



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 1H27 / pdb_00001h27
Title : CDK2/CyclinA in complex with an 11-residue recruitment peptide from p27
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 : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

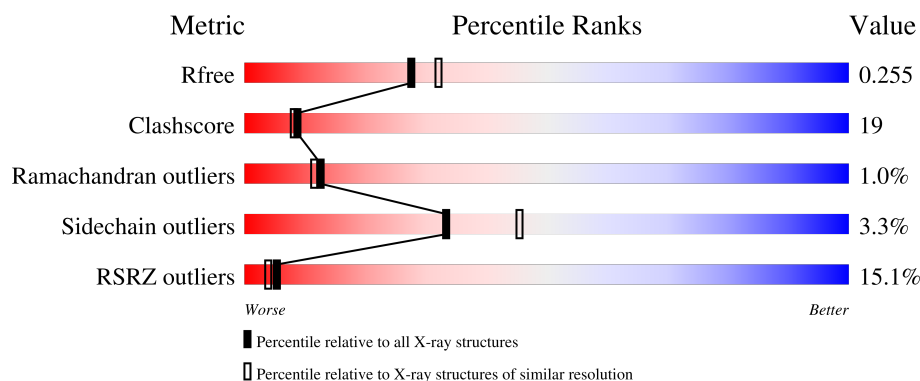
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	12% 67% 25% 5% ..
1	C	303	17% 63% 29%
2	B	259	2% 75% 23% .
2	D	259	27% 62% 35% .
3	E	11	55% 36% 18% 45%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	9	0	1
			2389	1550	405	425	1	8			
1	C	293	Total	C	N	O	P	S	0	0	1
			2342	1516	398	419	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
			2084	1350	339	384	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is a protein called CYCLIN-DEPENDENT KINASE INHIBITOR 1B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			50	32	10	8			

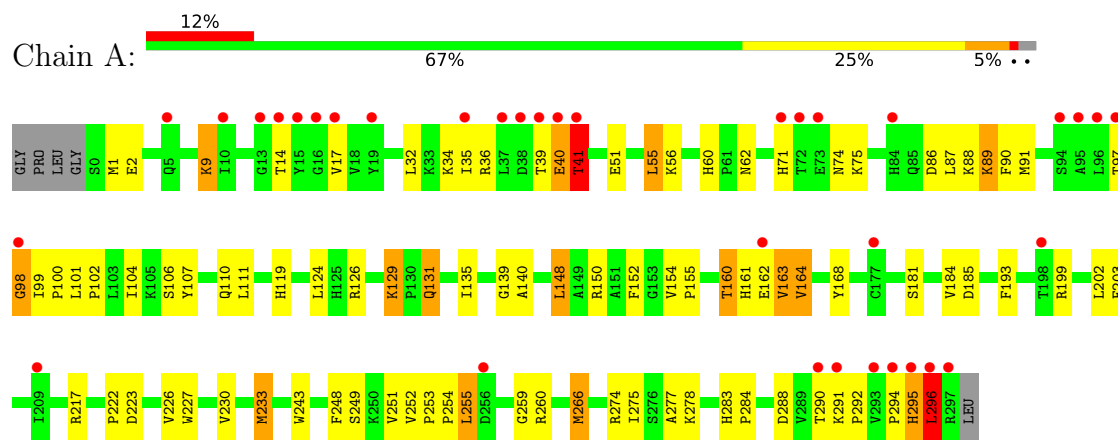
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	75	Total	O	0	0
			75	75		
4	C	45	Total	O	0	0
			45	45		
4	D	26	Total	O	0	0
			26	26		

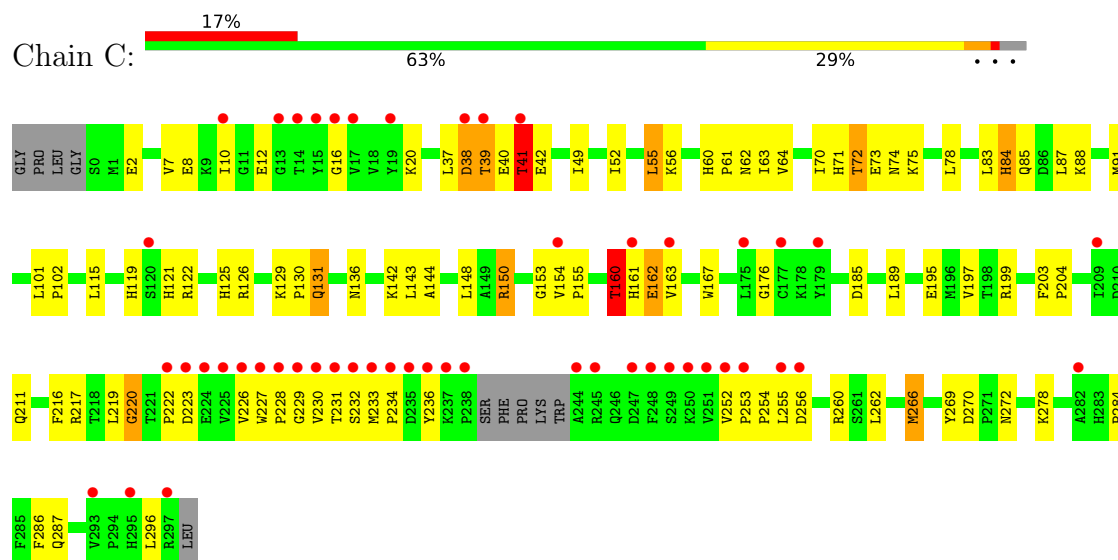
3 Residue-property plots

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

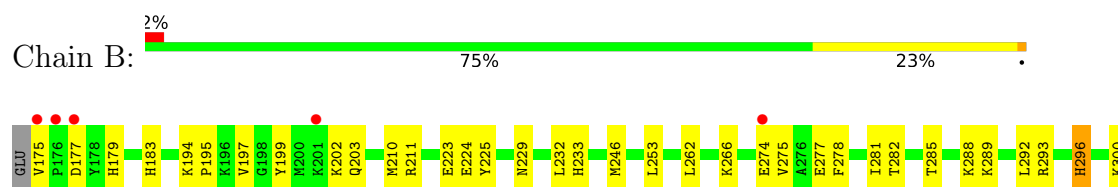
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 1: CELL DIVISION PROTEIN KINASE 2

