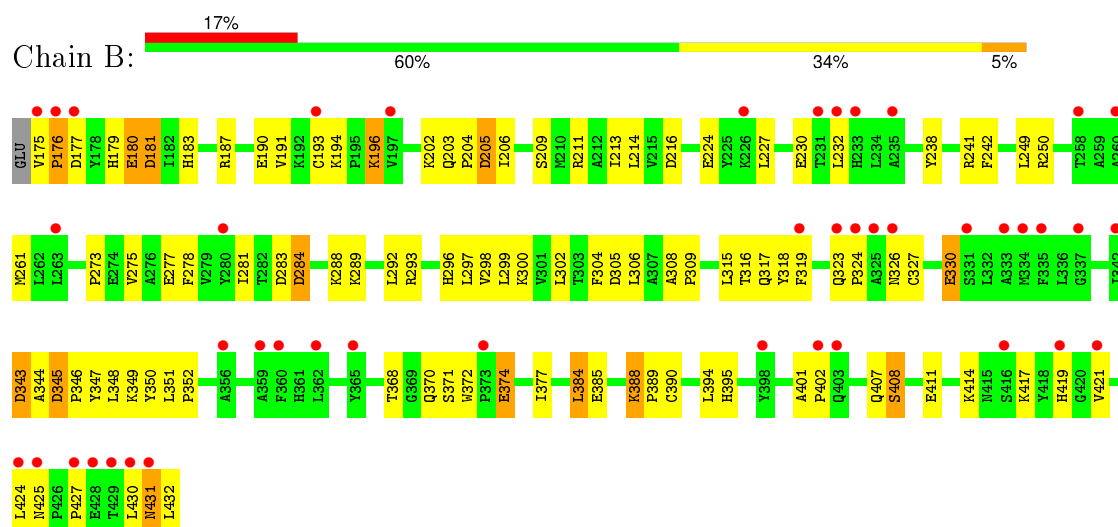
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

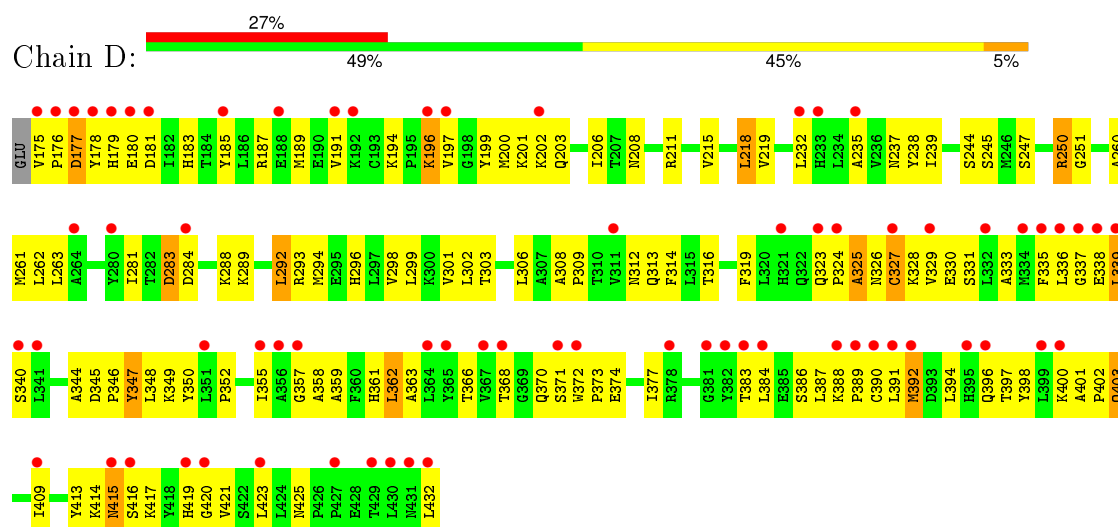
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	10	Total	C	N	O	0	0	0
			87	59	16	12			

- Molecule 4 is water.

