



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 PM GMT

PDB ID : 3WGU
Title : Crystal structure of a Na⁺-bound Na⁺,K⁺-ATPase preceding the E1P state without oligomycin
Authors : Kanai, R.; Ogawa, H.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2013-08-09
Resolution : 2.80 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

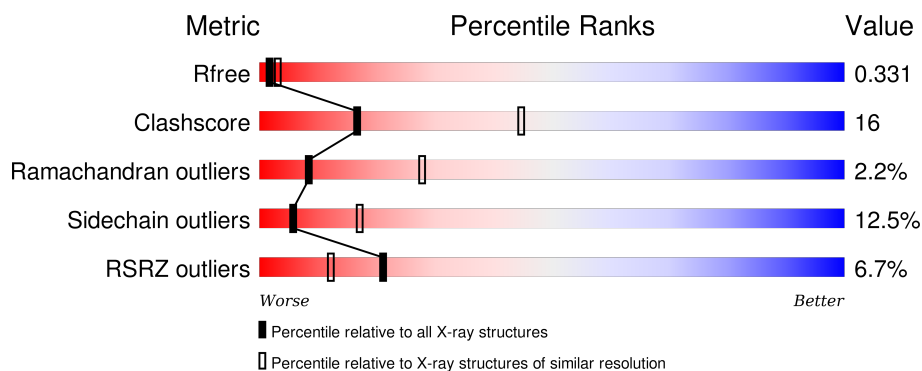
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1016	<div> <div>3%</div> <div>58%</div> <div>34%</div> <div>6%</div> </div>
1	C	1016	<div> <div>4%</div> <div>60%</div> <div>34%</div> <div>2%</div> </div>
2	B	303	<div> <div>15%</div> <div>51%</div> <div>42%</div> <div>6%</div> </div>
2	D	303	<div> <div>17%</div> <div>56%</div> <div>37%</div> <div>6%</div> </div>
3	E	65	<div> <div>8%</div> <div>28%</div> <div>23%</div> <div>46%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	65	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ALF	A	2002	-	-	-	X
5	ALF	C	2002	-	-	X	-
7	NA	A	2005	-	-	-	X
7	NA	A	2006	-	-	-	X
7	NA	A	2007	-	-	-	X
7	NA	C	2007	-	-	-	X
8	CLR	A	2009	-	-	-	X
8	CLR	A	2010	-	-	-	X
8	CLR	B	3001	-	-	-	X
8	CLR	C	2010	-	-	-	X
9	PC1	A	2012	-	-	-	X
9	PC1	A	2013	-	-	-	X
9	PC1	B	3002	-	-	-	X
9	PC1	C	2013	-	-	-	X
9	PC1	C	2014	-	-	-	X
9	PC1	C	2015	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21807 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			
1	C	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			
2	D	303	Total	C	N	O	S	0	0	0
			2479	1603	408	454	14			

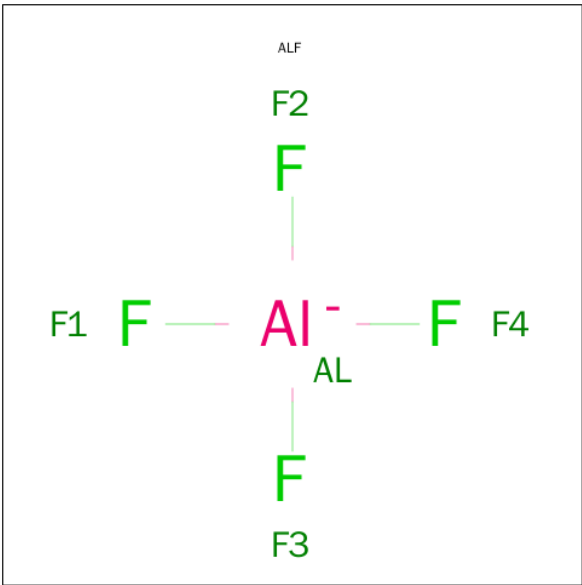
- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	34	Total	C	N	O	0	0	0
			270	183	39	48			
3	E	35	Total	C	N	O	0	0	0
			281	189	43	49			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

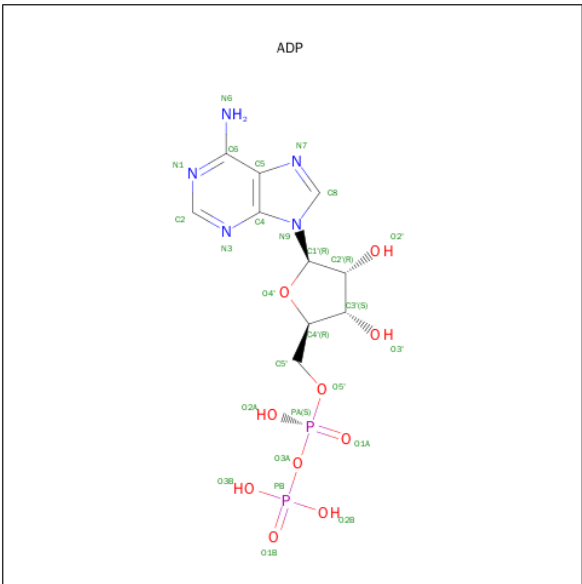
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	C	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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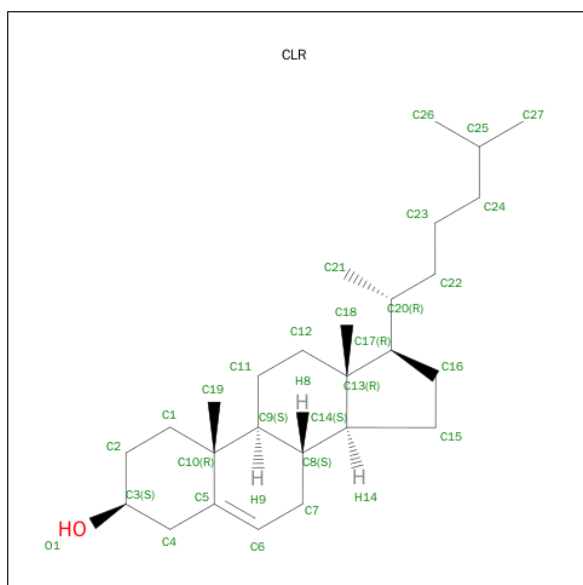
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

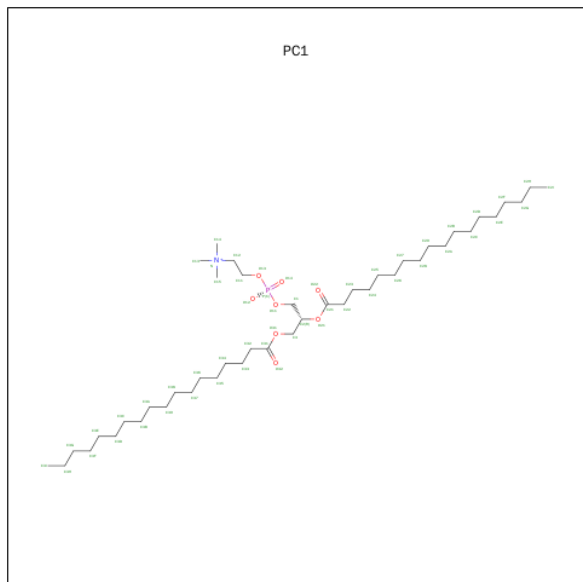
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		
7	C	4	Total	Na	0	0
			4	4		

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



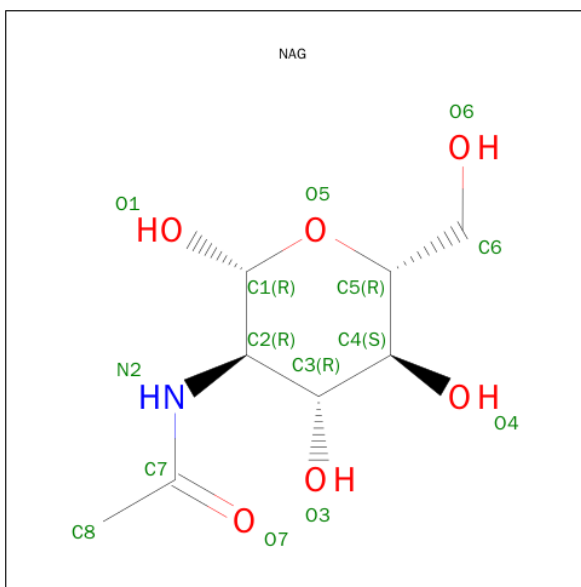
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			28	27	1		
8	A	1	Total	C	O	0	0
			28	27	1		
8	B	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		
8	C	1	Total	C	O	0	0
			28	27	1		

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	D	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

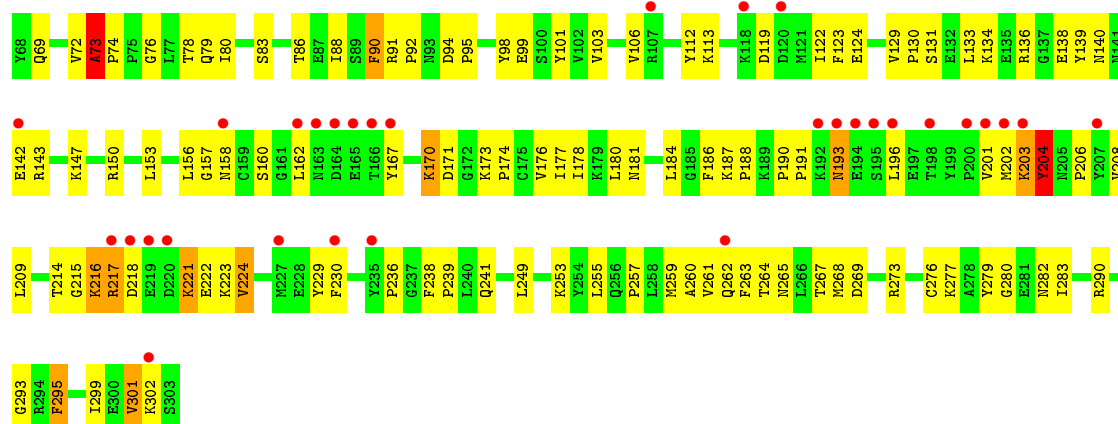
- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



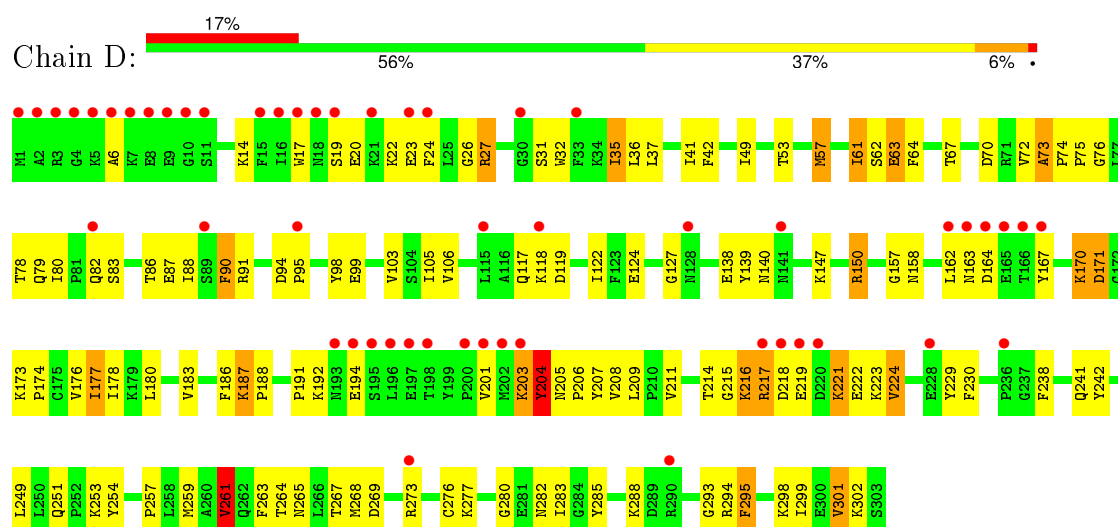
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is water.

