



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 10:55 AM 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 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/ValidationPDFNotes.html>

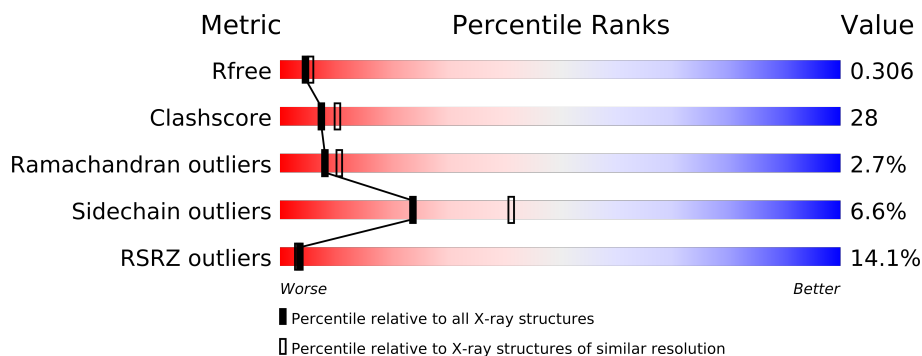
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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-ASSOCIATEDPROTEIN.

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

- Molecule 4 is water.

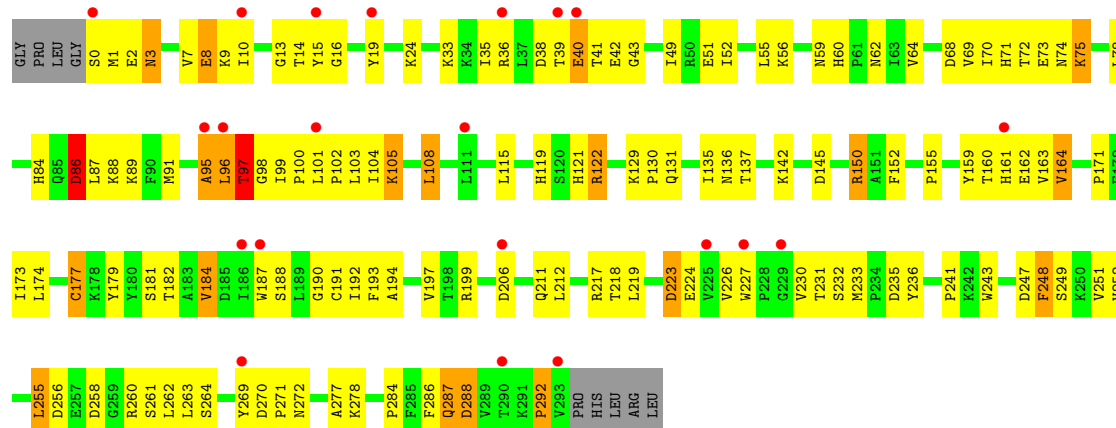
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	61	Total	O	0	0
			61	61		
4	C	47	Total	O	0	0
			47	47		
4	D	21	Total	O	0	0
			21	21		
4	E	1	Total	O	0	0
			1	1		

3 Residue-property plots

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.

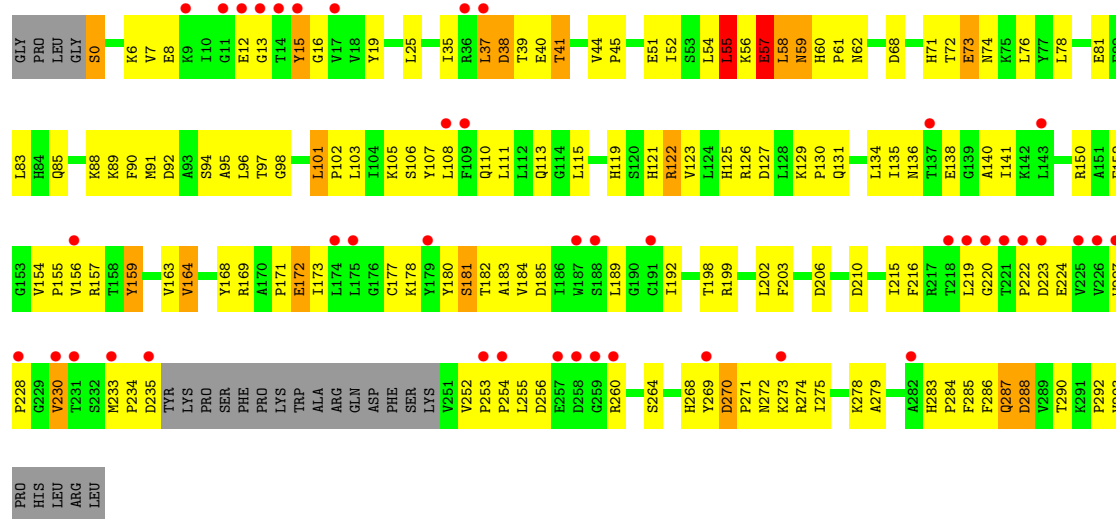
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 