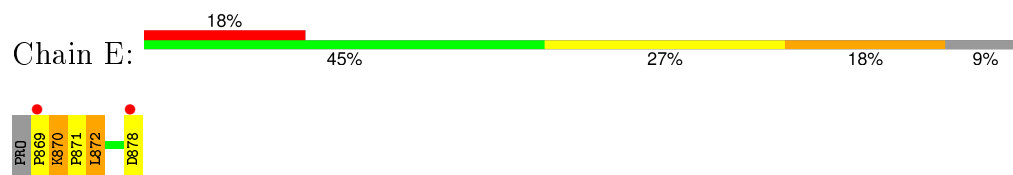
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	61	Total	O	0	0
			61	61		
4	C	47	Total	O	0	0
			47	47		
4	D	21	Total	O	0	0
			21	21		
4	E	1	Total	O	0	0
			1	1		



• 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 28.80 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.00-2.50) 98.8 (28.80-2.48)	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 0.295 , 0.307	Depositor DCC
R_{free} test set	2613 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 52041 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	0/2411	1.02	11/3270 (0.3%)
1	C	0.61	0/2269	0.87	10/3077 (0.3%)
2	B	0.82	0/2133	0.95	6/2897 (0.2%)
2	D	0.54	0/2133	0.81	4/2897 (0.1%)
3	E	0.62	0/89	0.97	0/116
All	All	0.70	0/9035	0.92	31/12257 (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	C	0	1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASP	CB-CG-OD2	9.24	126.61	118.30
2	B	345	ASP	CB-CG-OD2	8.18	125.66	118.30
1	C	38	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	247	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	256	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	127	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	223	ASP	CB-CG-OD2	6.58	124.23	118.30
2	B	205	ASP	CB-CG-OD2	6.44	124.09	118.30
2	B	305	ASP	CB-CG-OD2	6.14	123.82	118.30
1	C	235	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	86	ASP	CB-CG-OD2	6.07	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	38	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	92	ASP	CB-CG-OD2	5.98	123.68	118.30
2	D	177	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	68	ASP	CB-CG-OD2	5.77	123.50	118.30
1	C	270	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	258	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	288	ASP	CB-CG-OD2	5.65	123.38	118.30
2	D	181	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	145	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	256	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	206	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	108	LEU	CB-CG-CD1	-5.26	102.05	111.00
2	B	283	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	235	ASP	CB-CG-OD2	5.23	123.01	118.30
2	D	283	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	284	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	223	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	288	ASP	CB-CG-OD2	5.03	122.82	118.30
2	D	284	ASP	CB-CG-OD2	5.02	122.82	118.30

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 [\(i\)](#)

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	2363	0	2405	130	1
1	C	2229	0	2273	158	0
2	B	2083	0	2107	102	1
2	D	2083	0	2107	126	0
3	E	87	0	101	12	0
4	A	62	0	0	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	61	0	0	15	1
4	C	47	0	0	22	0
4	D	21	0	0	10	0
4	E	1	0	0	0	0
All	All	9037	0	8993	497	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 28.

All (497) 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
3:E:869:PRO:HB2	3:E:871:PRO:HD2	1.33	1.06
1:C:154:VAL:O	2:D:316:THR:HG23	1.55	1.06
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:HG	3:E:872:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:51:GLU:O	1:C:55:LEU:HB2	1.84	0.77
2:B:196:LYS:HB3	2:B:196:LYS:NZ	1.99	0.77
2:B:417:LYS:NZ	2:B:417:LYS:HB3	1.98	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
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
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