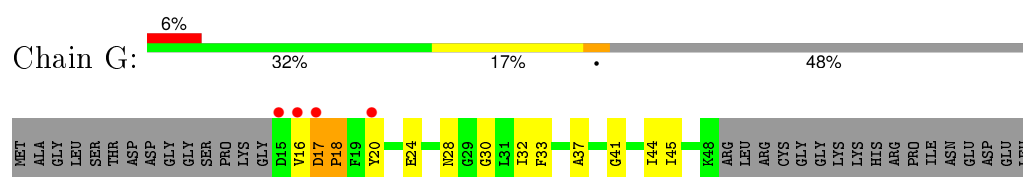
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	30	Total	O	0	0
			30	30		
11	B	2	Total	O	0	0
			2	2		
11	C	23	Total	O	0	0
			23	23		
11	D	3	Total	O	0	0
			3	3		



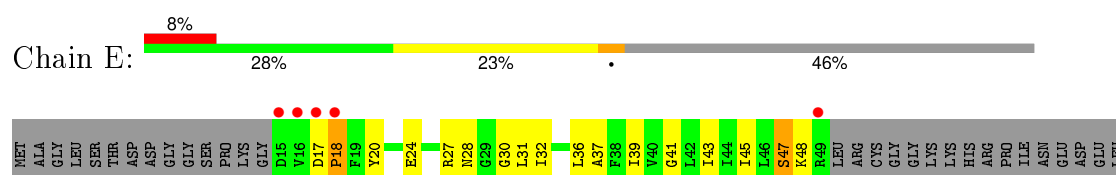
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.38Å 211.60Å 257.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.99-2.80) 88.9 (15.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.265 , 0.299 0.318 , 0.331	Depositor DCC
R_{free} test set	6460 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 126511 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	21807	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: MG, NAG, ADP, ALF, NA, PC1, CLR

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	0.48	1/7864 (0.0%)	0.65	5/10671 (0.0%)
1	C	0.41	0/7864	0.58	1/10671 (0.0%)
2	B	0.33	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.51	0/3426
3	E	0.59	1/287 (0.3%)	0.87	3/389 (0.8%)
3	G	0.43	0/276	0.57	0/375
All	All	0.43	2/21379 (0.0%)	0.60	10/28958 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	18	PRO	N-CD	7.79	1.58	1.47
1	A	511	CYS	CB-SG	-5.39	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	17	ASP	C-N-CD	-10.59	97.31	120.60
1	C	495	ARG	CB-CA-C	-8.16	94.09	110.40
1	A	495	ARG	CB-CA-C	-7.90	94.59	110.40
1	A	600	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	369	ASP	CB-CG-OD2	6.80	124.42	118.30
3	E	18	PRO	CA-N-CD	-6.62	102.23	111.50
3	E	18	PRO	N-CA-CB	6.58	111.19	103.30
1	A	600	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	360	LEU	CA-CB-CG	5.27	127.43	115.30
2	B	73	ALA	C-N-CD	5.03	138.96	128.40

There are no chirality outliers.

There are no planarity outliers.