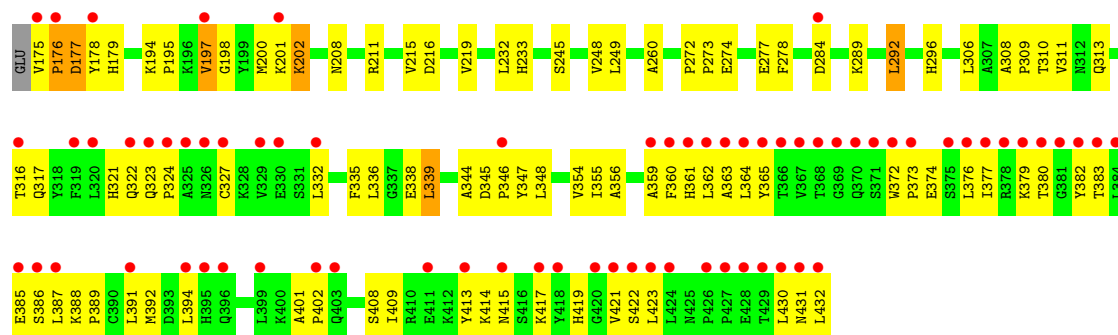


• Molecule 2: CYCLIN A2

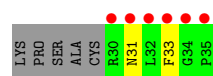
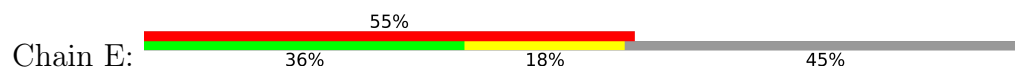




● Molecule 2: CYCLIN A2



● Molecule 3: CYCLIN-DEPENDENT KINASE INHIBITOR 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.69Å 133.55Å 148.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.20 29.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.75-2.20) 98.6 (29.75-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.269 0.229 , 0.255	Depositor DCC
R_{free} test set	3715 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9182	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.14	7/2439 (0.3%)	1.05	6/3310 (0.2%)
1	C	0.97	4/2387 (0.2%)	0.99	1/3237 (0.0%)
2	B	1.12	2/2134 (0.1%)	1.02	2/2897 (0.1%)
2	D	0.90	1/2134 (0.0%)	0.94	1/2897 (0.0%)
3	E	0.38	0/51	0.48	0/66
All	All	1.04	14/9145 (0.2%)	1.00	10/12407 (0.1%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	MET	SD-CE	-7.52	1.60	1.79
1	C	41	THR	CA-C	7.17	1.55	1.52
1	A	296	LEU	C-N	-6.88	1.23	1.33
1	C	296	LEU	C-N	-6.17	1.24	1.33
2	B	246	MET	SD-CE	-5.98	1.64	1.79
1	C	266	MET	SD-CE	-5.86	1.64	1.79
1	A	266	MET	SD-CE	5.80	1.94	1.79
1	C	70	ILE	CA-CB	-5.80	1.47	1.54
2	D	260	ALA	CA-CB	-5.69	1.44	1.53
1	A	275	ILE	CA-CB	-5.41	1.48	1.54
2	B	312	ASN	N-CA	-5.20	1.40	1.46
1	A	185	ASP	C-O	-5.17	1.18	1.24
1	A	277	ALA	CA-CB	-5.04	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	LYS	C-N	5.03	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	LYS	N-CA-C	-7.48	101.40	108.13
1	A	163	VAL	N-CA-C	6.41	117.93	108.45
1	C	72	THR	N-CA-C	-5.64	100.56	108.96
2	D	339	LEU	N-CA-C	-5.57	105.36	111.82
1	A	295	HIS	N-CA-C	-5.36	105.97	113.37
2	B	197	VAL	CB-CA-C	-5.33	105.06	112.04
2	B	211	ARG	N-CA-C	-5.24	105.68	111.71
1	A	193	PHE	N-CA-C	-5.17	105.53	111.07
1	A	40	GLU	N-CA-C	-5.16	105.87	113.72
1	A	168	TYR	N-CA-C	-5.04	106.05	113.61

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	160	TPO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2430	104	0
1	C	2342	0	2385	108	0
2	B	2084	0	2107	66	0
2	D	2084	0	2107	89	0
3	E	50	0	48	3	0
4	A	87	0	0	13	0
4	B	75	0	0	6	0
4	C	45	0	0	3	0
4	D	26	0	0	2	0
All	All	9182	0	9077	336	0

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 19.