3:E:869:PRO:HB2	3:E:871:PRO:CD	2.16	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
2:B:216:ASP:CG	2:B:408:SER:OG	2.28	0.72
2:B:417:LYS:NZ	2:B:417:LYS:CB	2.53	0.72
1:A:40:GLU:C	2:B:288:LYS:HE2	2.12	0.71
1:C:107:TYR:CE1	4:C:2026:HOH:O	2.44	0.71
1:A:2:GLU:HB2	1:C:73:GLU:OE1	1.90	0.71
2:D:176:PRO:O	4:D:2001:HOH:O	2.08	0.70
2:B:299:LEU:HD22	2:B:304:PHE:CD1	2.27	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:121:HIS:C	1:A:122:ARG:HG3	2.13	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
2:B:193:CYS:C	4:B:2015:HOH:O	2.33	0.67
2:D:238:TYR:CE1	2:D:306:LEU:HD22	2.29	0.67
1:C:121:HIS:C	1:C:122:ARG:HG3	2.14	0.67
1:A:249:SER:HA	1:A:260:ARG:HD3	1.77	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:194:LYS:HZ2	2:B:351:LEU:HD23	1.58	0.66
2:B:181:ASP:OD1	4:B:2010:HOH:O	2.13	0.66
1:A:86:ASP:C	1:A:86:ASP:OD1	2.34	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:227:TRP:CG	1:A:230:VAL:HG13	2.31	0.65
1:A:73:GLU:HA	4:A:2021:HOH:O	1.97	0.65
3:E:869:PRO:C	3:E:871:PRO:HD2	2.17	0.64
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.32	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:39:THR:C	1:A:41:THR:H	2.02	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:161:HIS:NE2	1:A:173:ILE:O	2.31	0.63
1:A:218:THR:HG23	1:A:251:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:41:THR:N	2.31	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: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:36:ARG:HD3	4:A:2010:HOH:O	1.98	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:C:60:HIS:CG	1:C:61:PRO:HD2	2.35	0.61
1:A:15:TYR:N	4:A:2007:HOH:O	2.24	0.61
1:A:71:HIS:HE2	2:B:304:PHE:HE2	1.47	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:HG3	2:D:294:MET:O	2.00	0.61
2:D:349:LYS:HE3	2:D:350:TYR:CZ	2.36	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
1:C:13:GLY:CA	4:C:2006:HOH:O	2.48	0.60
1:C:108:LEU:HD12	1:C:108:LEU:O	2.01	0.60
1:C:85:GLN:HB3	4:C:2023:HOH:O	2.00	0.60
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.82	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
2:B:216:ASP:OD2	2:B:408:SER:OG	2.21	0.59
1:A:252:VAL:HG11	1:A:255:LEU:HD22	1.82	0.59
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.85	0.59
1:A:39:THR:C	1:A:41:THR:N	2.53	0.59
1:C:177:CYS:SG	1:C:233:MET:SD	2.94	0.59
2:B:249:LEU:HD12	4:C:2008:HOH:O	2.02	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
1:C:62:ASN:ND2	1:C:110:GLN:HB3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:TYR:HE1	4:C:2026:HOH:O	1.80	0.58
2:D:211:ARG:HH11	2:D:211:ARG:HG2	1.67	0.58
2:D:237:ASN:HA	4:D:2008:HOH:O	2.03	0.58
2:B:421:VAL:O	4:B:2058:HOH:O	2.17	0.58
1:A:136:ASN:OD1	1:A:136:ASN:C	2.41	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
2:D:196:LYS:HB3	2:D:196:LYS:NZ	2.18	0.58
1:C:95:ALA:HA	1:C:199:ARG:HD2	1.86	0.58
1:C:122:ARG:HD3	4:C:2030:HOH:O	2.04	0.57
1:C:39:THR:O	1:C:40:GLU:HB2	2.02	0.57
2:D:298:VAL:HG13	2:D:302:LEU:HD12	1.85	0.57
1:C:106:SER:O	1:C:110:GLN:HG3	2.04	0.57
1:A:219:LEU:CD2	1:A:248:PHE:HE1	2.17	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
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:227:TRP:CD2	1:A:230:VAL:CG1	2.88	0.57
1:A:49:ILE:CG2	2:B:306:LEU:HD12	2.35	0.57
2:B:302:LEU:C	4:B:2028:HOH:O	2.43	0.57
1:C:270:ASP:HB3	1:C:273:LYS:HB2	1.88	0.56
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
2:D:362:LEU:HD12	2:D:362:LEU:O	2.05	0.56
1:A:64:VAL:HG13	1:A:64:VAL:O	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