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	7714	0	7769	262	0
1	C	7714	0	7768	248	0
2	B	2479	0	2458	92	0
2	D	2479	0	2458	80	0
3	E	281	0	285	9	0
3	G	270	0	272	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	27	0	12	5	0
6	C	27	0	12	6	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	A	56	0	87	12	0
8	B	28	0	44	4	0
8	C	84	0	131	23	0
9	A	216	0	352	14	0
9	B	54	0	88	0	0
9	C	216	0	352	21	0
9	D	54	0	88	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	30	0	0	0	0
11	B	2	0	0	0	0
11	C	23	0	0	3	0
11	D	3	0	0	1	0
All	All	21807	0	22202	724	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 16.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:HG3	1:C:495:ARG:O	1.61	0.97
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.52	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.54	0.90
8:C:2010:CLR:H272	9:C:2014:PC1:H2I2	1.54	0.88
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.56	0.87
1:C:166:ARG:NH1	1:C:182:ASP:OD1	2.08	0.87
1:A:600:ARG:HH11	1:A:600:ARG:HG2	1.39	0.87
1:C:44:LEU:HD11	1:C:197:ARG:HG2	1.58	0.86
1:C:985:PHE:HZ	8:C:2011:CLR:H221	1.40	0.85
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.57	0.85
1:C:454:GLU:HG2	1:C:460:VAL:HG23	1.58	0.85
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.41	0.83
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.60	0.83
2:D:221:LYS:HE3	2:D:223:LYS:HB2	1.60	0.82
2:D:269:ASP:HA	2:D:302:LYS:HA	1.60	0.82
1:A:44:LEU:HD11	1:A:197:ARG:HG2	1.61	0.82
1:C:493:GLU:HG2	1:C:495:ARG:H	1.43	0.82
2:B:216:LYS:HG2	2:B:221:LYS:HB2	1.62	0.81
1:A:369:ASP:OD2	5:A:2002:ALF:F4	1.88	0.81
1:C:384:MET:HE1	1:C:393:ALA:HB2	1.63	0.81
1:A:274:GLN:HE22	1:A:279:ALA:HB2	1.42	0.80
1:A:493:GLU:HG2	1:A:495:ARG:H	1.44	0.79
1:A:369:ASP:OD1	1:A:691:LYS:NZ	2.15	0.79
2:B:76:GLY:HA2	2:B:293:GLY:H	1.47	0.79
2:D:216:LYS:HG2	2:D:221:LYS:HB2	1.65	0.78
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.65	0.78
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.65	0.78
1:A:790:ASN:HD22	1:A:880:ARG:HD2	1.48	0.78
1:A:370:LYS:NZ	1:A:612:ASP:OD2	2.17	0.77
1:C:946:ILE:HG13	3:E:45:ILE:HD11	1.67	0.77
1:A:759:ARG:HH12	1:A:829:PRO:HA	1.48	0.76
1:A:495:ARG:HG3	1:A:495:ARG:O	1.83	0.76
1:A:565:ASP:H	1:A:570:ASN:HB2	1.49	0.76
8:C:2011:CLR:H121	8:C:2011:CLR:H212	1.65	0.76
1:A:443:ASP:HB2	1:A:446:GLU:HB2	1.68	0.76
1:C:565:ASP:H	1:C:570:ASN:HB2	1.47	0.76
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.68	0.75
9:A:2013:PC1:H3B2	9:A:2013:PC1:H292	1.68	0.75
1:C:495:ARG:O	1:C:495:ARG:CG	2.31	0.75
1:C:872:LEU:HD12	1:C:873:PRO:HD2	1.69	0.74
8:C:2009:CLR:H212	8:C:2009:CLR:H121	1.71	0.73
1:C:963:TYR:CE2	8:C:2011:CLR:H21	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.23	0.72
2:D:187:LYS:O	2:D:282:ASN:ND2	2.23	0.72
8:A:2009:CLR:H212	8:A:2009:CLR:H121	1.71	0.72
1:A:679:THR:HG23	1:A:680:GLU:HG3	1.72	0.72
1:C:801:LEU:HD13	1:C:805:LEU:HD21	1.71	0.72
8:C:2010:CLR:H212	8:C:2010:CLR:H121	1.71	0.72
2:B:269:ASP:HA	2:B:302:LYS:HA	1.72	0.72
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.71	0.72
1:C:986:PRO:HG3	8:C:2010:CLR:H152	1.70	0.71
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.55	0.71
1:A:831:ASN:HD21	2:B:6:ALA:HB2	1.55	0.71
1:A:50:THR:HG22	1:A:56:LEU:HB3	1.73	0.71
1:C:763:ASP:OD2	11:C:2118:HOH:O	2.09	0.70
1:A:57:THR:HG23	1:A:60:ARG:HB2	1.72	0.70
1:C:488:ASN:HB3	1:C:493:GLU:HG3	1.72	0.70
1:C:1003:ARG:HD2	9:C:2014:PC1:H122	1.73	0.70
1:A:166:ARG:NH1	1:A:182:ASP:OD1	2.23	0.70
8:B:3001:CLR:H121	8:B:3001:CLR:H212	1.71	0.70
1:A:445:SER:OG	1:A:544:ARG:NH1	2.25	0.70
1:C:365:THR:HB	1:C:705:VAL:HG12	1.73	0.69
2:B:14:LYS:HA	2:B:17:TRP:HB3	1.73	0.69
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.73	0.69
8:C:2010:CLR:H272	9:C:2014:PC1:C2I	2.22	0.69
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.73	0.69
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.28	0.68
9:C:2012:PC1:H2I3	9:C:2012:PC1:H3I1	1.75	0.68
9:C:2015:PC1:H351	9:C:2015:PC1:H251	1.76	0.68
1:A:544:ARG:NH2	6:A:2004:ADP:O2B	2.21	0.68
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.75	0.68
1:C:696:GLU:HG3	1:C:720:LYS:HE2	1.76	0.68
2:D:122:ILE:HG21	2:D:253:LYS:HE2	1.75	0.68
1:C:469:LYS:HA	1:C:486:HIS:HA	1.75	0.67
1:A:192:ILE:HD12	1:A:236:ALA:HB1	1.76	0.67
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.77	0.67
1:A:258:THR:HG23	1:A:261:GLY:H	1.59	0.67
1:A:986:PRO:HG3	8:A:2009:CLR:H181	1.78	0.66
1:A:495:ARG:O	1:A:495:ARG:CG	2.42	0.66
9:C:2012:PC1:H2D2	9:C:2015:PC1:H3F2	1.78	0.66
1:A:747:ASN:HD21	1:A:749:ALA:HB3	1.61	0.66
1:C:360:LEU:HG	1:C:723:ILE:HD13	1.76	0.66
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.77	0.65
1:C:309:THR:HG23	1:C:312:GLU:HB2	1.78	0.65
1:A:365:THR:HB	1:A:705:VAL:HG12	1.79	0.65
1:A:946:ILE:HG13	3:G:45:ILE:HD11	1.78	0.65
1:C:471:VAL:HG21	1:C:564:PHE:HB2	1.78	0.65
1:C:771:TYR:OH	11:C:2113:HOH:O	2.13	0.65
1:C:372:GLY:O	1:C:589:ARG:NH2	2.28	0.65
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.79	0.64
1:A:493:GLU:HG2	1:A:495:ARG:N	2.12	0.64
1:A:514:ILE:HG12	1:A:578:PHE:HB3	1.79	0.64
1:A:1009:TRP:HZ2	2:B:35:ILE:HG22	1.62	0.64
2:D:216:LYS:HB3	2:D:273:ARG:HB2	1.79	0.64
1:A:985:PHE:HZ	8:A:2010:CLR:H213	1.62	0.64
1:C:143:GLN:HE21	1:C:335:VAL:HG22	1.62	0.64
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.80	0.64
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.79	0.64
1:C:613:HIS:HD2	1:C:615:ILE:HB	1.63	0.63
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.80	0.63
1:C:531:PHE:HE2	1:C:581:LEU:HD21	1.64	0.63
1:C:56:LEU:HD11	1:C:182:ASP:HB3	1.79	0.63
1:A:777:ILE:HD11	1:A:847:TYR:HA	1.81	0.63
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.79	0.63
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.79	0.63
8:C:2010:CLR:H272	9:C:2014:PC1:C2H	2.29	0.63
2:B:229:TYR:HD1	2:B:261:VAL:HG12	1.62	0.63
1:A:385:TRP:HB3	1:A:581:LEU:HB2	1.81	0.62
2:B:224:VAL:HB	2:B:267:THR:HG21	1.80	0.62
1:A:154:PHE:HB3	1:A:350:LEU:HD13	1.81	0.62
2:D:191:PRO:HG3	2:D:280:GLY:HA2	1.82	0.62
2:D:229:TYR:HD1	2:D:261:VAL:HG12	1.64	0.62
1:C:31:GLU:HG3	1:C:32:VAL:H	1.65	0.61
2:D:70:ASP:OD1	11:D:501:HOH:O	2.16	0.61
1:C:902:GLU:O	1:C:906:ILE:HG12	2.00	0.61
2:D:91:ARG:HG3	2:D:302:LYS:O	2.01	0.61
1:C:191:ARG:HA	1:C:241:ASN:HB3	1.83	0.61
1:A:728:GLY:O	1:A:736:LYS:NZ	2.20	0.61
1:C:299:PHE:HB3	1:C:316:PHE:HE2	1.65	0.61
1:C:505:GLU:OE2	1:C:613:HIS:ND1	2.32	0.61
1:A:838:VAL:HG13	1:A:842:LEU:HD22	1.81	0.61
1:C:398:ASN:HB2	1:C:455:LEU:HD13	1.83	0.60
2:D:14:LYS:HA	2:D:17:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:ARG:HB3	1:C:600:ARG:HH11	1.67	0.60
3:E:47:SER:OG	3:E:47:SER:O	2.18	0.60
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.83	0.60
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.83	0.60
1:A:309:THR:HG23	1:A:312:GLU:HB2	1.83	0.60
2:D:224:VAL:HB	2:D:267:THR:HG21	1.83	0.60
1:C:446:GLU:OE2	1:C:482:GLN:NE2	2.34	0.60
1:A:360:LEU:HA	1:A:723:ILE:HD13	1.84	0.59
1:C:553:LEU:HD22	1:C:558:PHE:CE2	2.37	0.59
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.83	0.59
1:A:861:THR:HG21	1:A:918:SER:OG	2.02	0.59
1:A:300:PHE:HB2	1:A:317:LEU:HB2	1.85	0.59
1:C:777:ILE:HD12	1:C:777:ILE:H	1.67	0.59
1:A:340:THR:HG21	1:A:761:ILE:HD11	1.83	0.59
1:A:760:LEU:HD22	1:A:820:ALA:HB2	1.85	0.59
1:C:125:LEU:O	1:C:129:LEU:HB2	2.03	0.58
1:A:394:ASP:OD1	1:A:394:ASP:N	2.35	0.58
1:A:777:ILE:HD11	1:A:847:TYR:CG	2.37	0.58
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.83	0.58
1:A:191:ARG:HA	1:A:241:ASN:HB3	1.85	0.58
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.38	0.58
2:B:214:THR:OG1	2:B:215:GLY:N	2.35	0.58
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.38	0.58
2:B:216:LYS:HB3	2:B:273:ARG:HB2	1.86	0.58
1:A:777:ILE:H	1:A:777:ILE:HD12	1.68	0.58
2:B:216:LYS:H	2:B:216:LYS:HD2	1.69	0.58
2:B:35:ILE:HG13	2:B:36:LEU:N	2.18	0.58
1:C:170:LYS:NZ	1:C:185:GLU:OE2	2.36	0.58
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.85	0.58
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.84	0.58
2:D:106:VAL:HG22	2:D:167:TYR:HB2	1.86	0.58
8:C:2010:CLR:H272	9:C:2014:PC1:H2G1	1.86	0.57
1:A:258:THR:HG23	1:A:261:GLY:N	2.19	0.57
1:A:888:ILE:O	1:A:904:ARG:NH2	2.37	0.57
1:C:777:ILE:HD11	1:C:847:TYR:HA	1.86	0.57
1:A:944:ASN:ND2	1:A:947:LEU:HB2	2.18	0.57
1:A:422:ASN:OD1	1:A:423:ARG:N	2.37	0.57
2:D:83:SER:HB3	2:D:86:THR:HA	1.85	0.57
1:A:752:VAL:HA	1:A:755:VAL:HG12	1.85	0.57
8:C:2010:CLR:C27	9:C:2014:PC1:H2I2	2.31	0.57
1:A:902:GLU:O	1:A:906:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:ILE:HG13	2:D:36:LEU:N	2.18	0.57
3:G:17:ASP:HB3	3:G:18:PRO:HD2	1.86	0.57
1:A:298:SER:HB2	9:A:2014:PC1:H3F1	1.87	0.57
1:A:340:THR:HG22	1:A:757:GLU:OE1	2.04	0.57
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.39	0.57
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.87	0.57
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.87	0.57
1:C:440:VAL:HG21	1:C:451:LYS:HE3	1.86	0.57
1:A:294:PHE:HE2	9:A:2014:PC1:H3B2	1.70	0.56
1:A:152:GLU:HA	1:A:155:LYS:HG2	1.87	0.56
1:A:324:ASN:HA	1:A:776:ASN:OD1	2.04	0.56
1:A:483:LEU:HD21	1:A:571:PHE:HE2	1.71	0.56
1:C:238:PHE:O	1:C:260:MET:HG3	2.06	0.56
1:C:277:ILE:HD12	1:C:358:GLU:HG3	1.88	0.56
1:A:433:LEU:HD12	1:A:437:LYS:HB3	1.86	0.56
1:A:440:VAL:HG12	1:A:441:ALA:H	1.70	0.56
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.88	0.56
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.41	0.56
1:A:963:TYR:CE2	8:A:2010:CLR:H21	2.39	0.56
1:C:551:LEU:HD12	1:C:576:LEU:HA	1.88	0.56
1:C:998:ARG:HE	1:C:1014:THR:HB	1.71	0.56
2:D:173:LYS:HG2	2:D:264:THR:HA	1.86	0.56
1:A:857:GLY:O	1:A:861:THR:HG23	2.06	0.56
1:C:303:SER:O	1:C:308:TYR:HB2	2.05	0.56
1:C:956:ALA:HB2	3:E:37:ALA:HB3	1.88	0.55
1:A:790:ASN:ND2	1:A:880:ARG:HD2	2.19	0.55
1:A:889:ASN:ND2	1:A:901:TYR:H	2.04	0.55
1:A:551:LEU:HD22	1:A:553:LEU:HD23	1.88	0.55
1:A:255:GLY:O	1:A:258:THR:HG22	2.07	0.55
1:A:889:ASN:HD22	1:A:900:THR:HB	1.71	0.55
2:D:176:VAL:HB	2:D:261:VAL:HG23	1.89	0.55
1:C:854:GLN:HB3	1:C:922:VAL:HG21	1.88	0.55
1:C:483:LEU:HD21	1:C:571:PHE:HE2	1.71	0.55
1:C:426:PHE:HE2	1:C:454:GLU:HG3	1.72	0.55
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.89	0.55
1:C:600:ARG:HH21	1:C:680:GLU:HG2	1.72	0.55
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.89	0.55
2:B:106:VAL:HG22	2:B:167:TYR:HB2	1.89	0.54
1:A:613:HIS:NE2	1:A:615:ILE:HG12	2.21	0.54
1:C:850:ILE:O	1:C:854:GLN:HG3	2.07	0.54
1:C:283:HIS:NE2	1:C:287:ILE:HD11	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:TYR:CZ	8:C:2011:CLR:H21	2.42	0.54
1:A:343:ARG:HD2	1:A:757:GLU:OE2	2.07	0.54
2:D:268:MET:HA	2:D:301:VAL:HG23	1.89	0.54
2:B:268:MET:HA	2:B:301:VAL:HG23	1.89	0.54
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.90	0.54
1:A:613:HIS:CD2	1:A:615:ILE:HG12	2.43	0.54
1:A:372:GLY:HA2	1:A:377:ASN:HB2	1.88	0.54
1:C:778:PRO:HB3	1:C:855:ALA:HA	1.89	0.54
8:C:2011:CLR:H6	9:D:401:PC1:H242	1.90	0.54
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.72	0.54
8:C:2010:CLR:H272	9:C:2014:PC1:C2G	2.38	0.53
1:A:864:VAL:HA	2:B:57:MET:SD	2.48	0.53
1:C:50:THR:HG22	1:C:56:LEU:HD23	1.90	0.53
1:A:892:GLU:HA	1:A:897:GLN:O	2.08	0.53
1:C:301:ILE:O	1:C:305:ILE:HG12	2.09	0.53
5:C:2002:ALF:F4	6:C:2004:ADP:O3B	2.15	0.53
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.91	0.53
2:D:204:TYR:HB3	2:D:208:VAL:HB	1.89	0.53
1:C:1009:TRP:HZ2	2:D:35:ILE:HG22	1.73	0.53
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.89	0.53
1:C:997:VAL:O	1:C:1001:ILE:HG13	2.08	0.53
2:D:14:LYS:HZ3	2:D:17:TRP:HE3	1.56	0.53
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.91	0.53
1:C:933:ARG:HD2	1:C:1016:TYR:O	2.08	0.53
2:B:157:GLY:H	2:B:230:PHE:HB3	1.74	0.53
1:C:204:CYS:HA	1:C:245:GLY:HA3	1.91	0.53
1:C:324:ASN:HA	1:C:776:ASN:OD1	2.07	0.53
1:C:421:CYS:O	1:C:501:LYS:NZ	2.36	0.53
2:B:130:PRO:O	2:B:204:TYR:OH	2.13	0.53
1:A:55:GLY:HA2	1:A:183:LEU:HD22	1.91	0.53
1:A:882:ASN:HB3	1:A:888:ILE:HD12	1.91	0.53
2:D:186:PHE:CZ	2:D:282:ASN:HB3	2.43	0.53
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.90	0.53
1:A:303:SER:O	1:A:308:TYR:HB2	2.09	0.53
1:C:877:LEU:H	1:C:877:LEU:HD12	1.73	0.53
1:C:443:ASP:HB2	1:C:446:GLU:HB2	1.90	0.53
1:C:613:HIS:CD2	1:C:615:ILE:HB	2.44	0.52
1:A:387:ASP:O	1:A:389:GLN:N	2.42	0.52
1:C:759:ARG:HH12	1:C:829:PRO:HA	1.75	0.52
1:A:998:ARG:HH12	1:A:999:LYS:HG3	1.74	0.52
2:D:214:THR:OG1	2:D:215:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:2010:CLR:C27	9:C:2014:PC1:H2G1	2.39	0.52
2:B:191:PRO:HG3	2:B:280:GLY:HA2	1.92	0.52
1:C:99:ILE:O	1:C:103:LEU:HG	2.09	0.52
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.73	0.52
1:A:777:ILE:CD1	1:A:847:TYR:HA	2.39	0.52
1:C:670:GLN:O	1:C:674:ILE:HG13	2.10	0.52
1:A:80:PRO:HG2	1:A:83:VAL:HB	1.91	0.52
2:B:176:VAL:HB	2:B:261:VAL:HG23	1.91	0.52
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.91	0.52
1:A:628:SER:OG	1:A:680:GLU:OE2	2.28	0.52
1:C:544:ARG:NH2	6:C:2004:ADP:O1B	2.43	0.51
2:D:49:ILE:O	2:D:53:THR:HG22	2.10	0.51
1:A:413:ALA:HB1	1:A:550:HIS:HE1	1.74	0.51
2:D:216:LYS:HD2	2:D:216:LYS:H	1.74	0.51
2:B:193:ASN:OD1	2:B:193:ASN:N	2.43	0.51
1:C:906:ILE:O	1:C:910:THR:OG1	2.22	0.51
1:C:757:GLU:O	1:C:761:ILE:HG22	2.10	0.51
1:A:347:LYS:HG3	1:A:753:THR:HG21	1.92	0.51
1:C:55:GLY:HA2	1:C:183:LEU:HD22	1.93	0.51
1:C:679:THR:HG23	1:C:680:GLU:HG3	1.93	0.51
1:C:689:GLN:O	1:C:693:ILE:HG12	2.11	0.51
1:A:827:ARG:NH2	1:A:934:ARG:HD3	2.26	0.51
1:C:246:THR:OG1	1:C:423:ARG:NH2	2.44	0.51
1:C:824:ILE:HD12	1:C:825:MET:H	1.76	0.51
2:B:170:LYS:N	2:B:170:LYS:HD2	2.26	0.51
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.93	0.51
1:A:997:VAL:O	1:A:1001:ILE:HG13	2.11	0.51
1:A:928:VAL:O	1:A:931:LYS:HB3	2.10	0.51
2:B:95:PRO:HA	2:B:98:TYR:CE1	2.46	0.50
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.93	0.50
1:C:39:LEU:HD22	1:C:43:GLU:HB3	1.93	0.50
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.93	0.50
2:D:90:PHE:CD2	2:D:98:TYR:HB3	2.46	0.50
1:C:254:THR:HB	1:C:257:ARG:HH21	1.76	0.50
1:C:322:VAL:HG12	1:C:804:ASP:OD2	2.11	0.50
1:A:241:ASN:ND2	1:A:737:GLN:OE1	2.45	0.50
1:C:306:LEU:HD12	1:C:880:ARG:HE	1.75	0.50
1:C:781:THR:HG22	8:C:2009:CLR:H273	1.93	0.50
1:A:1009:TRP:CE2	1:A:1013:GLU:HG3	2.46	0.50
2:D:57:MET:HE3	2:D:61:ILE:HD11	1.93	0.50
3:G:24:GLU:O	3:G:28:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:HA	1:A:111:GLN:HE21	1.74	0.50
1:C:827:ARG:HH12	1:C:933:ARG:HH21	1.59	0.50
2:B:138:GLU:O	2:B:140:ASN:N	2.44	0.50
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.94	0.50
2:B:98:TYR:HA	2:B:101:TYR:HD1	1.77	0.50
1:C:255:GLY:O	1:C:258:THR:HG22	2.11	0.50
8:C:2011:CLR:C21	8:C:2011:CLR:H121	2.37	0.50
1:C:888:ILE:HG22	1:C:890:ASP:HB2	1.93	0.50
1:A:85:PHE:CZ	1:A:138:CYS:HB3	2.46	0.50
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.46	0.50
1:C:469:LYS:HB3	1:C:486:HIS:CE1	2.47	0.50
1:A:591:ALA:HB1	1:A:749:ALA:HB2	1.93	0.50
2:B:178:ILE:HD11	2:B:276:CYS:SG	2.51	0.50
2:D:178:ILE:HD11	2:D:276:CYS:SG	2.52	0.50
1:A:420:LEU:HD13	1:A:486:HIS:ND1	2.27	0.49
1:A:206:VAL:HA	1:A:242:CYS:HA	1.94	0.49
2:B:37:LEU:O	2:B:41:ILE:HG23	2.12	0.49
1:A:803:ILE:HG23	1:A:919:ILE:HG21	1.94	0.49
1:C:876:LEU:HD23	1:C:879:LEU:HD12	1.93	0.49
1:C:281:ILE:HD11	1:C:765:LEU:HD13	1.94	0.49
1:A:96:LEU:HD12	1:A:99:ILE:HD12	1.93	0.49
1:C:266:LEU:HD22	1:C:270:LEU:HA	1.93	0.49
1:A:793:LEU:HD12	1:A:794:PRO:HD2	1.95	0.49
1:A:55:GLY:HA3	1:A:165:ILE:O	2.11	0.49
1:A:998:ARG:NH1	1:A:999:LYS:HG3	2.28	0.49
1:A:1001:ILE:CG2	1:A:1010:VAL:HG21	2.43	0.49
2:D:117:GLN:OE1	2:D:150:ARG:HG2	2.13	0.49
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.93	0.49
1:A:842:LEU:HD12	1:A:1016:TYR:HD2	1.77	0.49
2:B:91:ARG:HH21	2:B:94:ASP:HB2	1.77	0.49
1:C:502:GLY:HA2	6:C:2004:ADP:N3	2.28	0.49
1:C:861:THR:HG21	1:C:918:SER:OG	2.11	0.49
2:D:157:GLY:H	2:D:230:PHE:HB3	1.77	0.49
1:A:333:VAL:HG22	1:A:765:LEU:HD11	1.95	0.49
1:A:553:LEU:HD22	1:A:558:PHE:CE2	2.48	0.49
1:A:182:ASP:O	1:A:251:VAL:HG23	2.12	0.49
1:C:985:PHE:CZ	8:C:2011:CLR:H221	2.32	0.48
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.48	0.48
1:A:228:ASN:HB3	1:A:231:GLU:HG2	1.95	0.48
1:A:335:VAL:HG11	1:A:817:TYR:CE2	2.47	0.48
2:B:27:ARG:HG3	2:B:31:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASP:HB2	1:A:570:ASN:HD22	1.78	0.48
1:C:781:THR:HG22	8:C:2009:CLR:C27	2.44	0.48
1:C:51:ASP:N	1:C:55:GLY:O	2.46	0.48
1:A:799:THR:O	1:A:803:ILE:HG12	2.14	0.48
1:A:505:GLU:HG3	1:A:506:ARG:H	1.79	0.48
1:C:953:GLU:OE2	3:E:41:GLY:HA3	2.14	0.48
2:B:202:MET:SD	2:B:236:PRO:HG2	2.54	0.48
1:C:802:CYS:HB3	1:C:916:PHE:CE1	2.48	0.48
1:C:799:THR:O	1:C:803:ILE:HG12	2.13	0.48
3:E:28:ASN:O	3:E:32:ILE:HG12	2.13	0.48
1:A:953:GLU:OE2	3:G:41:GLY:HA3	2.13	0.48
1:A:874:ILE:HD12	1:A:874:ILE:H	1.77	0.48
2:B:83:SER:HB3	2:B:86:THR:HA	1.95	0.48
9:C:2015:PC1:H282	9:C:2015:PC1:H3B1	1.94	0.48
1:A:350:LEU:HB2	1:A:744:LEU:HD21	1.95	0.48
1:C:332:THR:HG21	1:C:768:SER:OG	2.14	0.48
1:C:818:GLU:OE2	1:C:931:LYS:NZ	2.28	0.48
1:A:565:ASP:OD2	1:A:568:ASP:HB2	2.12	0.48
8:B:3001:CLR:H121	8:B:3001:CLR:C21	2.41	0.48
2:D:17:TRP:CZ2	2:D:19:SER:HB3	2.49	0.48