All (336) 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:A:230:VAL:HA	1:A:233:MET:HE2	1.21	1.18
2:B:177:ASP:HB2	4:B:2008:HOH:O	1.48	1.13
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.76	1.02
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.79	1.00
1:A:71:HIS:NE2	2:B:296:HIS:NE2	2.11	0.98
2:B:199:TYR:HA	2:B:202:LYS:HE2	1.50	0.94
1:A:71:HIS:NE2	2:B:296:HIS:CD2	2.36	0.92
2:D:388:LYS:HG3	2:D:432:LEU:HD13	1.53	0.91
1:A:230:VAL:CA	1:A:233:MET:HE2	2.01	0.90
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.40	0.90
1:A:106:SER:HB2	1:A:290:THR:O	1.71	0.89
1:A:154:VAL:O	2:B:316:THR:CG2	2.20	0.89
1:C:284:PRO:HA	1:C:287:GLN:HG2	1.56	0.88
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.55	0.88
1:A:154:VAL:O	2:B:316:THR:HG22	1.75	0.86
1:C:60:HIS:HD2	1:C:62:ASN:H	1.23	0.86
1:C:39:THR:N	4:C:2012:HOH:O	1.87	0.85
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.43	0.84
1:A:294:PRO:C	1:A:296:LEU:H	1.86	0.84
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.59	0.82
1:A:39:THR:HG21	2:B:289:LYS:NZ	1.94	0.82
2:D:284:ASP:N	4:D:2021:HOH:O	2.05	0.82
1:C:38:ASP:O	1:C:39:THR:CB	2.25	0.82
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.61	0.82
2:B:175:VAL:N	2:B:179:HIS:CE1	2.48	0.81
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.49	0.80
1:C:37:LEU:O	1:C:38:ASP:HB2	1.81	0.79
1:C:60:HIS:CD2	1:C:62:ASN:H	2.00	0.79
1:A:163:VAL:HG23	4:A:2021:HOH:O	1.81	0.79
2:D:197:VAL:HG13	2:D:198:GLY:N	1.98	0.78
1:C:38:ASP:O	1:C:39:THR:OG1	2.03	0.77
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.68	0.75
1:C:64:VAL:HG23	1:C:143:LEU:O	1.87	0.75
2:D:313:GLN:O	2:D:316:THR:HG22	1.87	0.74
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.16	0.74
1:C:256:ASP:O	1:C:260:ARG:HG3	1.87	0.74
2:D:387:LEU:O	2:D:391:LEU:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:H	1:C:226:VAL:HG12	1.52	0.74
1:C:160:TPO:N	1:C:160:TPO:O2P	2.16	0.73
1:A:107:TYR:OH	1:A:135:ILE:HD13	1.88	0.73
1:A:39:THR:HG21	2:B:289:LYS:CD	2.19	0.72
1:A:148:LEU:HD12	4:A:2027:HOH:O	1.90	0.71
2:D:322:GLN:HG2	2:D:324:PRO:O	1.90	0.70
1:C:262:LEU:HG	1:C:266:MET:HE2	1.73	0.70
2:B:334:MET:HE1	4:B:2024:HOH:O	1.91	0.69
1:C:39:THR:O	1:C:40:GLU:HB2	1.93	0.68
1:C:84:HIS:CD2	1:C:85:GLN:HG2	2.28	0.68
2:D:201:LYS:HD3	2:D:201:LYS:C	2.18	0.68
2:B:175:VAL:N	2:B:179:HIS:HE1	1.90	0.68
1:A:51:GLU:O	1:A:55:LEU:HB2	1.94	0.68
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.29	0.67
1:A:60:HIS:CD2	1:A:62:ASN:H	2.13	0.67
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.60	0.66
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.78	0.66
1:C:12:GLU:HG3	1:C:16:GLY:O	1.96	0.66
1:C:154:VAL:O	2:D:316:THR:HG23	1.96	0.66
2:B:203:GLN:O	4:B:2018:HOH:O	2.14	0.65
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.62	0.65
1:A:223:ASP:H	1:A:226:VAL:HG12	1.62	0.65
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.77	0.64
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.33	0.64
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.79	0.64
1:A:296:LEU:CD1	4:A:2006:HOH:O	2.45	0.64
2:D:413:TYR:O	2:D:422:SER:OG	2.14	0.63
1:C:38:ASP:C	1:C:39:THR:OG1	2.41	0.63
2:D:389:PRO:O	2:D:392:MET:HB2	1.99	0.63
2:B:293:ARG:HD3	1:C:2:GLU:OE1	1.99	0.62
1:A:88:LYS:C	1:A:90:PHE:H	2.08	0.62
1:A:161:HIS:HD2	4:A:2009:HOH:O	1.81	0.61
1:C:155:PRO:HD2	2:D:316:THR:OG1	1.99	0.61
1:A:2:GLU:OE1	1:C:73:GLU:OE2	2.17	0.61
4:A:2045:HOH:O	2:B:175:VAL:HG22	2.00	0.61
1:C:162:GLU:H	1:C:162:GLU:CD	2.08	0.61
1:A:97:THR:HG23	1:A:97:THR:O	1.99	0.61
1:C:230:VAL:HA	1:C:233:MET:HE2	1.82	0.60
2:D:197:VAL:CG1	2:D:198:GLY:N	2.64	0.60
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.36	0.60
2:B:210:MET:HB3	3:E:33:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:HA	1:C:233:MET:CE	2.30	0.60
2:B:175:VAL:HG23	2:B:175:VAL:O	2.02	0.60
1:A:290:THR:C	1:A:292:PRO:HD3	2.26	0.60
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.83	0.60
2:D:197:VAL:HG13	2:D:198:GLY:H	1.67	0.59