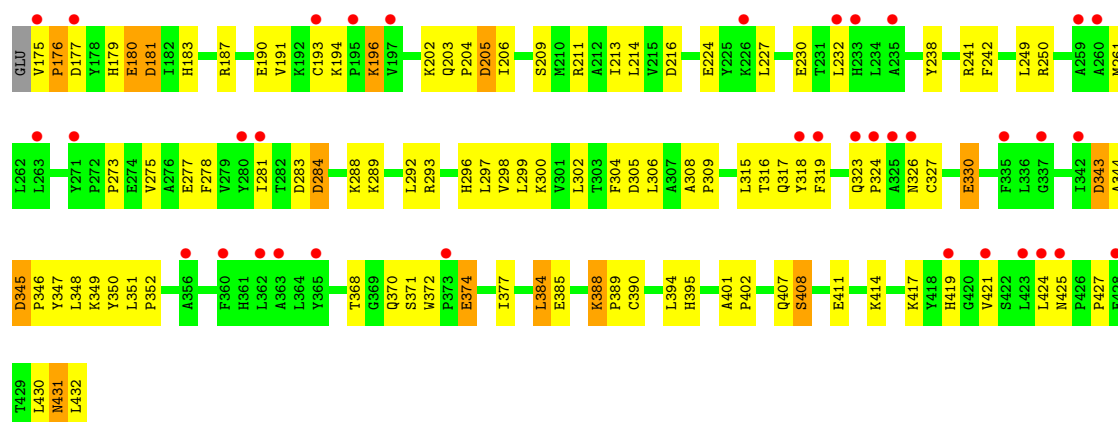
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C: 



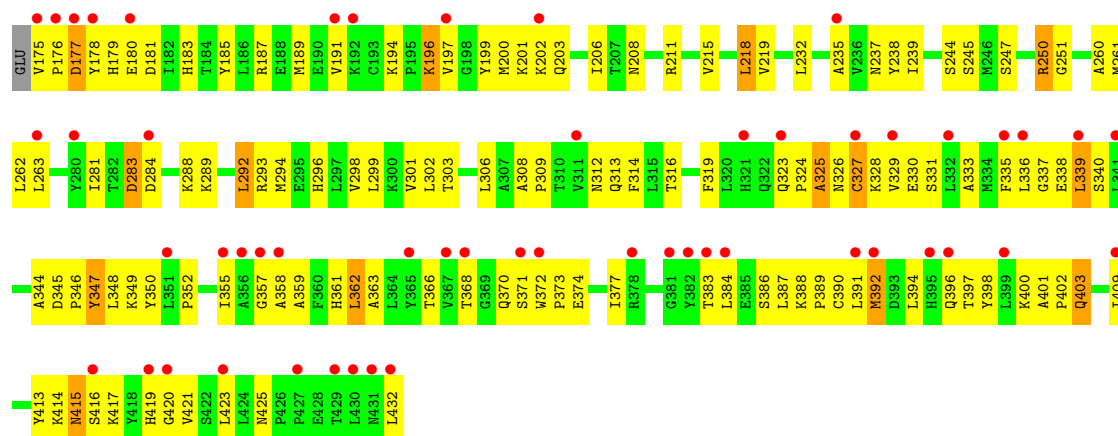
• Molecule 2: CYCLIN A2

Chain B: 



- Molecule 2: CYCLIN A2

Chain D:



- Molecule 3: RETINOBLASTOMA-ASSOCIATEDPROTEIN

Chain E:



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 0.296 , 0.306	Depositor DCC
R_{free} test set	2654 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)	0.33 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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.