1:C:553:LEU:HB3	1:C:558:PHE:CD2	2.48	0.48
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.49	0.48
1:C:768:SER:HA	1:C:815:LEU:HD23	1.96	0.48
2:D:23:GLU:HG2	2:D:24:PHE:H	1.78	0.48
2:D:76:GLY:HA2	2:D:293:GLY:H	1.78	0.48
1:A:488:ASN:HB3	1:A:493:GLU:HG3	1.95	0.47
1:C:777:ILE:CD1	1:C:847:TYR:HA	2.44	0.47
1:C:773:LEU:HD22	1:C:847:TYR:HE1	1.79	0.47
1:C:656:CYS:SG	1:C:681:ILE:HG22	2.54	0.47
2:D:41:ILE:HG13	2:D:42:PHE:N	2.29	0.47
1:C:565:ASP:H	1:C:570:ASN:CB	2.20	0.47
1:A:194:ALA:HA	1:A:238:PHE:HB2	1.95	0.47
1:C:908:GLU:O	1:C:911:CYS:HB2	2.14	0.47
1:A:371:THR:OG1	6:A:2004:ADP:O3B	2.29	0.47
1:C:311:LEU:O	1:C:315:ILE:HG12	2.14	0.47
2:B:173:LYS:HB3	2:B:264:THR:HA	1.96	0.47
1:A:280:GLU:OE1	1:A:830:ARG:NH2	2.48	0.47
1:A:402:VAL:HG23	1:A:404:PHE:H	1.79	0.47
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.50	0.47
1:C:613:HIS:CD2	1:C:615:ILE:H	2.33	0.47
1:A:393:ALA:HA	1:A:402:VAL:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HG	1:A:455:LEU:HD11	1.96	0.47
1:C:139:PHE:HD1	9:C:2013:PC1:H221	1.80	0.47
1:A:167:ASN:O	1:A:169:GLU:N	2.47	0.47
2:B:277:LYS:HD2	2:B:279:TYR:CE2	2.49	0.47
1:C:606:VAL:HG11	1:C:626:ILE:HD12	1.97	0.47
2:D:90:PHE:CE1	2:D:174:PRO:HG3	2.49	0.47
1:A:418:ALA:O	1:A:422:ASN:HB2	2.14	0.47
2:D:80:ILE:HG22	2:D:105:ILE:HA	1.97	0.47
1:C:305:ILE:C	1:C:307:GLU:H	2.18	0.47
1:C:1001:ILE:CG2	1:C:1010:VAL:HG21	2.44	0.47
1:C:841:ARG:HB2	1:C:1016:TYR:HA	1.95	0.47
1:A:387:ASP:C	1:A:389:GLN:H	2.17	0.47
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.72	0.47
1:A:968:GLY:HA2	1:A:973:MET:N	2.29	0.47
8:A:2009:CLR:H121	8:A:2009:CLR:C21	2.41	0.47
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.47	0.47
1:C:31:GLU:HG3	1:C:32:VAL:N	2.28	0.47
1:A:349:CYS:SG	1:A:741:MET:HG2	2.55	0.47
1:C:695:VAL:HG13	1:C:705:VAL:HG21	1.97	0.47
1:A:777:ILE:N	1:A:777:ILE:HD12	2.30	0.47
1:C:913:THR:O	1:C:917:VAL:HG23	2.15	0.47
1:A:616:THR:O	1:A:620:ILE:HG12	2.14	0.47
1:C:317:LEU:O	1:C:321:ILE:HG12	2.15	0.47
1:C:493:GLU:HG2	1:C:495:ARG:N	2.22	0.47
1:A:300:PHE:HE1	1:A:314:VAL:HG12	1.80	0.47
1:A:483:LEU:HD13	1:A:500:MET:HB3	1.96	0.47
1:A:951:LEU:O	1:A:955:THR:HG23	2.15	0.47
2:B:203:LYS:HB3	2:B:203:LYS:HE2	1.77	0.47
9:A:2011:PC1:H132	9:A:2011:PC1:H112	1.68	0.46
1:A:933:ARG:HD2	1:A:1016:TYR:O	2.15	0.46
2:D:27:ARG:HD3	2:D:32:TRP:HE3	1.79	0.46
1:A:633:THR:H	1:A:636:ASP:HB2	1.80	0.46
1:A:131:ALA:O	1:A:135:ILE:HG12	2.14	0.46
1:A:847:TYR:CD2	9:A:2011:PC1:H381	2.51	0.46
1:A:331:ALA:O	1:A:335:VAL:HG23	2.14	0.46
1:C:206:VAL:HA	1:C:242:CYS:HA	1.97	0.46
1:A:921:VAL:HG22	1:A:924:TRP:CH2	2.50	0.46
9:C:2012:PC1:H3H2	9:C:2015:PC1:H2H1	1.97	0.46
2:D:98:TYR:CZ	2:D:171:ASP:HB3	2.50	0.46
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.97	0.46
1:C:888:ILE:O	1:C:904:ARG:NH2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLY:HA2	1:A:973:MET:H	1.80	0.46
2:D:87:GLU:HA	2:D:298:LYS:O	2.15	0.46
1:A:937:VAL:HG21	1:A:992:PHE:CE1	2.50	0.46
1:C:801:LEU:O	1:C:805:LEU:HG	2.14	0.46
1:A:901:TYR:HA	1:A:904:ARG:CZ	2.45	0.46
2:D:277:LYS:HG2	2:D:285:TYR:CE2	2.50	0.46
1:C:383:HIS:CD2	1:C:392:GLU:HG2	2.50	0.46
1:C:982:PHE:HA	1:C:985:PHE:CD1	2.50	0.46
2:B:36:LEU:O	2:B:40:VAL:HG23	2.16	0.46
1:A:861:THR:HG22	1:A:983:CYS:CB	2.45	0.46
3:G:17:ASP:CB	3:G:18:PRO:HD2	2.46	0.46
2:B:173:LYS:HG2	2:B:264:THR:HA	1.98	0.46
1:C:220:ARG:HD3	1:C:233:ARG:O	2.15	0.46
1:A:122:ASN:ND2	1:A:315:ILE:HG13	2.31	0.46
1:A:592:VAL:O	1:A:596:VAL:HG22	2.16	0.46
8:C:2010:CLR:C21	8:C:2010:CLR:H121	2.42	0.46
1:C:924:TRP:HE1	1:C:955:THR:HG22	1.81	0.46
1:C:126:GLY:O	1:C:130:SER:OG	2.25	0.46
2:D:75:PRO:HG3	2:D:183:VAL:HG21	1.96	0.46
1:A:263:ILE:HG13	1:A:263:ILE:O	2.14	0.46
1:C:889:ASN:ND2	1:C:901:TYR:H	2.13	0.46
1:A:795:LEU:HD13	1:A:915:PHE:CD1	2.51	0.46
1:C:460:VAL:O	1:C:464:ARG:HB2	2.15	0.46
2:B:138:GLU:HG3	2:B:140:ASN:ND2	2.30	0.46
3:E:39:ILE:O	3:E:43:ILE:HG12	2.16	0.46
2:B:42:PHE:HD2	2:B:43:TYR:CD1	2.34	0.46
1:A:985:PHE:CZ	8:A:2010:CLR:H213	2.48	0.46
2:B:131:SER:HB2	2:B:241:GLN:HB3	1.98	0.46
1:C:622:LYS:HA	1:C:627:ILE:O	2.16	0.46
2:B:49:ILE:O	2:B:53:THR:HG22	2.16	0.46
2:B:90:PHE:CZ	2:B:174:PRO:HG3	2.52	0.45
1:C:202:ASN:HB2	1:C:246:THR:HG22	1.97	0.45
1:A:921:VAL:HG13	1:A:924:TRP:CZ3	2.50	0.45
1:C:366:ILE:HG12	1:C:706:ALA:HB3	1.98	0.45
1:C:950:GLY:O	1:C:954:GLU:HB2	2.16	0.45
1:C:801:LEU:CD1	1:C:805:LEU:HD21	2.44	0.45
1:A:818:GLU:HG2	1:A:944:ASN:HD22	1.80	0.45
1:A:402:VAL:HG21	1:A:404:PHE:CE1	2.51	0.45
1:C:535:TYR:CE2	1:C:545:VAL:HB	2.51	0.45
1:C:460:VAL:HG11	1:C:464:ARG:HH21	1.80	0.45
1:C:827:ARG:NH1	1:C:933:ARG:HH21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:TYR:OH	2:D:53:THR:HG21	2.17	0.45
1:A:332:THR:OG1	1:A:813:ILE:HD13	2.17	0.45
1:C:152:GLU:C	1:C:154:PHE:H	2.20	0.45
2:B:76:GLY:H	2:B:181:ASN:HD22	1.64	0.45
2:B:90:PHE:O	2:B:92:PRO:HD3	2.16	0.45
1:A:303:SER:HB2	1:A:308:TYR:CD2	2.51	0.45
2:B:66:PRO:HG2	2:B:69:GLN:HG3	1.97	0.45
1:C:331:ALA:O	1:C:335:VAL:HG23	2.16	0.45
1:C:28:LEU:C	1:C:31:GLU:HG2	2.37	0.45
1:C:685:ARG:NH2	6:C:2004:ADP:O3'	2.44	0.45
1:C:50:THR:HG21	1:C:181:GLY:C	2.37	0.45
1:C:551:LEU:HD13	1:C:576:LEU:HD23	1.99	0.45
1:C:99:ILE:HA	1:C:102:ILE:HD12	1.97	0.45
1:C:951:LEU:O	1:C:955:THR:HG23	2.17	0.45
1:A:860:PHE:CE1	2:B:53:THR:HG23	2.52	0.45
1:A:188:GLY:HA2	1:A:244:GLU:HA	1.99	0.45
1:C:25:MET:O	1:C:29:LYS:HG3	2.16	0.45
8:C:2009:CLR:C21	8:C:2009:CLR:H121	2.43	0.45
2:B:153:LEU:O	2:B:160:SER:OG	2.27	0.45
2:B:66:PRO:HD2	2:B:184:LEU:HD22	1.98	0.45
1:C:143:GLN:NE2	1:C:335:VAL:HG13	2.31	0.45
1:A:336:CYS:O	1:A:340:THR:HG23	2.17	0.45
1:C:785:ILE:HG22	1:C:791:ILE:HD12	1.98	0.45
1:A:688:PRO:O	1:A:691:LYS:HB2	2.17	0.45
2:B:209:LEU:HB3	2:B:238:PHE:HB2	1.98	0.45
9:C:2015:PC1:H221	9:C:2015:PC1:H2	1.78	0.45
1:A:504:PRO:HB3	1:A:581:LEU:HD21	1.99	0.45
2:B:90:PHE:HD2	2:B:98:TYR:HB3	1.82	0.45
1:C:131:ALA:O	1:C:135:ILE:HG12	2.17	0.44
1:A:956:ALA:HB2	3:G:37:ALA:HB3	1.99	0.44
3:G:45:ILE:HA	3:G:45:ILE:HD12	1.73	0.44
1:C:589:ARG:NH1	1:C:746:ASP:HB3	2.33	0.44
1:A:60:ARG:O	1:A:64:ILE:HG13	2.17	0.44
8:A:2010:CLR:H212	8:A:2010:CLR:H121	1.99	0.44
1:C:901:TYR:OH	1:C:905:LYS:HE3	2.18	0.44
1:C:209:SER:HB3	1:C:215:SER:HA	1.99	0.44
2:D:163:ASN:HB3	2:D:164:ASP:H	1.62	0.44
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.62	0.44
5:C:2002:ALF:F1	6:C:2004:ADP:O3B	2.25	0.44
1:C:423:ARG:HD2	1:C:472:GLU:OE2	2.18	0.44
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLY:HA3	1:A:974:TYR:CE2	2.52	0.44
1:C:494:PRO:HG2	1:C:552:PHE:HB3	1.98	0.44
3:E:45:ILE:HA	3:E:45:ILE:HD12	1.86	0.44
2:B:17:TRP:CZ2	2:B:19:SER:HB3	2.52	0.44
1:A:300:PHE:CE1	1:A:314:VAL:HG12	2.53	0.44
3:G:28:ASN:O	3:G:32:ILE:HG12	2.18	0.44
1:A:504:PRO:HB3	1:A:581:LEU:CD2	2.48	0.44
2:B:177:ILE:HA	2:B:260:ALA:HA	1.98	0.44
2:B:204:TYR:HB3	2:B:208:VAL:HB	1.98	0.44
1:C:480:LYS:HG2	6:C:2004:ADP:H5'1	1.99	0.44
1:A:413:ALA:HB1	1:A:550:HIS:CE1	2.53	0.44
1:A:512:SER:O	1:A:523:LEU:HB2	2.18	0.44
1:A:492:ALA:O	1:A:494:PRO:HD3	2.18	0.44
9:D:401:PC1:H2B2	9:D:401:PC1:H282	1.65	0.44
9:C:2015:PC1:H361	9:C:2015:PC1:H3B2	2.00	0.44
1:C:531:PHE:CE2	1:C:581:LEU:HD21	2.48	0.44
1:A:204:CYS:HA	1:A:245:GLY:HA3	2.00	0.44
1:C:512:SER:O	1:C:523:LEU:HB2	2.18	0.44
2:B:99:GLU:O	2:B:103:VAL:HG23	2.18	0.44
1:C:1016:TYR:HD1	1:C:1016:TYR:H	1.66	0.44
2:B:27:ARG:HD3	2:B:32:TRP:HE3	1.83	0.44
2:D:217:ARG:HD2	2:D:218:ASP:H	1.82	0.44
1:A:883:TRP:NE1	1:A:908:GLU:OE1	2.50	0.44
1:C:436:LEU:HG	1:C:455:LEU:HD11	2.00	0.43
1:C:258:THR:HG23	1:C:261:GLY:H	1.83	0.43
1:C:857:GLY:O	1:C:861:THR:HG23	2.17	0.43
1:A:921:VAL:HG12	1:A:988:SER:HB2	2.00	0.43
1:A:351:VAL:HG11	1:A:357:VAL:HG23	2.00	0.43
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.99	0.43
2:B:157:GLY:N	2:B:230:PHE:HB3	2.33	0.43
1:C:43:GLU:O	1:C:46:ARG:HG2	2.18	0.43
1:C:804:ASP:O	1:C:808:ASP:HB2	2.17	0.43
1:A:948:ILE:HG21	3:G:44:ILE:HD13	2.00	0.43
1:A:318:ILE:O	1:A:322:VAL:HG23	2.18	0.43
2:D:192:LYS:HZ1	2:D:205:ASN:HB3	1.83	0.43
1:C:460:VAL:HG12	1:C:464:ARG:HE	1.82	0.43
1:A:340:THR:HG21	1:A:761:ILE:CD1	2.48	0.43
2:B:193:ASN:HA	2:B:196:LEU:HD21	2.00	0.43
1:C:430:GLN:HE21	1:C:433:LEU:HD21	1.84	0.43
2:D:62:SER:C	2:D:64:PHE:H	2.22	0.43
2:B:217:ARG:HD2	2:B:218:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HD2	1:A:157:MET:HG3	1.82	0.43
1:A:103:LEU:HA	1:A:106:LEU:HB3	2.00	0.43
1:C:91:GLY:O	1:C:93:PHE:N	2.51	0.43
9:C:2013:PC1:H272	9:C:2013:PC1:H331	1.99	0.43
2:D:203:LYS:HE2	2:D:203:LYS:HB3	1.79	0.43
1:C:185:GLU:HG3	1:C:248:ARG:HE	1.84	0.43
1:C:924:TRP:O	1:C:928:VAL:HG23	2.18	0.43
1:C:884:ASP:OD1	1:C:905:LYS:NZ	2.48	0.43
1:C:592:VAL:O	1:C:596:VAL:HG13	2.19	0.43
1:A:32:VAL:O	1:A:262:ARG:NH1	2.52	0.43
8:C:2010:CLR:C24	9:C:2014:PC1:H2I2	2.48	0.43
1:C:297:VAL:O	1:C:301:ILE:HG23	2.19	0.43
1:A:827:ARG:HH21	1:A:934:ARG:HD3	1.83	0.43
1:C:209:SER:C	1:C:211:LEU:H	2.22	0.43
1:C:618:LYS:HB2	1:C:657:VAL:HG21	2.01	0.43
1:C:295:LEU:HD13	1:C:780:ILE:HD13	2.01	0.43
1:A:514:ILE:HG22	1:A:516:ILE:HG12	2.01	0.43
1:A:285:ILE:HA	1:A:288:ILE:HG22	1.99	0.43
2:D:251:GLN:HB3	2:D:254:TYR:HB2	2.00	0.43
2:B:94:ASP:HA	2:B:95:PRO:HD3	1.79	0.43
2:D:178:ILE:HD13	2:D:211:VAL:HG11	2.01	0.43
2:D:24:PHE:C	2:D:26:GLY:H	2.22	0.43
2:D:138:GLU:HG3	2:D:140:ASN:ND2	2.34	0.43
1:C:611:GLY:HA2	1:C:686:THR:H	1.83	0.43
1:C:707:VAL:HG23	1:C:721:ALA:HB2	2.00	0.43
1:A:667:THR:OG1	1:A:668:SER:N	2.51	0.43
1:A:986:PRO:CG	8:A:2009:CLR:H181	2.48	0.42
1:A:544:ARG:O	1:A:583:SER:HA	2.19	0.42
1:C:777:ILE:HD12	1:C:777:ILE:N	2.31	0.42
9:A:2012:PC1:H152	9:A:2012:PC1:H112	1.85	0.42
1:C:1013:GLU:OE1	2:D:27:ARG:NH2	2.52	0.42
1:A:667:THR:HG23	1:A:670:GLN:H	1.83	0.42
2:B:136:ARG:HD2	2:B:143:ARG:HH12	1.84	0.42
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.99	0.42
1:C:84:LYS:HE2	1:C:84:LYS:HB3	1.88	0.42
1:A:35:ASP:HB2	1:A:37:HIS:ND1	2.34	0.42
1:A:340:THR:HG21	1:A:761:ILE:CG1	2.49	0.42
1:C:889:ASN:HD22	1:C:900:THR:HB	1.84	0.42
1:C:431:GLU:OE2	1:C:438:ARG:NH1	2.52	0.42
2:D:170:LYS:N	2:D:170:LYS:HD2	2.34	0.42
1:C:925:ALA:O	1:C:929:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:PHE:HE2	2:B:262:GLN:HB3	1.84	0.42
1:A:99:ILE:O	1:A:103:LEU:HG	2.19	0.42
1:A:231:GLU:H	1:A:231:GLU:HG2	1.66	0.42
1:C:831:ASN:HD21	2:D:6:ALA:HB2	1.84	0.42
1:A:819:GLN:H	1:A:819:GLN:HG3	1.42	0.42
2:B:123:PHE:HB3	2:B:150:ARG:HG3	2.00	0.42
2:D:37:LEU:O	2:D:41:ILE:HG23	2.18	0.42
1:C:27:GLU:C	1:C:29:LYS:H	2.22	0.42
1:C:115:GLU:HG2	1:C:116:GLU:H	1.84	0.42
3:E:27:ARG:O	3:E:31:LEU:HG	2.20	0.42
1:C:39:LEU:HA	1:C:39:LEU:HD23	1.85	0.42
1:A:365:THR:HG23	1:A:605:LYS:HB3	2.02	0.42
1:A:963:TYR:CZ	8:A:2010:CLR:H21	2.55	0.42
1:A:505:GLU:CD	1:A:685:ARG:HH11	2.21	0.42
2:D:242:TYR:CG	2:D:257:PRO:HG3	2.54	0.42
1:A:476:ASN:ND2	1:A:479:ASN:HB2	2.33	0.42
1:C:462:GLU:O	1:C:466:ARG:HG3	2.20	0.42
1:C:781:THR:N	1:C:782:PRO:HD2	2.35	0.42
1:A:501:LYS:HE3	6:A:2004:ADP:N1	2.35	0.42
1:C:815:LEU:HD12	1:C:815:LEU:HA	1.76	0.42
1:C:430:GLN:HA	1:C:430:GLN:HE21	1.85	0.42
8:A:2010:CLR:H211	8:A:2010:CLR:H232	1.83	0.42
1:C:613:HIS:HD2	1:C:615:ILE:H	1.66	0.42
1:A:191:ARG:NH2	1:A:239:SER:HA	2.35	0.42
2:D:204:TYR:HD2	2:D:207:TYR:H	1.68	0.42
1:A:1001:ILE:O	1:A:1005:ARG:HB2	2.20	0.42
1:A:226:ASN:HB3	1:A:231:GLU:HB2	2.00	0.42
9:A:2012:PC1:H2A2	9:A:2012:PC1:H2E2	2.02	0.42
1:A:953:GLU:HB3	9:A:2012:PC1:H2D2	2.02	0.42
1:A:71:ASN:HB3	1:A:175:ALA:O	2.20	0.42
1:C:814:SER:HB3	1:C:946:ILE:HG22	2.02	0.42
1:A:781:THR:HG22	8:B:3001:CLR:H271	2.02	0.42
1:C:420:LEU:C	1:C:422:ASN:H	2.23	0.42
1:A:386:PHE:CE2	1:A:391:HIS:CD2	3.08	0.42
1:C:180:VAL:HG23	11:C:2108:HOH:O	2.19	0.42
9:A:2013:PC1:H381	9:A:2013:PC1:H2A2	2.02	0.42
2:D:94:ASP:HA	2:D:95:PRO:HD3	1.90	0.42
1:C:154:PHE:HA	1:C:154:PHE:HD2	1.75	0.42
1:A:327:GLU:H	1:A:327:GLU:CD	2.23	0.42
1:A:411:TRP:CE3	1:A:414:LEU:HD23	2.55	0.42
9:D:401:PC1:H291	9:D:401:PC1:H351	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLN:HG3	1:C:589:ARG:HA	2.01	0.41
9:A:2011:PC1:H372	9:A:2014:PC1:H351	2.02	0.41
1:A:882:ASN:HA	1:A:885:ASP:HB2	2.01	0.41
2:D:157:GLY:N	2:D:230:PHE:HB3	2.35	0.41
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.90	0.41
1:C:375:THR:HA	1:C:588:PRO:HA	2.02	0.41
1:A:638:ALA:HB2	1:A:648:VAL:HG21	2.00	0.41
1:A:216:GLU:HA	1:A:217:PRO:HD3	1.87	0.41
1:C:129:LEU:HA	1:C:129:LEU:HD23	1.86	0.41
1:A:31:GLU:HG3	1:A:32:VAL:H	1.84	0.41
1:A:410:THR:HG23	1:A:515:LEU:HD22	2.01	0.41
1:A:537:GLU:O	1:A:541:LEU:HD22	2.19	0.41
1:A:398:ASN:ND2	1:A:400:SER:O	2.53	0.41
1:C:1009:TRP:CZ2	2:D:35:ILE:HG22	2.53	0.41
1:C:916:PHE:O	1:C:920:VAL:HG23	2.20	0.41
1:C:587:PRO:HA	1:C:588:PRO:HD3	1.96	0.41
1:A:637:ILE:HD13	1:A:640:ARG:NH1	2.35	0.41
1:C:41:LEU:O	1:C:52:LEU:HD11	2.20	0.41
1:C:195:ASP:O	1:C:252:VAL:HG22	2.20	0.41
2:D:95:PRO:HA	2:D:98:TYR:CE1	2.56	0.41
2:B:25:LEU:HG	2:B:25:LEU:O	2.20	0.41
2:B:238:PHE:HA	2:B:239:PRO:HD2	1.87	0.41
1:A:861:THR:HG22	1:A:983:CYS:HB3	2.02	0.41
1:C:504:PRO:HA	1:C:547:GLY:HA3	2.02	0.41
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.91	0.41
1:A:778:PRO:HB3	1:A:855:ALA:HA	2.01	0.41
1:C:860:PHE:HZ	8:C:2010:CLR:H193	1.85	0.41
1:A:472:GLU:CB	1:A:484:SER:HB3	2.51	0.41
2:D:99:GLU:O	2:D:103:VAL:HG23	2.19	0.41
1:A:663:LEU:HD21	1:A:671:LEU:HG	2.02	0.41
1:C:199:ILE:HA	1:C:199:ILE:HD13	1.75	0.41
1:A:384:MET:SD	1:A:384:MET:N	2.93	0.41
2:B:39:TYR:CZ	8:B:3001:CLR:H191	2.56	0.41
8:A:2010:CLR:H183	3:G:33:PHE:CZ	2.56	0.41
1:A:505:GLU:OE2	1:A:613:HIS:ND1	2.38	0.41
2:D:27:ARG:HG3	2:D:31:SER:HB3	2.01	0.41
2:B:24:PHE:HA	2:B:24:PHE:HD2	1.74	0.41
1:A:430:GLN:HA	1:A:430:GLN:HE21	1.86	0.41
2:B:61:ILE:HG23	2:B:67:THR:HG23	2.02	0.41
1:A:565:ASP:H	1:A:570:ASN:CB	2.27	0.41
1:A:501:LYS:HG3	6:A:2004:ADP:H2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ASN:HA	9:A:2011:PC1:O11	2.21	0.41
1:C:842:LEU:HD12	1:C:1016:TYR:HD2	1.86	0.41
1:C:36:ASP:HB2	1:C:39:LEU:HD12	2.02	0.41
2:B:27:ARG:HB2	2:B:28:THR:H	1.71	0.41
1:C:132:VAL:HG22	9:C:2013:PC1:H3A2	2.03	0.41
1:A:971:LEU:HB2	1:A:973:MET:HG3	2.03	0.41
1:C:75:PRO:O	1:C:77:PRO:HD3	2.21	0.41
2:D:216:LYS:HE2	2:D:273:ARG:O	2.21	0.41
1:A:301:ILE:HD11	9:A:2014:PC1:H3I1	2.03	0.41
1:A:350:LEU:HD23	1:A:742:ILE:HD12	2.03	0.41
2:B:190:PRO:HA	2:B:191:PRO:HD3	1.80	0.41
1:A:765:LEU:O	1:A:769:ILE:HG13	2.21	0.41
1:A:228:ASN:HB3	1:A:231:GLU:CG	2.51	0.41
1:A:451:LYS:O	1:A:455:LEU:HD12	2.21	0.41
1:A:263:ILE:HD12	1:A:265:THR:OG1	2.20	0.41
1:C:889:ASN:HD22	1:C:901:TYR:H	1.68	0.41
1:A:860:PHE:HA	2:B:50:PHE:HE2	1.86	0.41
1:A:908:GLU:O	1:A:911:CYS:HB2	2.21	0.41
1:A:637:ILE:HD13	1:A:640:ARG:HH12	1.86	0.41
2:B:112:TYR:CE2	2:B:255:LEU:HB3	2.55	0.41
1:A:209:SER:HB3	1:A:215:SER:HA	2.03	0.41
8:A:2010:CLR:C12	8:A:2010:CLR:H212	2.51	0.41
2:B:91:ARG:NH2	2:D:94:ASP:OD1	2.54	0.41
1:C:445:SER:OG	1:C:544:ARG:NH1	2.54	0.41
1:C:228:ASN:OD1	1:C:230:LEU:N	2.53	0.41
2:B:27:ARG:HG3	2:B:31:SER:CB	2.51	0.41
2:B:186:PHE:HZ	2:B:282:ASN:HB3	1.84	0.41
1:C:122:ASN:OD1	1:C:315:ILE:HG13	2.21	0.41
1:A:315:ILE:HA	1:A:315:ILE:HD13	1.85	0.41
1:C:889:ASN:HB3	1:C:900:THR:HA	2.03	0.41
2:B:134:LYS:HB2	2:B:136:ARG:HH12	1.86	0.41
2:D:79:GLN:HE21	2:D:83:SER:H	1.69	0.40
3:G:16:VAL:HG12	3:G:17:ASP:N	2.36	0.40
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.54	0.40
2:B:27:ARG:H	2:B:27:ARG:CD	2.34	0.40
9:A:2012:PC1:H2B1	9:A:2012:PC1:H281	1.91	0.40
2:D:27:ARG:HD3	2:D:32:TRP:CE3	2.56	0.40
1:C:921:VAL:HG12	1:C:924:TRP:CZ2	2.56	0.40
2:B:23:GLU:HG2	2:B:24:PHE:H	1.86	0.40
1:C:964:CYS:HA	1:C:965:PRO:HD2	1.83	0.40
1:C:972:ARG:HH12	2:D:288:LYS:HZ1	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:O	1:A:128:VAL:HG23	2.21	0.40
1:A:470:ILE:H	1:A:470:ILE:HG13	1.51	0.40
9:A:2013:PC1:H292	9:A:2013:PC1:C3B	2.45	0.40
1:A:1009:TRP:CZ2	2:B:35:ILE:HG22	2.49	0.40
1:A:183:LEU:HD23	1:A:183:LEU:H	1.86	0.40
1:A:293:VAL:O	1:A:297:VAL:HG13	2.21	0.40
1:C:1000:LEU:HG	9:C:2014:PC1:H12	2.04	0.40
1:C:626:ILE:O	1:C:680:GLU:HB3	2.20	0.40
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.85	0.40
1:A:815:LEU:O	1:A:818:GLU:HB2	2.22	0.40
1:A:483:LEU:HD12	1:A:484:SER:N	2.37	0.40
2:D:241:GLN:HG3	2:D:242:TYR:CD1	2.56	0.40
1:A:801:LEU:O	1:A:805:LEU:HG	2.22	0.40
1:C:1002:ILE:HG23	1:C:1011:GLU:HB2	2.03	0.40
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.56	0.40
1:A:501:LYS:HG3	6:A:2004:ADP:C2	2.57	0.40
1:C:287:ILE:H	1:C:287:ILE:HG13	1.57	0.40
2:D:61:ILE:HG23	2:D:67:THR:HG23	2.03	0.40
1:C:783:PHE:CE2	1:C:787:ILE:HD11	2.57	0.40
1:A:926:ASP:HA	1:A:929:ILE:HG12	2.02	0.40
2:B:52:GLY:O	2:B:56:VAL:HG23	2.22	0.40
9:C:2014:PC1:H2A1	9:C:2014:PC1:H272	1.71	0.40
1:A:318:ILE:HD13	1:A:318:ILE:HA	1.89	0.40
1:A:634:VAL:HG23	1:A:645:VAL:HG12	2.03	0.40
1:C:410:THR:HA	1:C:515:LEU:HD22	2.02	0.40
1:A:115:GLU:HG2	1:A:116:GLU:N	2.37	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	992/1016 (98%)	882 (89%)	97 (10%)	13 (1%)	15	44
1	C	992/1016 (98%)	890 (90%)	88 (9%)	14 (1%)	14	42
2	B	301/303 (99%)	234 (78%)	55 (18%)	12 (4%)	4	12
2	D	301/303 (99%)	231 (77%)	55 (18%)	15 (5%)	3	8
3	E	33/65 (51%)	32 (97%)	0	1 (3%)	5	18
3	G	32/65 (49%)	27 (84%)	3 (9%)	2 (6%)	2	4
All	All	2651/2768 (96%)	2296 (87%)	298 (11%)	57 (2%)	8	28