2:B:253:LEU:HD23	3:E:33:PHE:CZ	2.38	0.59
1:C:39:THR:CA	4:C:2012:HOH:O	2.40	0.59
1:A:71:HIS:NE2	2:B:296:HIS:CG	2.71	0.59
1:C:39:THR:O	1:C:40:GLU:CB	2.49	0.59
1:C:129:LYS:HG3	1:C:131:GLN:HG2	1.83	0.59
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.84	0.59
1:C:64:VAL:HG21	1:C:144:ALA:CB	2.30	0.58
1:A:154:VAL:O	2:B:316:THR:HG23	2.04	0.58
1:C:84:HIS:HD2	1:C:85:GLN:HG2	1.69	0.58
1:A:39:THR:C	1:A:41:THR:H	2.12	0.58
1:A:39:THR:HG22	1:A:40:GLU:H	1.69	0.57
2:B:396:GLN:HB3	2:B:400:LYS:HE2	1.87	0.57
2:B:392:MET:HE2	2:B:392:MET:HA	1.85	0.57
2:D:373:PRO:O	2:D:377:ILE:HG13	2.05	0.57
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.57
1:A:296:LEU:HD12	4:A:2006:HOH:O	2.03	0.57
1:A:39:THR:HG21	2:B:289:LYS:HZ2	1.67	0.56
2:B:275:VAL:HG11	2:B:292:LEU:HD11	1.86	0.56
1:C:38:ASP:O	1:C:39:THR:HB	2.04	0.56
1:A:260:ARG:HD3	4:A:2067:HOH:O	2.05	0.56
1:C:121:HIS:O	1:C:122:ARG:HG3	2.06	0.56
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.32	0.56
2:B:274:GLU:HG2	2:B:277:GLU:HG3	1.87	0.56
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.41	0.56
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.87	0.56
1:A:101:LEU:N	1:A:102:PRO:CD	2.68	0.56
1:A:288:ASP:HB3	4:A:2085:HOH:O	2.04	0.55
2:D:233:HIS:HD2	4:D:2024:HOH:O	1.89	0.55
1:C:230:VAL:HG23	1:C:231:THR:H	1.71	0.55
1:A:294:PRO:C	1:A:296:LEU:N	2.54	0.55
4:A:2045:HOH:O	2:B:175:VAL:CG2	2.55	0.55
2:D:361:HIS:O	2:D:362:LEU:C	2.50	0.55
2:B:233:HIS:HD2	4:B:2042:HOH:O	1.89	0.55
1:A:88:LYS:C	1:A:90:PHE:N	2.65	0.54
1:A:39:THR:HG21	2:B:289:LYS:CE	2.37	0.54
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ILE:CD1	1:C:78:LEU:HD21	2.35	0.54
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.88	0.54
1:A:56:LYS:NZ	2:B:303:THR:O	2.40	0.54
1:A:139:GLY:HA2	1:A:294:PRO:HD3	1.88	0.54
2:B:338:GLU:OE2	2:B:413:TYR:OH	2.26	0.54
1:C:121:HIS:C	1:C:122:ARG:HG3	2.33	0.54
2:D:415:ASN:OD1	2:D:417:LYS:N	2.22	0.53
1:A:99:ILE:HG22	1:A:104:ILE:HG13	1.90	0.53
1:C:153:GLY:O	1:C:155:PRO:C	2.52	0.53
1:A:97:THR:C	1:A:98:GLY:O	2.50	0.53
2:D:176:PRO:HA	2:D:179:HIS:CE1	2.44	0.53
2:D:389:PRO:O	2:D:392:MET:N	2.41	0.53
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.90	0.53
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.36	0.53
2:B:288:LYS:O	2:B:292:LEU:HD13	2.08	0.53
1:C:40:GLU:OE2	2:D:289:LYS:NZ	2.43	0.52
1:C:262:LEU:HG	1:C:266:MET:CE	2.39	0.52
1:A:39:THR:HG22	1:A:40:GLU:N	2.24	0.52
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.92	0.52
1:A:230:VAL:HA	1:A:233:MET:CE	2.15	0.52
2:D:414:LYS:HE2	2:D:423:LEU:HD21	1.92	0.52
1:C:83:LEU:HD23	1:C:136:ASN:HB3	1.92	0.51
1:C:219:LEU:O	1:C:220:GLY:O	2.27	0.51
1:C:223:ASP:H	1:C:226:VAL:CG1	2.20	0.51
1:C:262:LEU:CG	1:C:266:MET:HE2	2.39	0.51
1:C:61:PRO:O	1:C:142:LYS:HE2	2.11	0.51
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.69	0.51
1:C:284:PRO:CA	1:C:287:GLN:HG2	2.36	0.51
1:A:295:HIS:O	1:A:296:LEU:CB	2.59	0.50
1:C:10:ILE:HD11	1:C:20:LYS:HB2	1.94	0.50
1:A:253:PRO:N	1:A:254:PRO:CD	2.75	0.50
1:C:74:ASN:ND2	4:C:2025:HOH:O	2.45	0.50
2:D:175:VAL:N	2:D:176:PRO:HD3	2.27	0.50
1:A:227:TRP:HB3	1:A:230:VAL:HG13	1.93	0.50
1:C:231:THR:HA	1:C:236:TYR:CD1	2.47	0.50
2:D:211:ARG:HD3	2:D:344:ALA:HB2	1.94	0.50
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.42	0.50
1:A:119:HIS:HD2	4:B:2009:HOH:O	1.95	0.50
2:D:430:LEU:O	2:D:431:ASN:HB2	2.12	0.50
1:A:296:LEU:HD11	4:A:2006:HOH:O	2.08	0.49
1:C:230:VAL:HG23	1:C:231:THR:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:O	1:C:40:GLU:CD	2.55	0.49
1:C:219:LEU:HB2	1:C:269:TYR:OH	2.12	0.49
1:A:148:LEU:HB3	4:A:2027:HOH:O	2.12	0.49
2:B:199:TYR:CD1	2:B:199:TYR:C	2.90	0.49
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.96	0.49
2:D:197:VAL:CG1	2:D:198:GLY:H	2.25	0.49
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.99	0.49
1:C:7:VAL:O	1:C:8:GLU:HB3	2.12	0.49
1:A:160:TPO:O3P	1:A:160:TPO:N	2.39	0.48
2:D:176:PRO:HA	2:D:179:HIS:CG	2.48	0.48
1:A:39:THR:C	1:A:41:THR:N	2.70	0.48
1:A:106:SER:OG	1:A:291:LYS:HA	2.13	0.48