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
2:D:361:HIS:O	2:D:363:ALA:N	2.40	0.55
1:C:37:LEU:HD21	1:C:76:LEU:HD13	1.87	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
1:C:94:SER:O	1:C:199:ARG:CD	2.54	0.55
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:129:LYS:HD2	1:C:131:GLN:OE1	2.07	0.55
2:D:199:TYR:O	2:D:202:LYS:HB2	2.07	0.55
1:A:51:GLU:O	1:A:55:LEU:HB2	2.06	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
2:B:395:HIS:HE1	2:B:427:PRO:O	1.90	0.54
2:B:350:TYR:CE1	2:B:390:CYS:HB2	2.41	0.54
1:A:9:LYS:HA	1:A:19:TYR:HD2	1.73	0.54
2:D:387:LEU:O	2:D:391:LEU:HB2	2.08	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
1:C:0:SER:C	4:C:2002:HOH:O	2.47	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:C:57:GLU:O	1:C:58:LEU:C	2.46	0.53
1:C:54:LEU:O	1:C:55:LEU:C	2.46	0.53
2:D:323:GLN:N	2:D:324:PRO:CD	2.71	0.53
1:A:101:LEU:N	1:A:102:PRO:CD	2.72	0.53
1:A:84:HIS:CE1	1:A:137:THR:HG23	2.43	0.53
1:C:38:ASP:HA	4:C:2013:HOH:O	2.08	0.53
2:B:202:LYS:O	2:B:204:PRO:HD3	2.10	0.52
2:D:361:HIS:C	2:D:363:ALA:H	2.13	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:C:39:THR:HG21	2:D:289:LYS:HZ2	1.75	0.52
1:A:217:ARG:HD3	1:A:243:TRP:CE2	2.44	0.52
1:A:190:GLY:O	1:A:191:CYS:C	2.48	0.52
2:B:417:LYS:HZ2	2:B:417:LYS:CB	2.23	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
2:D:377:ILE:HG22	4:D:2017:HOH:O	2.11	0.51
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:D:301:VAL:CG1	2:D:301:VAL:O	2.58	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
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.34	0.51
1:A:262:LEU:O	1:A:263:LEU:C	2.49	0.51
1:A:122:ARG:HA	1:A:152:PHE:CZ	2.45	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
3:E:869:PRO:C	3:E:871:PRO:CD	2.78	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:C:39:THR:CG2	2:D:289:LYS:HZ2	2.25	0.50
1:A:218:THR:HG23	1:A:251:VAL:CG2	2.41	0.50
1:A:184:VAL:O	4:A:2041:HOH:O	2.17	0.50
1:A:162:GLU:HG2	4:A:2035:HOH:O	2.11	0.50
2:D:302:LEU:O	2:D:303:THR:C	2.50	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:131:GLN:H	1:A:131:GLN:CD	2.15	0.50
2:B:175:VAL:C	2:B:177:ASP:H	2.15	0.50
1:A:161:HIS:HB3	1:A:162:GLU:OE2	2.12	0.50
1:A:193:PHE:O	1:A:194:ALA:C	2.47	0.50
1:C:293:VAL:O	1:C:293:VAL:HG12	2.12	0.50
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
1:A:96:LEU:O	1:A:97:THR:C	2.49	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
1:A:100:PRO:C	1:A:102:PRO:HD2	2.33	0.49
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.95	0.49
2:B:175:VAL:O	2:B:177:ASP:N	2.46	0.49
2:B:194:LYS:HZ3	2:B:351:LEU:CD2	2.25	0.49
2:D:196:LYS:HZ3	2:D:196:LYS:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:ILE:O	3:E:872:LEU:HA	2.12	0.49
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:175:VAL:C	2:B:177:ASP:N	2.66	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
2:B:327:CYS:HG	2:B:419:HIS:CD2	2.31	0.48
1:A:159:TYR:O	1:A:160:TPO:C	2.61	0.48
1:A:98:GLY:HA2	1:A:199:ARG:CD	2.42	0.48
2:D:298:VAL:HG13	2:D:302:LEU:CD1	2.44	0.48
1:C:157:ARG:NH1	1:C:159:TYR:HE1	2.11	0.48
1:A:3:ASN:O	1:A:24:LYS:HG3	2.12	0.48
3:E:870:LYS:N	3:E:871:PRO:CD	2.76	0.48
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.49	0.48
2:D:191:VAL:O	2:D:194:LYS:HB3	2.14	0.48
1:C:95:ALA:C	1:C:199:ARG:HH11	2.16	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
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
1:A:230:VAL:HA	1:A:233:MET:SD	2.54	0.47
1:C:76:LEU:HA	1:C:76:LEU:HD12	1.71	0.47