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	139	TYR
3	G	17	ASP
3	G	18	PRO
1	C	267	ALA
1	C	398	ASN
1	C	880	ARG
3	E	18	PRO
2	B	19	SER
2	B	201	VAL
2	B	204	TYR
1	C	34	MET
1	C	92	GLY
1	C	629	GLU
2	D	82	GLN
2	D	201	VAL
2	D	204	TYR
1	A	362	SER
1	A	560	GLU
1	A	775	SER
1	A	804	ASP
2	B	142	GLU
2	B	265	ASN
1	C	775	SER
2	D	73	ALA
2	D	118	LYS
2	D	206	PRO
1	A	34	MET
1	A	394	ASP

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Mol	Chain	Res	Type
2	B	21	LYS
2	B	133	LEU
1	C	373	THR
1	C	432	ASN
1	C	804	ASP
2	D	139	TYR
2	D	158	ASN
2	D	265	ASN
1	A	118	PRO
2	B	73	ALA
2	B	156	LEU
1	C	306	LEU
2	D	63	GLU
2	D	194	GLU
2	D	203	LYS
1	A	629	GLU
1	A	893	ASP
2	B	203	LYS
2	B	206	PRO
1	C	210	SER
2	D	219	GLU
1	A	92	GLY
1	C	593	PRO
1	C	630	GLY
2	D	261	VAL
1	A	489	PRO
2	D	127	GLY