1:C:41:THR:HB	1:C:42:GLU:H	1.55	0.48
1:A:71:HIS:CE1	2:B:300:LYS:HG3	2.48	0.48
1:C:125:HIS:O	1:C:126:ARG:HB2	2.14	0.48
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.95	0.48
1:A:86:ASP:C	1:A:86:ASP:OD1	2.56	0.48
1:A:107:TYR:CZ	1:A:135:ILE:HD13	2.48	0.48
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.28	0.48
1:A:98:GLY:HA3	1:A:199:ARG:NH2	2.29	0.47
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.95	0.47
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.28	0.47
1:A:290:THR:O	1:A:292:PRO:HD3	2.13	0.47
2:D:361:HIS:O	2:D:363:ALA:N	2.47	0.47
1:C:101:LEU:O	1:C:101:LEU:HG	2.14	0.47
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.49	0.47
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.96	0.47
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.49	0.47
2:D:354:VAL:O	2:D:355:ILE:C	2.57	0.47
2:D:345:ASP:HA	2:D:346:PRO:HA	1.69	0.47
2:B:285:THR:HG23	3:E:31:ASN:ND2	2.30	0.47
1:C:203:PHE:HB3	1:C:211:GLN:NE2	2.30	0.47
1:A:249:SER:HA	4:A:2067:HOH:O	2.13	0.46
2:D:321:HIS:HE1	2:D:379:LYS:HD2	1.79	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.75	0.46
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.71	0.46
2:D:388:LYS:O	2:D:392:MET:N	2.48	0.46
2:D:201:LYS:HD3	2:D:201:LYS:O	2.15	0.46
1:A:227:TRP:CG	1:A:230:VAL:HG13	2.50	0.46
1:C:60:HIS:HB3	1:C:63:ILE:HD12	1.97	0.46
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.97	0.46
1:A:107:TYR:O	1:A:111:LEU:HG	2.16	0.46
1:A:106:SER:CB	1:A:290:THR:O	2.54	0.46
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.51	0.46
2:B:417:LYS:HE3	2:B:418:TYR:OH	2.15	0.46
2:D:194:LYS:CE	2:D:195:PRO:HD2	2.46	0.46
1:C:38:ASP:C	1:C:39:THR:HG1	2.18	0.46
2:D:215:VAL:O	2:D:219:VAL:HG23	2.15	0.46
2:D:372:TRP:CD1	2:D:377:ILE:HG12	2.51	0.46
1:C:222:PRO:HB3	1:C:269:TYR:CD2	2.51	0.46
1:C:227:TRP:HB3	1:C:230:VAL:HG13	1.98	0.45
2:D:216:ASP:OD2	2:D:408:SER:HB2	2.16	0.45
1:A:87:LEU:O	1:A:91:MET:HG3	2.16	0.45
2:B:183:HIS:HB2	2:B:317:GLN:NE2	2.30	0.45
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.78	0.45
2:D:274:GLU:HG2	2:D:277:GLU:OE2	2.17	0.45
1:A:106:SER:CB	1:A:292:PRO:HD2	2.46	0.45
1:C:87:LEU:HG	1:C:91:MET:HE2	1.99	0.45
1:C:230:VAL:C	1:C:232:SER:H	2.24	0.45
2:B:229:ASN:ND2	2:B:334:MET:HE2	2.23	0.45
2:D:313:GLN:O	2:D:316:THR:CG2	2.63	0.45
1:A:202:LEU:HD23	1:A:203:PHE:CE2	2.52	0.44
2:D:200:MET:HG2	2:D:208:ASN:OD1	2.16	0.44
1:A:39:THR:CG2	2:B:289:LYS:NZ	2.75	0.44
2:D:248:VAL:HG12	2:D:249:LEU:O	2.17	0.44
2:B:175:VAL:C	2:B:179:HIS:CE1	2.95	0.44
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.78	0.44
1:A:148:LEU:HD13	1:A:148:LEU:HA	1.89	0.44
2:D:388:LYS:HE3	2:D:432:LEU:HB3	1.98	0.44
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.98	0.44
1:C:203:PHE:CB	1:C:211:GLN:HE22	2.31	0.44
2:D:361:HIS:C	2:D:363:ALA:N	2.75	0.44
1:A:97:THR:O	1:A:98:GLY:O	2.35	0.44
2:B:316:THR:HG21	4:B:2003:HOH:O	2.18	0.44
2:D:401:ALA:N	2:D:402:PRO:CD	2.80	0.44
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.82	0.44
1:A:140:ALA:HA	1:A:291:LYS:HE3	2.00	0.44
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.99	0.44
2:D:365:TYR:O	2:D:365:TYR:CG	2.70	0.44
1:A:223:ASP:H	1:A:226:VAL:CG1	2.30	0.43
2:D:361:HIS:O	2:D:364:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.43
1:C:195:GLU:O	1:C:199:ARG:N	2.47	0.43
1:A:88:LYS:HD2	1:A:131:GLN:OE1	2.18	0.43
2:D:380:THR:HB	2:D:382:TYR:CD2	2.53	0.43
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.48	0.43
2:D:308:ALA:O	2:D:313:GLN:NE2	2.51	0.43
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.00	0.43
1:C:161:HIS:O	1:C:163:VAL:HG12	2.17	0.43
1:A:181:SER:O	1:A:184:VAL:HG22	2.18	0.43
1:C:217:ARG:HH11	1:C:217:ARG:HB3	1.83	0.43
1:A:9:LYS:HE3	1:A:17:VAL:HG13	2.01	0.43
1:C:217:ARG:HB3	1:C:217:ARG:NH1	2.34	0.43
2:D:175:VAL:O	2:D:177:ASP:N	2.46	0.43
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.33	0.43
1:A:278:LYS:HD2	2:B:177:ASP:OD1	2.18	0.43
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.54	0.43