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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	87	0	101	12	0
4	A	62	0	0	15	1
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (497) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:A:72:THR:HB	1:A:75:LYS:H	1.58	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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%)	6	7
1	C	274/303 (90%)	240 (88%)	25 (9%)	9 (3%)	6	7
2	B	256/259 (99%)	245 (96%)	7 (3%)	4 (2%)	14	23
2	D	256/259 (99%)	225 (88%)	26 (10%)	5 (2%)	11	17
3	E	8/11 (73%)	5 (62%)	2 (25%)	1 (12%)	1	0
All	All	1085/1135 (96%)	980 (90%)	76 (7%)	29 (3%)	8	10

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

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Mol	Chain	Res	Type
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%)	20	35
1	C	244/265 (92%)	229 (94%)	15 (6%)	26	46
2	B	232/233 (100%)	219 (94%)	13 (6%)	30	51
2	D	232/233 (100%)	217 (94%)	15 (6%)	24	42
3	E	10/11 (91%)	8 (80%)	2 (20%)	2	3
All	All	976/1007 (97%)	912 (93%)	64 (7%)	24	41

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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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 chains 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	10,10,11	15.53	5 (50%)	12,14,16	1.40	2 (16%)
1	TPO	C	160	1	10,10,11	14.79	5 (50%)	12,14,16	0.67	0