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	844/861 (98%)	723 (86%)	121 (14%)	4	12
1	C	844/861 (98%)	751 (89%)	93 (11%)	8	23
2	B	269/269 (100%)	234 (87%)	35 (13%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	269/269 (100%)	238 (88%)	31 (12%)	7	21
3	E	29/52 (56%)	24 (83%)	5 (17%)	2	7
3	G	28/52 (54%)	27 (96%)	1 (4%)	42	76
All	All	2283/2364 (97%)	1997 (88%)	286 (12%)	6	17

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	44	LEU
1	A	56	LEU
1	A	57	THR
1	A	60	ARG
1	A	81	GLU
1	A	82	TRP
1	A	83	VAL
1	A	121	ASP
1	A	125	LEU
1	A	129	LEU
1	A	152	GLU
1	A	158	VAL
1	A	161	GLN
1	A	171	MET
1	A	192	ILE
1	A	210	SER
1	A	211	LEU
1	A	231	GLU
1	A	239	SER
1	A	241	ASN
1	A	242	CYS
1	A	252	VAL
1	A	266	LEU
1	A	268	SER
1	A	270	LEU
1	A	274	GLN
1	A	291	VAL
1	A	297	VAL
1	A	305	ILE
1	A	308	TYR
1	A	309	THR
1	A	310	TRP

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Mol	Chain	Res	Type
1	A	314	VAL
1	A	317	LEU
1	A	318	ILE
1	A	337	LEU
1	A	360	LEU
1	A	364	SER
1	A	365	THR
1	A	371	THR
1	A	379	MET
1	A	380	THR
1	A	384	MET
1	A	394	ASP
1	A	410	THR
1	A	417	ILE
1	A	425	VAL
1	A	430	GLN
1	A	433	LEU
1	A	437	LYS
1	A	438	ARG
1	A	440	VAL
1	A	450	LEU
1	A	455	LEU
1	A	461	LYS
1	A	469	LYS
1	A	471	VAL
1	A	473	ILE
1	A	476	ASN
1	A	478	THR
1	A	485	ILE
1	A	487	LYS
1	A	493	GLU
1	A	495	ARG
1	A	508	LEU
1	A	513	SER
1	A	514	ILE
1	A	515	LEU
1	A	519	LYS
1	A	520	GLU
1	A	521	GLN
1	A	523	LEU
1	A	535	TYR
1	A	541	LEU