2:D:314:PHE:HE2	2:D:352:PRO:HB2	1.78	0.47
2:B:395:HIS:CE1	2:B:427:PRO:O	2.67	0.47
1:C:171:PRO:O	1:C:173:ILE:N	2.47	0.47
1:A:10:ILE:O	1:A:10:ILE:HG12	2.15	0.47
1:A:131:GLN:N	1:A:131:GLN:CD	2.68	0.47
1:C:111:LEU:CD2	1:C:141:ILE:HD13	2.44	0.47
2:D:175:VAL:O	2:D:177:ASP:N	2.48	0.47
2:B:224:GLU:HB2	3:E:871:PRO:CG	2.44	0.47
1:C:136:ASN:HD21	1:C:140:ALA:CB	2.18	0.47
1:A:73:GLU:CA	4:A:2021:HOH:O	2.61	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
2:D:281:ILE:C	2:D:283:ASP:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ALA:O	2:D:403:GLN:N	2.48	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:B:191:VAL:CG1	2:B:191:VAL:O	2.63	0.47
1:C:12:GLU:HG3	1:C:16:GLY:O	2.14	0.47
1:C:269:TYR:O	1:C:271:PRO:HD3	2.16	0.46
2:D:361:HIS:C	2:D:363:ALA:N	2.69	0.46
2:B:315:LEU:O	2:B:316:THR:C	2.52	0.46
2:D:350:TYR:CZ	2:D:390:CYS:HA	2.50	0.46
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.96	0.46
2:D:373:PRO:O	2:D:377:ILE:HG13	2.16	0.46
1:C:96:LEU:C	4:C:2025:HOH:O	2.53	0.46
1:C:57:GLU:HB2	1:C:58:LEU:H	1.36	0.46
1:A:0:SER:HA	1:A:70:ILE:HD13	1.96	0.46
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.84	0.46
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.51	0.46
1:C:107:TYR:O	1:C:111:LEU:HG	2.16	0.46
2:D:355:ILE:HA	2:D:390:CYS:SG	2.55	0.46
2:B:323:GLN:CB	4:B:2036:HOH:O	2.63	0.46
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.89	0.46
1:A:39:THR:HG22	1:A:40:GLU:H	1.81	0.46
1:A:197:VAL:HG11	1:A:252:VAL:HG13	1.98	0.46
1:C:108:LEU:HG	1:C:286:PHE:HZ	1.81	0.46
1:A:188:SER:O	1:A:192:ILE:HG13	2.15	0.46
2:B:205:ASP:OD1	2:B:250:ARG:NH2	2.37	0.46
2:B:343:ASP:O	2:B:344:ALA:C	2.53	0.46
2:B:319:PHE:CZ	2:B:330:GLU:HA	2.50	0.46
1:A:231:THR:HA	1:A:236:TYR:CD1	2.51	0.46
2:B:350:TYR:CD1	2:B:390:CYS:HB2	2.51	0.46
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.62	0.46
2:D:383:THR:H	2:D:386:SER:HG	1.62	0.46
1:A:88:LYS:HA	1:A:91:MET:HE2	1.97	0.46
1:A:224:GLU:OE2	1:A:231:THR:HG23	2.16	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
2:D:306:LEU:O	2:D:308:ALA:N	2.46	0.45
1:C:125:HIS:O	1:C:126:ARG:HB2	2.16	0.45
1:A:2:GLU:HG3	1:C:73:GLU:CD	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:194:ALA:O	1:A:197:VAL:HB	2.17	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:91:MET:HE1	1:C:130:PRO:HB3	1.99	0.45
1:C:168:TYR:N	1:C:168:TYR:CD2	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:D:345:ASP:HA	2:D:346:PRO:HA	1.57	0.44
1:A:13:GLY:C	4:A:2007:HOH:O	2.55	0.44
2:D:237:ASN:ND2	4:D:2008:HOH:O	2.49	0.44
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.31	0.44
2:D:403:GLN:HB2	2:D:403:GLN:HE21	1.57	0.44
2:D:196:LYS:NZ	2:D:196:LYS:CB	2.80	0.44
2:D:263:LEU:HA	2:D:263:LEU:HD23	1.89	0.44
1:C:72:THR:HG22	1:C:73:GLU:N	2.32	0.44
2:B:430:LEU:O	2:B:431:ASN:CB	2.62	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:C:88:LYS:O	1:C:89:LYS:C	2.55	0.44
1:C:54:LEU:C	1:C:56:LYS:N	2.71	0.44
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.99	0.44
1:A:155:PRO:HD2	2:B:316:THR:HB	2.00	0.43
2:B:345:ASP:HA	2:B:346:PRO:HA	1.73	0.43
1:C:115:LEU:HD21	1:C:185:ASP:HB3	2.00	0.43
1:C:152:PHE:C	4:C:2030:HOH:O	2.57	0.43
1:A:252:VAL:HG12	1:A:252:VAL:O	2.18	0.43
2:B:430:LEU:HD12	2:B:432:LEU:HD11	2.00	0.43
2:B:407:GLN:O	2:B:411:GLU:HG2	2.18	0.43
1:A:33:LYS:HE2	4:A:2003:HOH:O	2.18	0.43
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.99	0.43
1:C:154:VAL:HA	1:C:155:PRO:HA	1.80	0.43
1:A:64:VAL:CG1	1:A:64:VAL:O	2.66	0.43
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:262:LEU:C	1:A:264:SER:N	2.67	0.43