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	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	48.32	1.45	1.11
1	C	160	TPO	O-C	45.92	1.43	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	5.78	1.70	1.51
1	C	160	TPO	P-O1P	5.66	1.70	1.51
1	C	160	TPO	P-O3P	4.33	1.70	1.54
1	A	160	TPO	P-O2P	3.96	1.69	1.54
1	A	160	TPO	P-O3P	3.95	1.69	1.54
1	C	160	TPO	P-O2P	3.88	1.68	1.54
1	A	160	TPO	CA-C	3.29	1.54	1.48
1	C	160	TPO	CA-C	2.95	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	OG1-CB-CA	3.12	112.78	107.55
1	A	160	TPO	O3P-P-OG1	2.29	113.69	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	294/303 (97%)	0.80	21 (7%) 16 15	28, 40, 70, 79	0
1	C	279/303 (92%)	1.04	43 (15%) 3 2	38, 60, 99, 109	0
2	B	258/259 (99%)	1.07	36 (13%) 3 3	27, 42, 57, 76	0
2	D	258/259 (99%)	1.30	53 (20%) 1 1	36, 71, 107, 114	0
3	E	10/11 (90%)	1.84	2 (20%) 2 1	58, 65, 72, 73	0
All	All	1099/1135 (96%)	1.05	155 (14%) 3 3	27, 51, 98, 114	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	10.9
2	D	432	LEU	8.2
1	C	225	VAL	7.6
1	C	14	THR	6.1
1	C	227	TRP	6.0
2	D	323	GLN	5.8
1	A	40	GLU	5.5
2	B	175	VAL	5.4
2	D	372	TRP	5.3
1	C	223	ASP	5.1
1	A	39	THR	4.9
2	D	327	CYS	4.8
2	D	416	SER	4.7
2	D	335	PHE	4.6
2	D	175	VAL	4.5
2	D	368	THR	4.5
3	E	878	ASP	4.3
1	C	235	ASP	4.3
1	A	15	TYR	4.2
1	A	96	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	273	LYS	4.0
1	C	15	TYR	4.0
2	D	423	LEU	3.9
2	D	430	LEU	3.9
2	D	391	LEU	3.9
1	C	188	SER	3.9
1	C	230	VAL	3.7
2	D	351	LEU	3.6
1	C	259	GLY	3.6
2	D	357	GLY	3.6
2	B	424	LEU	3.5
2	D	356	ALA	3.5
3	E	869	PRO	3.5
2	B	428	GLU	3.5
2	D	197	VAL	3.4
2	B	425	ASN	3.4
2	D	378	ARG	3.3
1	C	221	THR	3.3
2	B	324	PRO	3.3
1	C	258	ASP	3.2
1	C	13	GLY	3.2
2	B	232	LEU	3.2
2	D	381	GLY	3.2
2	D	180	GLU	3.2
1	C	222	PRO	3.1
2	B	323	GLN	3.1
2	D	392	MET	3.1
1	C	109	PHE	3.1
2	B	356	ALA	3.1
2	D	280	TYR	3.1
2	D	339	LEU	3.0
1	C	187	TRP	3.0
2	D	395	HIS	3.0
2	B	197	VAL	3.0
1	C	269	TYR	3.0
2	D	384	LEU	2.9
1	C	11	GLY	2.9
2	D	399	LEU	2.9
2	D	176	PRO	2.9
2	D	178	TYR	2.9
2	D	419	HIS	2.8
1	C	233	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	179	TYR	2.8
1	A	19	TYR	2.8
2	B	260	ALA	2.8
2	D	177	ASP	2.8
1	C	260	ARG	2.8
1	A	36	ARG	2.7
2	B	335	PHE	2.7
1	A	161	HIS	2.7
1	C	282	ALA	2.7
2	B	365	TYR	2.7
2	D	235	ALA	2.7
1	A	0	SER	2.7
2	D	355	ILE	2.7
2	B	419	HIS	2.7
1	C	220	GLY	2.6
1	C	175	LEU	2.6
1	C	12	GLU	2.6
1	A	290	THR	2.6
1	C	174	LEU	2.6
1	C	253	PRO	2.5
1	A	229	GLY	2.5
1	A	95	ALA	2.5
2	D	367	VAL	2.5
1	C	108	LEU	2.5
1	C	17	VAL	2.5
2	B	325	ALA	2.5
1	C	257	GLU	2.4
2	D	311	VAL	2.4
2	B	195	PRO	2.4
2	B	193	CYS	2.4
1	A	186	ILE	2.4
2	B	342	ILE	2.4
2	D	365	TYR	2.4
2	D	284	ASP	2.4
2	B	263	LEU	2.4
2	D	332	LEU	2.4
1	C	191	CYS	2.4
2	D	431	ASN	2.4
1	C	254	PRO	2.3
2	B	259	ALA	2.3
2	D	321	HIS	2.3
1	A	269	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	382	TYR	2.3
2	D	420	GLY	2.3
1	A	111	LEU	2.3
1	A	293	VAL	2.3
2	D	396	GLN	2.3
2	B	360	PHE	2.3
2	B	226	LYS	2.2
1	C	143	LEU	2.2
2	B	319	PHE	2.2
2	B	271	TYR	2.2
2	B	280	TYR	2.2
1	A	187	TRP	2.2
2	D	358	ALA	2.2
1	C	228	PRO	2.2
1	C	231	THR	2.2
2	D	371	SER	2.2
2	B	281	ILE	2.2
1	C	219	LEU	2.2
2	B	326	ASN	2.2
2	B	373	PRO	2.2
2	D	427	PRO	2.2
2	D	336	LEU	2.2
2	D	202	LYS	2.2
1	C	37	LEU	2.1
2	D	409	ILE	2.1
1	C	36	ARG	2.1
1	A	225	VAL	2.1
1	C	9	LYS	2.1
1	C	156	VAL	2.1
2	D	383	THR	2.1
2	D	192	LYS	2.1
2	B	423	LEU	2.1
2	B	337	GLY	2.1
2	B	363	ALA	2.1
1	A	227	TRP	2.1
1	C	137	THR	2.1
2	B	233	HIS	2.1
2	D	429	THR	2.1
1	A	10	ILE	2.1
2	B	362	LEU	2.1
2	D	341	LEU	2.1
1	C	218	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	329	VAL	2.0
2	D	263	LEU	2.0
1	A	206	ASP	2.0
2	B	318	TYR	2.0
1	A	101	LEU	2.0
2	B	421	VAL	2.0
2	D	191	VAL	2.0
2	B	235	ALA	2.0
2	B	177	ASP	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.17	-0.65	57,62,66,66	0
1	TPO	A	160	11/12	0.14	-2.37	39,41,43,44	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.