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Mol	Chain	Res	Type
1	A	570	ASN
1	A	589	ARG
1	A	600	ARG
1	A	628	SER
1	A	629	GLU
1	A	634	VAL
1	A	635	GLU
1	A	663	LEU
1	A	666	MET
1	A	667	THR
1	A	671	LEU
1	A	675	LEU
1	A	681	ILE
1	A	687	SER
1	A	723	ILE
1	A	741	MET
1	A	744	LEU
1	A	750	SER
1	A	751	ILE
1	A	753	THR
1	A	763	ASP
1	A	765	LEU
1	A	775	SER
1	A	781	THR
1	A	791	ILE
1	A	805	LEU
1	A	814	SER
1	A	815	LEU
1	A	818	GLU
1	A	819	GLN
1	A	822	SER
1	A	823	ASP
1	A	824	ILE
1	A	830	ARG
1	A	845	MET
1	A	880	ARG
1	A	881	VAL
1	A	882	ASN
1	A	884	ASP
1	A	900	THR
1	A	936	SER
1	A	957	LEU

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Mol	Chain	Res	Type
1	A	969	VAL
1	A	998	ARG
1	A	1004	ARG
1	A	1010	VAL
2	B	20	GLU
2	B	22	LYS
2	B	24	PHE
2	B	27	ARG
2	B	37	LEU
2	B	41	ILE
2	B	45	CYS
2	B	54	ILE
2	B	57	MET
2	B	61	ILE
2	B	63	GLU
2	B	72	VAL
2	B	78	THR
2	B	90	PHE
2	B	119	ASP
2	B	129	VAL
2	B	158	ASN
2	B	162	LEU
2	B	170	LYS
2	B	171	ASP
2	B	180	LEU
2	B	187	LYS
2	B	193	ASN
2	B	204	TYR
2	B	216	LYS
2	B	217	ARG
2	B	221	LYS
2	B	222	GLU
2	B	224	VAL
2	B	249	LEU
2	B	259	MET
2	B	263	PHE
2	B	290	ARG
2	B	295	PHE
2	B	301	VAL
3	G	20	TYR
1	C	28	LEU
1	C	36	ASP

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Mol	Chain	Res	Type
1	C	44	LEU
1	C	56	LEU
1	C	57	THR
1	C	60	ARG
1	C	82	TRP
1	C	85	PHE
1	C	86	CYS
1	C	95	MET
1	C	114	THR
1	C	125	LEU
1	C	129	LEU
1	C	154	PHE
1	C	161	GLN
1	C	166	ARG
1	C	172	SER
1	C	191	ARG
1	C	241	ASN
1	C	242	CYS
1	C	244	GLU
1	C	254	THR
1	C	274	GLN
1	C	277	ILE
1	C	287	ILE
1	C	293	VAL
1	C	308	TYR
1	C	309	THR
1	C	310	TRP
1	C	317	LEU
1	C	336	CYS
1	C	360	LEU
1	C	371	THR
1	C	379	MET
1	C	380	THR
1	C	394	ASP
1	C	403	SER
1	C	412	LEU
1	C	423	ARG
1	C	430	GLN
1	C	433	LEU
1	C	450	LEU
1	C	454	GLU
1	C	469	LYS

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Mol	Chain	Res	Type
1	C	473	ILE
1	C	476	ASN
1	C	478	THR
1	C	491	THR
1	C	493	GLU
1	C	495	ARG
1	C	500	MET
1	C	514	ILE
1	C	519	LYS
1	C	520	GLU
1	C	521	GLN
1	C	523	LEU
1	C	535	TYR
1	C	541	LEU
1	C	550	HIS
1	C	600	ARG
1	C	612	ASP
1	C	629	GLU
1	C	645	VAL
1	C	662	ASP
1	C	667	THR
1	C	671	LEU
1	C	681	ILE
1	C	687	SER
1	C	708	THR
1	C	719	LYS
1	C	723	ILE
1	C	744	LEU
1	C	750	SER
1	C	772	THR
1	C	791	ILE
1	C	805	LEU
1	C	815	LEU
1	C	818	GLU
1	C	824	ILE
1	C	859	PHE
1	C	861	THR
1	C	880	ARG
1	C	881	VAL
1	C	886	ARG
1	C	888	ILE
1	C	894	SER

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Mol	Chain	Res	Type
1	C	900	THR
1	C	936	SER
1	C	969	VAL
1	C	980	TRP
1	C	1000	LEU
1	C	1004	ARG
1	C	1010	VAL
2	D	20	GLU
2	D	22	LYS
2	D	27	ARG
2	D	35	ILE
2	D	57	MET
2	D	61	ILE
2	D	63	GLU
2	D	72	VAL
2	D	78	THR
2	D	90	PHE
2	D	119	ASP
2	D	150	ARG
2	D	162	LEU
2	D	170	LYS
2	D	171	ASP
2	D	177	ILE
2	D	180	LEU
2	D	187	LYS
2	D	204	TYR
2	D	216	LYS
2	D	217	ARG
2	D	221	LYS
2	D	222	GLU
2	D	224	VAL
2	D	249	LEU
2	D	259	MET
2	D	261	VAL
2	D	263	PHE
2	D	294	ARG
2	D	295	PHE
2	D	301	VAL
3	E	20	TYR
3	E	24	GLU
3	E	36	LEU
3	E	47	SER

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Mol	Chain	Res	Type
3	E	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	GLN
1	A	143	GLN
1	A	156	ASN
1	A	161	GLN
1	A	274	GLN
1	A	432	ASN
1	A	550	HIS
1	A	570	ASN
1	A	575	ASN
1	A	699	GLN
1	A	747	ASN
1	A	790	ASN
1	A	819	GLN
1	A	889	ASN
1	A	903	GLN
1	A	944	ASN
2	B	181	ASN
2	B	262	GLN
2	B	292	GLN
3	G	28	ASN
1	C	119	GLN
1	C	120	ASN
1	C	143	GLN
1	C	156	ASN
1	C	161	GLN
1	C	274	GLN
1	C	388	ASN
1	C	430	GLN
1	C	550	HIS
1	C	570	ASN
1	C	699	GLN
1	C	790	ASN
1	C	854	GLN
1	C	889	ASN
1	C	897	GLN
1	C	903	GLN

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Mol	Chain	Res	Type
1	C	923	GLN
1	C	940	GLN
2	D	69	GLN
2	D	140	ASN
2	D	262	GLN
2	D	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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	$\# Z > 2$
5	ALF	A	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	A	2004	4	22,29,29	1.27	2 (9%)	27,45,45	1.88	6 (22%)
8	CLR	A	2009	-	31,31,31	4.38	14 (45%)	48,48,48	2.45	16 (33%)
8	CLR	A	2010	-	31,31,31	4.41	14 (45%)	48,48,48	2.96	20 (41%)
9	PC1	A	2011	-	53,53,53	0.86	3 (5%)	57,61,61	1.18	5 (8%)
9	PC1	A	2012	-	53,53,53	0.88	3 (5%)	57,61,61	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PC1	A	2013	-	53,53,53	0.87	3 (5%)	57,61,61	1.16	4 (7%)
9	PC1	A	2014	-	53,53,53	0.88	4 (7%)	57,61,61	1.30	4 (7%)
8	CLR	B	3001	-	31,31,31	4.38	13 (41%)	48,48,48	2.35	16 (33%)
9	PC1	B	3002	-	53,53,53	0.85	3 (5%)	57,61,61	1.17	4 (7%)
10	NAG	B	3003	-	14,14,15	0.40	0	15,19,21	0.75	0
5	ALF	C	2002	-	0,4,4	0.00	-	0,6,6	0.00	-
6	ADP	C	2004	-	22,29,29	0.98	2 (9%)	27,45,45	1.78	5 (18%)
8	CLR	C	2009	-	31,31,31	4.31	14 (45%)	48,48,48	2.38	16 (33%)
8	CLR	C	2010	-	31,31,31	4.40	13 (41%)	48,48,48	2.43	19 (39%)
8	CLR	C	2011	-	31,31,31	4.50	13 (41%)	48,48,48	2.46	19 (39%)
9	PC1	C	2012	-	53,53,53	0.87	4 (7%)	57,61,61	1.25	5 (8%)
9	PC1	C	2013	-	53,53,53	0.88	3 (5%)	57,61,61	1.30	5 (8%)
9	PC1	C	2014	-	53,53,53	0.91	4 (7%)	57,61,61	1.28	6 (10%)
9	PC1	C	2015	-	53,53,53	0.86	3 (5%)	57,61,61	1.26	5 (8%)
9	PC1	D	401	-	53,53,53	0.88	3 (5%)	57,61,61	1.21	4 (7%)
10	NAG	D	402	-	14,14,15	0.44	0	15,19,21	0.74	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
5	ALF	A	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	A	2004	4	-	0/12/32/32	0/3/3/3
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	A	2010	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2012	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2013	-	-	0/57/57/57	0/0/0/0
9	PC1	A	2014	-	-	0/57/57/57	0/0/0/0
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4
9	PC1	B	3002	-	-	0/57/57/57	0/0/0/0
10	NAG	B	3003	-	-	0/6/23/26	0/1/1/1
5	ALF	C	2002	-	-	0/0/0/0	0/0/0/0
6	ADP	C	2004	-	-	0/12/32/32	0/3/3/3
8	CLR	C	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	C	2010	-	-	0/10/68/68	0/4/4/4
8	CLR	C	2011	-	-	0/10/68/68	0/4/4/4
9	PC1	C	2012	-	-	0/57/57/57	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	C	2013	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2014	-	-	0/57/57/57	0/0/0/0
9	PC1	C	2015	-	-	2/57/57/57	0/0/0/0
9	PC1	D	401	-	-	0/57/57/57	0/0/0/0
10	NAG	D	402	-	-	0/6/23/26	0/1/1/1