2:D:338:GLU:HB3	2:D:409:ILE:HD13	2.00	0.43
1:A:249:SER:HA	1:A:260:ARG:HD3	2.01	0.42
1:C:52:ILE:O	1:C:56:LYS:HG3	2.19	0.42
2:D:388:LYS:N	2:D:389:PRO:CD	2.82	0.42
1:A:288:ASP:OD1	1:A:288:ASP:N	2.49	0.42
1:C:216:PHE:O	1:C:220:GLY:N	2.52	0.42
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.54	0.42
2:D:392:MET:HE3	2:D:432:LEU:HD12	2.01	0.42
1:C:39:THR:C	1:C:41:THR:H	2.26	0.42
1:A:154:VAL:HA	1:A:155:PRO:HA	1.89	0.42
2:B:223:GLU:O	2:B:224:GLU:C	2.61	0.42
1:C:126:ARG:CD	1:C:163:VAL:HG21	2.45	0.42
2:D:360:PHE:CE2	2:D:376:LEU:HD11	2.55	0.42
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.92	0.42
2:D:310:THR:O	2:D:311:VAL:C	2.62	0.42
1:A:34:LYS:HG2	1:A:35:ILE:N	2.34	0.42
2:D:202:LYS:HA	2:D:202:LYS:HD2	1.78	0.42
2:D:316:THR:HG23	2:D:317:GLN:N	2.35	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.74	0.42
1:C:62:ASN:HA	1:C:142:LYS:HG2	2.01	0.42
1:C:229:GLY:O	1:C:233:MET:HG3	2.20	0.42
1:A:97:THR:O	1:A:97:THR:CG2	2.65	0.42
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.49	0.42
2:D:383:THR:C	2:D:385:GLU:N	2.75	0.42
1:C:286:PHE:O	1:C:287:GLN:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.54	0.41
1:A:266:MET:O	1:A:274:ARG:HD3	2.20	0.41
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.01	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41
2:D:327:CYS:HG	2:D:419:HIS:CD2	2.38	0.41
1:C:49:ILE:CG2	2:D:306:LEU:HD12	2.51	0.41
1:C:155:PRO:HD2	2:D:316:THR:HG1	1.84	0.41
1:A:88:LYS:O	1:A:90:PHE:N	2.53	0.41
2:B:345:ASP:HA	2:B:346:PRO:HA	1.74	0.41
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.72	0.41
1:C:227:TRP:HB3	1:C:230:VAL:CG1	2.49	0.41
2:D:383:THR:O	2:D:386:SER:OG	2.33	0.41
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.35	0.41
1:A:101:LEU:N	1:A:102:PRO:HD2	2.36	0.41
1:A:161:HIS:CD2	4:A:2009:HOH:O	2.63	0.41
1:A:163:VAL:HG22	1:A:164:VAL:N	2.35	0.41
1:C:60:HIS:HD2	1:C:62:ASN:N	2.04	0.41
1:C:71:HIS:C	1:C:72:THR:CG2	2.94	0.41
1:C:154:VAL:HA	1:C:155:PRO:HA	1.84	0.41
2:D:175:VAL:O	2:D:179:HIS:CE1	2.74	0.41
1:A:100:PRO:O	1:A:101:LEU:C	2.64	0.41
2:B:388:LYS:O	2:B:392:MET:HG2	2.21	0.41
1:C:131:GLN:CD	1:C:131:GLN:H	2.28	0.41
2:D:273:PRO:HB2	2:D:278:PHE:CE2	2.56	0.41
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.55	0.41
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.07	0.41
1:A:106:SER:O	1:A:110:GLN:HG3	2.20	0.41
1:A:227:TRP:O	1:A:230:VAL:HG22	2.21	0.41
1:A:255:LEU:HG	1:A:259:GLY:HA3	2.03	0.41
2:B:282:THR:O	2:B:285:THR:OG1	2.22	0.41
2:D:332:LEU:HD13	2:D:421:VAL:HB	2.03	0.41
1:A:126:ARG:HD2	1:A:163:VAL:HG21	2.03	0.41
1:A:162:GLU:CD	1:A:162:GLU:N	2.79	0.41
1:A:222:PRO:HA	1:A:226:VAL:HG11	2.02	0.41
1:C:176:GLY:O	1:C:234:PRO:HG2	2.22	0.41
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	0.40
2:B:289:LYS:HE2	2:B:293:ARG:HH21	1.87	0.40
1:C:270:ASP:OD1	1:C:272:ASN:N	2.54	0.40
1:C:278:LYS:HE2	2:D:178:TYR:CE1	2.56	0.40
2:D:311:VAL:HG13	2:D:356:ALA:HB2	2.02	0.40
2:B:194:LYS:HD2	2:B:351:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:ND1	1:C:161:HIS:C	2.79	0.40
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.56	0.40
2:D:272:PRO:HA	2:D:273:PRO:HD3	2.00	0.40
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.90	0.40
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.98	0.40
2:D:372:TRP:HA	2:D:373:PRO:HD2	1.94	0.40
2:D:383:THR:C	2:D:385:GLU:H	2.30	0.40
2:D:383:THR:O	2:D:386:SER:N	2.54	0.40
1:C:150:ARG:HH21	1:C:160:TPO:P	2.45	0.40
1:C:284:PRO:HA	1:C:287:GLN:HE21	1.86	0.40
2:D:292:LEU:HD12	2:D:292:LEU:HA	1.88	0.40
2:D:359:ALA:HA	2:D:394:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/303 (97%)	277 (94%)	14 (5%)	4 (1%)	9	7
1	C	288/303 (95%)	267 (93%)	16 (6%)	5 (2%)	7	5
2	B	256/259 (99%)	253 (99%)	3 (1%)	0	100	100
2	D	256/259 (99%)	236 (92%)	18 (7%)	2 (1%)	16	16
3	E	4/11 (36%)	3 (75%)	1 (25%)	0	100	100
All	All	1099/1135 (97%)	1036 (94%)	52 (5%)	11 (1%)	12	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	197	VAL
1	A	98	GLY