2:D:324:PRO:O	2:D:325:ALA:HB3	2.18	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:263:LEU:HD12	1:A:263:LEU:HA	1.73	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
1:C:202:LEU:O	1:C:203:PHE:CD1	2.72	0.43
2:D:250:ARG:HG3	2:D:251:GLY:N	2.34	0.43
2:B:238:TYR:N	2:B:238:TYR:CD1	2.83	0.43
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:NH1	1:C:260:ARG:HG3	2.34	0.42
2:D:203:GLN:OE1	2:D:247:SER:HA	2.17	0.42
1:A:87:LEU:HD12	1:A:87:LEU:O	2.19	0.42
1:A:135:ILE:HG13	1:A:135:ILE:O	2.18	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:C:60:HIS:CD2	1:C:61:PRO:N	2.88	0.42
1:A:69:VAL:O	1:A:69:VAL:HG12	2.18	0.42
1:A:223:ASP:H	1:A:226:VAL:CG1	2.31	0.42
1:C:270:ASP:HA	1:C:271:PRO:HD3	1.87	0.42
1:A:13:GLY:O	1:A:16:GLY:N	2.50	0.42
2:B:181:ASP:N	2:B:181:ASP:OD1	2.52	0.42
1:A:223:ASP:O	1:A:226:VAL:HG12	2.20	0.42
2:D:323:GLN:N	2:D:324:PRO:HD3	2.34	0.42
1:C:97:THR:N	4:C:2025:HOH:O	2.53	0.42
1:C:182:THR:O	1:C:183:ALA:C	2.58	0.42
2:D:185:TYR:O	2:D:189:MET:HG2	2.19	0.42
1:C:180:TYR:C	1:C:180:TYR:CD1	2.93	0.42
1:C:135:ILE:HA	1:C:140:ALA:O	2.20	0.42
1:C:39:THR:C	1:C:41:THR:H	2.23	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
2:D:208:ASN:HD22	2:D:208:ASN:H	1.68	0.42
1:C:7:VAL:O	1:C:8:GLU:HB3	2.20	0.42
2:B:175:VAL:HG23	2:B:177:ASP:CG	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.55	0.42
2:D:294:MET:HB2	2:D:294:MET:HE2	1.89	0.42
1:C:171:PRO:C	1:C:173:ILE:N	2.71	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: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:C:129:LYS:HB2	1:C:130:PRO:HD2	2.02	0.41
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.01	0.41
2:D:327:CYS:HG	2:D:419:HIS:CE1	2.37	0.41
2:B:411:GLU:O	2:B:414:LYS:HB2	2.20	0.41
1:C:110:GLN:HA	1:C:113:GLN:HE21	1.85	0.41
1:A:161:HIS:CG	1:A:161:HIS:O	2.73	0.41
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.50	0.41
1:C:40:GLU:O	2:D:288:LYS:NZ	2.51	0.41
2:D:260:ALA:O	2:D:263:LEU:N	2.53	0.41
1:C:189:LEU:CA	1:C:192:ILE:HD12	2.50	0.41
1:C:6:LYS:HD3	1:C:19:TYR:CD2	2.55	0.41
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.63	0.41
1:A:174:LEU:HD11	1:A:211:GLN:HG2	2.03	0.41
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.91	0.41
2:D:312:ASN:O	2:D:316:THR:HB	2.21	0.41
1:C:39:THR:HG22	2:D:289:LYS:HZ3	1.85	0.41
2:B:211:ARG:O	2:B:214:LEU:N	2.52	0.41
2:D:208:ASN:HD22	2:D:208:ASN:N	2.18	0.41
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.56	0.41
1:C:275:ILE:CG1	1:C:279:ALA:HB3	2.50	0.41
1:A:41:THR:HB	1:A:43:GLY:H	1.85	0.41
2:B:317:GLN:O	2:B:318:TYR:C	2.57	0.41
2:B:318:TYR:O	2:B:319:PHE:C	2.56	0.41
1:C:51:GLU:CD	4:C:2014:HOH:O	2.59	0.41
1:C:59:ASN:HD22	1:C:59:ASN:HA	1.54	0.41
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.93	0.41
3:E:872:LEU:CG	3:E:872:LEU:O	2.54	0.41
1:A:277:ALA:O	1:A:278:LYS:C	2.59	0.41
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.92	0.41
2:D:261:MET:O	2:D:262:LEU:C	2.59	0.41
2:D:366:THR:HG22	2:D:366:THR:O	2.21	0.41
1:C:136:ASN:OD1	1:C:138:GLU:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:HIS:HA	1:C:284:PRO:HD3	1.82	0.41
2:B:371:SER:O	2:B:372:TRP:C	2.60	0.41
2:B:296:HIS:O	2:B:297:LEU:C	2.59	0.41
1:A:270:ASP:O	1:A:271:PRO:C	2.58	0.40
1:A:104:ILE:O	1:A:105:LYS:C	2.60	0.40
1:C:278:LYS:HG3	2:D:178:TYR:CE1	2.56	0.40
1:C:85:GLN:NE2	1:C:90:PHE:HB2	2.37	0.40
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.51	0.40
1:C:101:LEU:HD13	1:C:101:LEU:O	2.21	0.40
1:A:52:ILE:O	1:A:56:LYS:HG3	2.22	0.40