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Mol	Chain	Res	Type
1	A	164	VAL
1	C	84	HIS
1	C	162	GLU
1	C	220	GLY
1	C	38	ASP
1	A	41	THR
1	A	296	LEU
2	D	176	PRO
1	C	228	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/265 (98%)	249 (95%)	12 (5%)	24	32
1	C	256/265 (97%)	248 (97%)	8 (3%)	35	48
2	B	232/233 (100%)	225 (97%)	7 (3%)	36	49
2	D	232/233 (100%)	226 (97%)	6 (3%)	40	55
3	E	5/9 (56%)	5 (100%)	0	100	100
All	All	986/1005 (98%)	953 (97%)	33 (3%)	33	45

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	14	THR
1	A	41	THR
1	A	55	LEU
1	A	74	ASN
1	A	75	LYS
1	A	89	LYS
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	248	PHE
1	A	255	LEU
2	B	232	LEU
2	B	296	HIS
2	B	316	THR
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
2	B	416	SER
1	C	39	THR
1	C	41	THR
1	C	55	LEU
1	C	75	LYS
1	C	88	LYS
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
2	D	177	ASP
2	D	202	LYS
2	D	232	LEU
2	D	245	SER
2	D	292	LEU
2	D	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	85	GLN
1	A	119	HIS
1	A	265	GLN
1	A	268	HIS
2	B	179	HIS
2	B	229	ASN
2	B	254	GLN
2	B	312	ASN
2	B	317	GLN
2	B	431	ASN
1	C	60	HIS
1	C	71	HIS
1	C	84	HIS

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	119	HIS
1	C	121	HIS
1	C	211	GLN
1	C	265	GLN
1	C	268	HIS
1	C	287	GLN
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	326	ASN
2	D	361	HIS
2	D	396	GLN
2	D	403	GLN
2	D	431	ASN
3	E	31	ASN

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	3.24	4 (50%)	10,14,16	2.16	2 (20%)
1	TPO	C	160	1	8,10,11	3.55	4 (50%)	10,14,16	3.06	4 (40%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	6.34	1.44	1.20
1	A	160	TPO	O-C	5.97	1.42	1.20
1	C	160	TPO	P-O1P	5.36	1.67	1.50
1	A	160	TPO	P-O1P	4.34	1.64	1.50
1	C	160	TPO	P-O2P	3.92	1.69	1.54
1	A	160	TPO	P-O2P	3.76	1.68	1.54
1	A	160	TPO	P-O3P	3.52	1.67	1.54
1	C	160	TPO	P-O3P	3.50	1.67	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O2P-P-OG1	-6.37	81.02	105.85
1	C	160	TPO	O-C-CA	-4.82	112.38	124.77
1	A	160	TPO	O-C-CA	-4.38	113.52	124.77
1	A	160	TPO	O3P-P-OG1	-3.97	90.37	105.85
1	C	160	TPO	O3P-P-O2P	3.12	119.52	107.80
1	C	160	TPO	O2P-P-O1P	2.90	122.13	110.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB
1	A	160	TPO	C-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/303 (97%)	0.42	35 (11%) 9 7	20, 33, 82, 103	0
1	C	292/303 (96%)	0.92	50 (17%) 4 3	27, 47, 121, 150	0
2	B	258/259 (99%)	-0.01	6 (2%) 61 58	21, 33, 55, 86	0
2	D	258/259 (99%)	1.25	71 (27%) 1 1	24, 52, 116, 146	0
3	E	6/11 (54%)	4.90	6 (100%) 0 0	142, 143, 148, 149	0
All	All	1110/1135 (97%)	0.67	168 (15%) 5 4	20, 40, 106, 150	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	9.8
1	A	97	THR	7.5
1	C	244	ALA	7.5
1	C	238	PRO	7.3
3	E	32	LEU	6.8
2	D	424	LEU	6.3
2	D	175	VAL	6.2
1	A	294	PRO	6.1
2	D	178	TYR	6.1
1	C	225	VAL	6.0
3	E	33	PHE	5.7
1	C	15	TYR	5.6
2	D	421	VAL	5.6
2	D	284	ASP	5.5
1	A	293	VAL	5.5
1	C	226	VAL	5.5
2	D	426	PRO	5.5
2	D	420	GLY	5.3
1	A	95	ALA	5.2
1	A	96	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	430	LEU	5.0
1	C	38	ASP	5.0
3	E	30	ARG	4.9
2	B	175	VAL	4.8
1	C	161	HIS	4.8
2	D	176	PRO	4.7
2	B	176	PRO	4.7
2	D	365	TYR	4.5
1	A	296	LEU	4.5
1	C	251	VAL	4.4
2	D	423	LEU	4.4
3	E	31	ASN	4.4
2	D	427	PRO	4.3
2	D	367	VAL	4.1
2	D	428	GLU	4.1
1	A	71	HIS	4.0
2	B	432	LEU	4.0
3	E	34	GLY	3.9
1	A	17	VAL	3.9
1	C	17	VAL	3.9
1	A	37	LEU	3.9
1	C	249	SER	3.9
2	D	375	SER	3.9
1	C	248	PHE	3.8
2	D	320	LEU	3.8
1	C	234	PRO	3.8
3	E	35	PRO	3.8
2	D	368	THR	3.7
2	D	325	ALA	3.7
2	D	363	ALA	3.7
1	C	235	ASP	3.6
1	A	295	HIS	3.6
2	D	431	ASN	3.6
2	D	372	TRP	3.6
1	C	233	MET	3.5
1	C	163	VAL	3.5
1	C	231	THR	3.5
2	D	364	LEU	3.5
1	C	229	GLY	3.5
2	D	382	TYR	3.5
2	D	324	PRO	3.4
1	C	14	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	250	LYS	3.4
2	D	197	VAL	3.4
1	A	41	THR	3.4
2	D	373	PRO	3.4
2	D	379	LYS	3.3
1	C	230	VAL	3.3
1	C	223	ASP	3.3
1	A	39	THR	3.3
2	D	418	TYR	3.3
2	D	432	LEU	3.2
2	D	384	LEU	3.2
1	A	98	GLY	3.1
2	D	402	PRO	3.1
1	C	41	THR	3.1
2	D	366	THR	3.1
2	D	327	CYS	3.1
1	C	297	ARG	3.1
1	A	13	GLY	3.0
1	C	237	LYS	3.0
2	D	386	SER	3.0
1	C	252	VAL	3.0
1	C	16	GLY	3.0
2	D	322	GLN	2.9
1	A	15	TYR	2.9
2	D	329	VAL	2.9
1	C	10	ILE	2.9
2	D	429	THR	2.9
1	C	236	TYR	2.8
2	D	399	LEU	2.8
1	C	227	TRP	2.8
2	D	371	SER	2.8
1	C	293	VAL	2.8
1	C	228	PRO	2.8
1	A	19	TYR	2.8
1	C	13	GLY	2.7
1	C	245	ARG	2.7
2	D	395	HIS	2.7
1	C	209	ILE	2.7
2	D	369	GLY	2.7
2	D	413	TYR	2.7
1	C	295	HIS	2.7
2	D	381	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLU	2.7
2	D	376	LEU	2.7
1	C	39	THR	2.7
2	D	316	THR	2.7
2	D	326	ASN	2.7
1	C	222	PRO	2.7
2	B	177	ASP	2.6
2	D	385	GLU	2.6
1	A	72	THR	2.6
2	D	362	LEU	2.6
1	C	120	SER	2.6
2	D	411	GLU	2.5
2	D	422	SER	2.5
1	A	38	ASP	2.5
2	D	415	ASN	2.5
2	D	360	PHE	2.5
1	A	10	ILE	2.5
1	C	175	LEU	2.5
1	A	5	GLN	2.5
2	D	323	GLN	2.4
2	D	378	ARG	2.4
1	A	14	THR	2.4
2	D	396	GLN	2.4
1	A	16	GLY	2.4
2	D	380	THR	2.4
1	A	290	THR	2.4
2	D	319	PHE	2.3
2	D	332	LEU	2.3
1	A	40	GLU	2.3
2	B	274	GLU	2.3
2	D	403	GLN	2.3
1	C	256	ASP	2.3
1	C	232	SER	2.3
1	C	255	LEU	2.3
1	C	154	VAL	2.3
1	C	224	GLU	2.3
2	D	370	GLN	2.3
2	D	377	ILE	2.3
2	D	387	LEU	2.2
1	C	253	PRO	2.2
1	C	19	TYR	2.2
1	A	162	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	201	LYS	2.2
2	D	361	HIS	2.2
1	C	247	ASP	2.2
1	C	177	CYS	2.1
1	A	94	SER	2.1
1	C	282	ALA	2.1
1	C	179	TYR	2.1
1	A	84	HIS	2.1
1	A	198	THR	2.1
1	A	256	ASP	2.1
1	A	177	CYS	2.1
2	D	383	THR	2.1
2	D	391	LEU	2.1
1	A	35	ILE	2.1
2	D	417	LYS	2.0
2	D	330	GLU	2.0
2	D	359	ALA	2.0
2	D	394	LEU	2.0
1	A	209	ILE	2.0
2	D	346	PRO	2.0
1	A	291	LYS	2.0
2	D	201	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	160	11/12	0.97	0.07	25,28,31,31	0
1	TPO	C	160	11/12	0.97	0.08	34,37,40,44	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.