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.86	0.40
1:C:287:GLN:HG3	1:C:288:ASP:N	2.35	0.40
1:A:122:ARG:HD2	1:A:122:ARG:O	2.21	0.40
1:C:215:ILE:HG23	1:C:219:LEU:CD1	2.50	0.40
2:D:211:ARG:NH1	2:D:211:ARG:HG2	2.35	0.40
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.93	0.40
2:B:326:ASN:OD1	2:B:326:ASN:C	2.59	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%)	5	6
1	C	274/303 (90%)	240 (88%)	25 (9%)	9 (3%)	5	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	256/259 (99%)	245 (96%)	7 (3%)	4 (2%)	12	21
2	D	256/259 (99%)	225 (88%)	26 (10%)	5 (2%)	9	15
3	E	8/11 (73%)	5 (62%)	2 (25%)	1 (12%)	0	0
All	All	1085/1135 (96%)	980 (90%)	76 (7%)	29 (3%)	6	9

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
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%)	239 (93%)	19 (7%)	17	31
1	C	244/265 (92%)	229 (94%)	15 (6%)	23	42
2	B	232/233 (100%)	219 (94%)	13 (6%)	26	47
2	D	232/233 (100%)	217 (94%)	15 (6%)	21	39
3	E	10/11 (91%)	8 (80%)	2 (20%)	1	3
All	All	976/1007 (97%)	912 (93%)	64 (7%)	21	38

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
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	105	LYS
1	A	122	ARG
1	A	150	ARG
1	A	177	CYS
1	A	184	VAL
1	A	206	ASP
1	A	232	SER
1	A	248	PHE
1	A	255	LEU
1	A	261	SER
1	A	272	ASN
2	B	179	HIS
2	B	180	GLU
2	B	181	ASP
2	B	196	LYS

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Mol	Chain	Res	Type
2	B	232	LEU
2	B	261	MET
2	B	277	GLU
2	B	374	GLU
2	B	384	LEU
2	B	385	GLU
2	B	388	LYS
2	B	408	SER
2	B	425	ASN
1	C	0	SER
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	122	ARG
1	C	150	ARG
1	C	178	LYS
1	C	210	ASP
1	C	290	THR
2	D	180	GLU
2	D	196	LYS
2	D	201	LYS
2	D	218	LEU
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	398	TYR
2	D	403	GLN
2	D	417	LYS
2	D	425	ASN
2	D	432	LEU
3	E	872	LEU
3	E	878	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	85	GLN
1	A	119	HIS
1	A	131	GLN
1	A	272	ASN
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	431	ASN
1	C	59	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	85	GLN
1	C	113	GLN
1	C	131	GLN
1	C	268	HIS
2	D	254	GLN
2	D	313	GLN
2	D	361	HIS
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	3.51	4 (50%)	7,14,16	3.09	1 (14%)
1	TPO	C	160	1	8,10,11	3.46	4 (50%)	7,14,16	2.57	1 (14%)

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O2P	3.95	1.68	1.54
1	A	160	TPO	P-O3P	4.02	1.69	1.54
1	A	160	TPO	P-O2P	4.03	1.69	1.54
1	C	160	TPO	P-O3P	4.41	1.70	1.54
1	C	160	TPO	O-C	5.10	1.43	1.19
1	A	160	TPO	O-C	5.46	1.45	1.19
1	C	160	TPO	P-O1P	5.79	1.70	1.51
1	A	160	TPO	P-O1P	5.91	1.70	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-8.02	104.26	125.44
1	C	160	TPO	O-C-CA	-6.35	108.66	125.44

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/303 (96%)	0.92	31 (10%) 8 8	28, 40, 70, 79	0
1	C	278/303 (91%)	1.30	61 (21%) 1 1	38, 60, 99, 109	0
2	B	258/259 (99%)	1.17	44 (17%) 2 2	27, 42, 57, 76	0
2	D	258/259 (99%)	1.51	70 (27%) 1 1	36, 71, 107, 114	0
3	E	10/11 (90%)	2.05	2 (20%) 1 1	58, 65, 72, 73	0
All	All	1097/1135 (96%)	1.22	208 (18%) 2 1	27, 51, 98, 114	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	12.5
2	D	432	LEU	9.7
1	C	225	VAL	8.1
2	D	323	GLN	7.1
1	C	227	TRP	7.0
2	B	175	VAL	6.9
1	C	14	THR	6.7
1	A	40	GLU	6.1
2	D	430	LEU	5.8
1	A	39	THR	5.7
1	C	15	TYR	5.4
2	D	416	SER	5.3
1	C	223	ASP	5.2
2	D	175	VAL	4.9
2	D	368	THR	4.9
2	D	197	VAL	4.9
3	E	878	ASP	4.8
2	D	391	LEU	4.8
2	D	372	TRP	4.8
1	A	96	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	188	SER	4.7
1	C	259	GLY	4.7
2	D	335	PHE	4.7
1	A	15	TYR	4.6
2	D	423	LEU	4.5
1	C	235	ASP	4.5
2	D	327	CYS	4.5
1	C	273	LYS	4.3
1	C	221	THR	4.2
1	C	230	VAL	4.1
2	B	324	PRO	4.1
1	C	13	GLY	4.1
2	D	356	ALA	4.0
2	D	384	LEU	4.0
1	C	258	ASP	4.0
2	D	419	HIS	4.0
2	D	311	VAL	3.9
1	C	222	PRO	3.9
1	C	11	GLY	3.9
1	C	269	TYR	3.9
2	D	357	GLY	3.9
2	B	424	LEU	3.8
2	B	232	LEU	3.8
3	E	869	PRO	3.8
2	B	323	GLN	3.8
2	D	351	LEU	3.7
2	D	176	PRO	3.7
1	C	220	GLY	3.7
1	C	179	TYR	3.6
2	D	235	ALA	3.5
1	C	233	MET	3.5
2	D	392	MET	3.5
2	B	428	GLU	3.5
2	D	383	THR	3.4
2	D	381	GLY	3.4
2	D	429	THR	3.4
1	C	229	GLY	3.4
2	D	339	LEU	3.4
2	D	395	HIS	3.4
2	D	378	ARG	3.3
2	B	356	ALA	3.3
1	C	175	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	161	HIS	3.3
1	C	109	PHE	3.3
1	A	95	ALA	3.3
1	C	36	ARG	3.2
1	C	254	PRO	3.2
2	D	180	GLU	3.2
1	C	257	GLU	3.2
1	C	191	CYS	3.2
1	C	108	LEU	3.1
1	C	143	LEU	3.1
2	D	409	ILE	3.1
1	C	228	PRO	3.1
2	D	280	TYR	3.1
1	C	12	GLU	3.1
2	B	425	ASN	3.1
1	A	36	ARG	3.1
2	D	178	TYR	3.0
2	D	355	ILE	3.0
2	D	427	PRO	3.0
1	C	187	TRP	3.0
1	C	260	ARG	3.0
1	C	128	LEU	3.0
1	C	17	VAL	3.0
2	D	364	LEU	2.9
1	C	189	LEU	2.9
2	D	341	LEU	2.9
1	C	253	PRO	2.9
1	C	282	ALA	2.8
1	A	16	GLY	2.8
1	A	229	GLY	2.8
1	C	218	THR	2.8
2	B	419	HIS	2.8
1	C	231	THR	2.8
2	D	420	GLY	2.8
2	D	324	PRO	2.8
1	C	174	LEU	2.8
1	C	184	VAL	2.8
2	D	367	VAL	2.8
2	D	431	ASN	2.8
2	B	260	ALA	2.8
1	C	164	VAL	2.7
2	D	415	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	336	LEU	2.7
2	D	179	HIS	2.7
1	C	190	GLY	2.7
2	B	402	PRO	2.7
1	A	186	ILE	2.7
1	A	111	LEU	2.7
2	D	192	LYS	2.7
2	D	321	HIS	2.7
2	D	191	VAL	2.7
2	B	325	ALA	2.7
2	D	329	VAL	2.6
2	D	177	ASP	2.6
2	B	365	TYR	2.6
2	D	232	LEU	2.6
1	A	225	VAL	2.6
1	A	0	SER	2.6
2	D	399	LEU	2.6
2	B	335	PHE	2.6
2	B	226	LYS	2.6
2	D	382	TYR	2.5
1	C	10	ILE	2.5
2	B	421	VAL	2.5
1	C	37	LEU	2.5
2	B	193	CYS	2.5
1	C	219	LEU	2.5
2	D	284	ASP	2.5
2	B	177	ASP	2.5
2	B	233	HIS	2.5
2	D	202	LYS	2.5
1	A	269	TYR	2.5
2	B	431	ASN	2.5
2	B	235	ALA	2.5
1	A	293	VAL	2.5
2	B	197	VAL	2.4
1	A	19	TYR	2.4
2	B	373	PRO	2.4
2	D	188	GLU	2.4
2	B	280	TYR	2.4
2	D	396	GLN	2.3
1	A	189	LEU	2.3
2	B	342	ILE	2.3
2	D	388	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	236	TYR	2.3
1	C	213	PHE	2.3
2	D	337	GLY	2.3
2	B	176	PRO	2.3
2	B	319	PHE	2.3
2	D	340	SER	2.3
1	C	9	LYS	2.3
1	C	102	PRO	2.3
2	B	359	ALA	2.3
1	A	114	GLY	2.3
2	B	398	TYR	2.3
1	A	187	TRP	2.3
2	B	333	ALA	2.2
2	D	264	ALA	2.2
2	D	334	MET	2.2
2	D	338	GLU	2.2
2	D	371	SER	2.2
1	C	209	ILE	2.2
2	B	430	LEU	2.2
2	D	332	LEU	2.2
2	B	258	THR	2.2
2	B	429	THR	2.2
2	B	331	SER	2.2
2	D	365	TYR	2.2
2	D	181	ASP	2.2
1	A	227	TRP	2.2
1	A	290	THR	2.2
1	C	178	LYS	2.2
1	A	181	SER	2.2
2	B	334	MET	2.2
1	A	228	PRO	2.2
2	B	326	ASN	2.2
1	C	77	TYR	2.2
2	D	233	HIS	2.2
1	C	192	ILE	2.2
1	C	137	THR	2.2
1	A	71	HIS	2.1
1	A	73	GLU	2.1
2	B	337	GLY	2.1
1	A	291	LYS	2.1
2	B	403	GLN	2.1
1	C	156	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	362	LEU	2.1
2	B	427	PRO	2.1
2	B	416	SER	2.1
2	B	360	PHE	2.1
2	D	389	PRO	2.1
1	A	243	TRP	2.1
2	D	390	CYS	2.1
2	D	185	TYR	2.1
1	C	84	HIS	2.1
2	D	196	LYS	2.1
1	C	162	GLU	2.1
2	B	263	LEU	2.1
2	D	400	LYS	2.1
1	C	157	ARG	2.0
1	A	7	VAL	2.0
1	A	206	ASP	2.0
1	C	161	HIS	2.0
1	C	202	LEU	2.0
1	A	41	THR	2.0
2	B	231	THR	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	0.93	0.14	-	39,41,43,44	0
1	TPO	C	160	11/12	0.93	0.18	-	57,62,66,66	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 ⓘ

There are no such residues in this entry.