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2011	CLR	C10-C9	-12.49	1.33	1.56
8	A	2010	CLR	C10-C9	-12.40	1.33	1.56
8	A	2009	CLR	C10-C9	-12.19	1.34	1.56
8	C	2010	CLR	C10-C9	-11.95	1.34	1.56
8	B	3001	CLR	C10-C9	-11.93	1.34	1.56
8	C	2009	CLR	C10-C9	-11.92	1.34	1.56
8	B	3001	CLR	C12-C13	-9.52	1.35	1.54
8	C	2011	CLR	C12-C13	-9.45	1.35	1.54
8	C	2010	CLR	C12-C13	-9.19	1.36	1.54
8	C	2009	CLR	C12-C13	-8.95	1.36	1.54
8	A	2009	CLR	C12-C13	-8.94	1.36	1.54
8	A	2010	CLR	C13-C14	-8.88	1.37	1.55
8	A	2010	CLR	C12-C13	-8.68	1.37	1.54
8	B	3001	CLR	C13-C14	-8.60	1.37	1.55
8	C	2011	CLR	C13-C14	-8.57	1.37	1.55
8	C	2010	CLR	C13-C14	-8.40	1.38	1.55
8	C	2009	CLR	C13-C14	-8.20	1.38	1.55
8	A	2009	CLR	C13-C14	-8.12	1.38	1.55
8	C	2011	CLR	C18-C13	-5.41	1.44	1.54
8	B	3001	CLR	C18-C13	-5.25	1.44	1.54
8	C	2011	CLR	C8-C14	-5.18	1.43	1.53
8	A	2010	CLR	C18-C13	-5.10	1.44	1.54
8	C	2010	CLR	C18-C13	-5.08	1.44	1.54
8	C	2010	CLR	C8-C14	-4.91	1.43	1.53
8	B	3001	CLR	C8-C14	-4.86	1.44	1.53
8	C	2009	CLR	C18-C13	-4.84	1.45	1.54
8	A	2009	CLR	C8-C14	-4.78	1.44	1.53
8	A	2010	CLR	C8-C14	-4.72	1.44	1.53
8	C	2009	CLR	C8-C14	-4.70	1.44	1.53
8	A	2009	CLR	C18-C13	-4.61	1.45	1.54
8	C	2010	CLR	C20-C17	-4.29	1.46	1.54
8	C	2011	CLR	C20-C17	-4.24	1.46	1.54
8	C	2011	CLR	C19-C10	-4.24	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2010	CLR	C19-C10	-4.17	1.47	1.54
8	A	2009	CLR	C19-C10	-4.15	1.47	1.54
8	B	3001	CLR	C20-C17	-4.12	1.46	1.54
8	A	2009	CLR	C20-C17	-4.02	1.46	1.54
8	C	2009	CLR	C20-C17	-3.88	1.47	1.54
8	C	2010	CLR	C19-C10	-3.84	1.47	1.54
8	B	3001	CLR	C19-C10	-3.59	1.48	1.54
8	C	2011	CLR	C16-C17	-3.37	1.46	1.54
8	C	2009	CLR	C19-C10	-3.35	1.48	1.54
8	A	2010	CLR	C16-C17	-3.10	1.47	1.54
8	A	2009	CLR	C16-C17	-2.82	1.47	1.54
8	B	3001	CLR	C16-C17	-2.74	1.48	1.54
8	C	2010	CLR	C16-C17	-2.69	1.48	1.54
8	A	2010	CLR	C20-C17	-2.62	1.49	1.54
8	A	2009	CLR	O1-C3	-2.58	1.35	1.43
8	C	2009	CLR	C16-C17	-2.54	1.48	1.54
9	A	2013	PC1	O21-C2	-2.47	1.40	1.46
8	A	2009	CLR	C1-C2	-2.40	1.48	1.53
9	B	3002	PC1	O21-C2	-2.38	1.40	1.46
8	C	2010	CLR	O1-C3	-2.34	1.36	1.43
8	A	2010	CLR	C1-C2	-2.31	1.48	1.53
9	A	2011	PC1	O21-C2	-2.30	1.40	1.46
9	A	2011	PC1	C3A-C39	-2.28	1.38	1.51
9	C	2015	PC1	C3A-C39	-2.20	1.38	1.51
9	B	3002	PC1	C3A-C39	-2.20	1.38	1.51
9	A	2013	PC1	C3A-C39	-2.19	1.38	1.51
8	B	3001	CLR	O1-C3	-2.17	1.37	1.43
8	C	2009	CLR	O1-C3	-2.15	1.37	1.43
9	C	2015	PC1	O21-C2	-2.15	1.41	1.46
9	C	2013	PC1	C3A-C39	-2.14	1.39	1.51
9	C	2014	PC1	C3A-C39	-2.14	1.39	1.51
9	A	2012	PC1	O21-C2	-2.14	1.41	1.46
9	C	2012	PC1	C3A-C39	-2.11	1.39	1.51
9	C	2012	PC1	O21-C2	-2.10	1.41	1.46
8	A	2010	CLR	O1-C3	-2.10	1.37	1.43
9	A	2012	PC1	C3A-C39	-2.10	1.39	1.51
9	D	401	PC1	O21-C2	-2.09	1.41	1.46
9	A	2014	PC1	O21-C2	-2.09	1.41	1.46
9	C	2014	PC1	O21-C2	-2.07	1.41	1.46
9	A	2014	PC1	C3A-C39	-2.05	1.39	1.51
8	C	2009	CLR	C1-C2	-2.04	1.48	1.53
8	C	2011	CLR	C1-C2	-2.03	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	401	PC1	C3A-C39	-2.00	1.40	1.51
9	A	2014	PC1	O21-C21	2.05	1.40	1.34
9	C	2014	PC1	O21-C21	2.05	1.40	1.34
9	C	2013	PC1	O21-C21	2.07	1.40	1.34
9	C	2012	PC1	O21-C21	2.09	1.40	1.34
6	C	2004	ADP	O4'-C1'	2.13	1.43	1.41
8	A	2010	CLR	C16-C15	2.18	1.60	1.54
8	C	2011	CLR	C16-C15	2.41	1.60	1.54
9	B	3002	PC1	O31-C31	2.62	1.41	1.33
6	C	2004	ADP	C5-C4	2.65	1.46	1.40
8	B	3001	CLR	C16-C15	2.86	1.62	1.54
8	A	2009	CLR	C16-C15	2.88	1.62	1.54
9	A	2013	PC1	O31-C31	2.94	1.42	1.33
9	C	2014	PC1	O31-C31	2.94	1.42	1.33
6	A	2004	ADP	O4'-C1'	2.96	1.45	1.41
9	A	2011	PC1	O31-C31	2.97	1.42	1.33
9	C	2015	PC1	O31-C31	2.99	1.42	1.33
8	C	2011	CLR	C6-C5	3.12	1.40	1.33
8	C	2010	CLR	C16-C15	3.13	1.62	1.54
8	C	2010	CLR	C6-C5	3.14	1.40	1.33
9	A	2014	PC1	O31-C31	3.24	1.43	1.33
9	C	2012	PC1	O31-C31	3.26	1.43	1.33
8	A	2010	CLR	C6-C5	3.28	1.41	1.33
9	A	2012	PC1	O31-C31	3.28	1.43	1.33
8	C	2009	CLR	C16-C15	3.28	1.63	1.54
9	D	401	PC1	O31-C31	3.30	1.43	1.33
9	C	2013	PC1	O31-C31	3.41	1.43	1.33
8	A	2009	CLR	C6-C5	3.44	1.41	1.33
8	B	3001	CLR	C6-C5	3.53	1.41	1.33
6	A	2004	ADP	C5-C4	3.55	1.48	1.40
8	C	2009	CLR	C6-C5	3.71	1.42	1.33
8	C	2009	CLR	C12-C11	5.23	1.65	1.53
8	B	3001	CLR	C12-C11	5.32	1.65	1.53
8	C	2010	CLR	C12-C11	5.54	1.65	1.53
8	C	2011	CLR	C12-C11	5.75	1.66	1.53
8	A	2009	CLR	C12-C11	5.83	1.66	1.53
8	A	2010	CLR	C12-C11	6.27	1.67	1.53
8	B	3001	CLR	C11-C9	11.07	1.73	1.53
8	A	2009	CLR	C11-C9	11.24	1.73	1.53
8	C	2009	CLR	C11-C9	11.30	1.73	1.53
8	C	2010	CLR	C11-C9	11.35	1.73	1.53
8	C	2011	CLR	C11-C9	11.42	1.74	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2010	CLR	C11-C9	11.57	1.74	1.53

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2010	CLR	C21-C20-C22	-10.07	93.56	110.35
8	A	2010	CLR	C21-C20-C17	-7.74	100.07	112.96
6	C	2004	ADP	N3-C2-N1	-5.97	124.32	128.89
6	A	2004	ADP	N3-C2-N1	-5.59	124.61	128.89
8	C	2010	CLR	C10-C5-C6	-4.55	114.50	122.92
8	C	2011	CLR	C11-C9-C8	-4.40	105.36	111.74
8	A	2010	CLR	C11-C9-C8	-4.39	105.36	111.74
8	A	2009	CLR	C19-C10-C9	-4.38	106.07	111.67
8	B	3001	CLR	C10-C5-C6	-4.35	114.88	122.92
8	C	2010	CLR	C11-C9-C8	-4.35	105.43	111.74
8	C	2011	CLR	C10-C5-C6	-4.31	114.95	122.92
8	C	2009	CLR	C10-C5-C6	-4.24	115.09	122.92
8	A	2009	CLR	C11-C9-C8	-4.09	105.80	111.74
8	B	3001	CLR	C11-C9-C8	-3.90	106.08	111.74
8	B	3001	CLR	C19-C10-C9	-3.73	106.90	111.67
6	C	2004	ADP	C4-C5-N7	-3.65	106.12	109.48
8	C	2009	CLR	C11-C9-C8	-3.65	106.45	111.74
8	A	2010	CLR	C10-C5-C6	-3.59	116.28	122.92
8	A	2009	CLR	C10-C5-C6	-3.51	116.43	122.92
6	A	2004	ADP	C4-C5-N7	-3.48	106.28	109.48
8	C	2010	CLR	C12-C13-C17	-3.45	110.43	116.56
8	C	2009	CLR	C19-C10-C9	-3.41	107.31	111.67
8	C	2010	CLR	C19-C10-C9	-3.38	107.34	111.67
8	B	3001	CLR	C12-C13-C17	-3.37	110.57	116.56
8	C	2011	CLR	C19-C10-C9	-3.37	107.37	111.67
8	A	2009	CLR	C18-C13-C12	-3.32	104.87	110.54
8	C	2009	CLR	C12-C13-C17	-3.20	110.88	116.56
6	A	2004	ADP	C2'-C1'-N9	-3.12	109.53	114.29
6	C	2004	ADP	C2'-C1'-N9	-3.03	109.67	114.29
8	A	2009	CLR	C12-C13-C17	-2.94	111.33	116.56
6	C	2004	ADP	PA-O3A-PB	-2.92	122.87	132.67
8	A	2010	CLR	C19-C10-C9	-2.91	107.95	111.67
8	C	2010	CLR	C23-C24-C25	-2.84	101.57	115.87
8	C	2010	CLR	C22-C20-C17	-2.76	104.43	110.24
8	C	2011	CLR	C12-C13-C17	-2.75	111.67	116.56
6	A	2004	ADP	O3A-PA-O5'	-2.75	95.65	102.94
8	A	2009	CLR	C19-C10-C1	-2.72	105.35	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2010	CLR	C18-C13-C12	-2.63	106.06	110.54
8	C	2010	CLR	C7-C8-C14	-2.60	106.80	110.86
8	C	2011	CLR	C18-C13-C12	-2.54	106.21	110.54
8	C	2011	CLR	C16-C17-C20	-2.52	107.55	112.05
8	A	2010	CLR	C19-C10-C1	-2.44	105.77	109.43
8	C	2009	CLR	C16-C17-C20	-2.44	107.71	112.05
8	C	2011	CLR	C3-C4-C5	-2.43	106.81	111.82
9	C	2014	PC1	O31-C31-O32	-2.40	117.28	123.49
8	C	2011	CLR	C27-C25-C26	-2.36	98.67	110.55
8	A	2010	CLR	C15-C14-C8	-2.34	115.33	119.03
8	C	2011	CLR	C2-C3-C4	-2.31	106.20	110.32
8	B	3001	CLR	C19-C10-C1	-2.31	105.97	109.43
8	A	2010	CLR	C18-C13-C17	-2.29	107.26	111.75
8	C	2011	CLR	C18-C13-C17	-2.26	107.33	111.75
9	A	2011	PC1	O31-C31-O32	-2.25	117.69	123.49
8	C	2009	CLR	C21-C20-C22	-2.24	106.61	110.35
8	A	2010	CLR	C7-C8-C14	-2.22	107.40	110.86
8	C	2010	CLR	C19-C10-C1	-2.19	106.14	109.43
8	A	2010	CLR	C18-C13-C12	-2.15	106.88	110.54
9	A	2012	PC1	O21-C21-O22	-2.13	117.94	123.67
8	C	2011	CLR	C21-C20-C22	-2.09	106.86	110.35
8	A	2009	CLR	C8-C7-C6	-2.06	109.63	112.75
8	B	3001	CLR	C21-C20-C22	-2.05	106.93	110.35
8	A	2010	CLR	C2-C3-C4	-2.04	106.69	110.32
8	C	2009	CLR	C18-C13-C17	-2.02	107.79	111.75
9	C	2015	PC1	O21-C21-O22	-2.01	118.26	123.67
8	A	2010	CLR	C23-C22-C20	-2.01	108.12	115.06
9	C	2012	PC1	O31-C31-O32	-2.00	118.32	123.49
8	A	2009	CLR	C1-C10-C9	2.03	111.25	108.64
9	C	2014	PC1	C2G-C2F-C2E	2.08	125.28	114.53
6	A	2004	ADP	O3B-PB-O2B	2.09	115.33	107.38
8	B	3001	CLR	C4-C5-C10	2.13	119.53	116.43
8	C	2009	CLR	C1-C10-C9	2.14	111.39	108.64
9	A	2013	PC1	O31-C31-C32	2.15	118.45	111.90
6	C	2004	ADP	O4'-C1'-N9	2.15	112.60	108.10
9	C	2013	PC1	C2-O21-C21	2.15	123.05	117.89
8	B	3001	CLR	C1-C10-C9	2.20	111.47	108.64
9	A	2012	PC1	C2-O21-C21	2.25	123.28	117.89
8	A	2010	CLR	C4-C5-C10	2.39	119.90	116.43
8	C	2010	CLR	C1-C10-C9	2.39	111.72	108.64
8	A	2010	CLR	C12-C13-C14	2.45	111.29	107.31
9	D	401	PC1	O31-C31-C32	2.45	119.37	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	3002	PC1	O31-C31-C32	2.48	119.47	111.90
9	C	2012	PC1	O31-C31-C32	2.59	119.80	111.90
8	A	2009	CLR	C4-C5-C6	2.62	125.02	120.57
9	A	2012	PC1	O31-C31-C32	2.62	119.90	111.90
8	C	2010	CLR	C4-C5-C10	2.63	120.25	116.43
9	C	2014	PC1	O31-C31-C32	2.63	119.92	111.90
9	A	2011	PC1	O31-C3-C2	2.64	115.80	108.69
9	B	3002	PC1	O31-C3-C2	2.64	115.81	108.69
9	C	2015	PC1	O31-C31-C32	2.67	120.03	111.90
8	C	2010	CLR	C4-C5-C6	2.72	125.19	120.57
9	C	2014	PC1	O31-C3-C2	2.78	116.17	108.69
9	A	2014	PC1	O31-C31-C32	2.80	120.42	111.90
8	C	2011	CLR	C10-C9-C8	2.86	116.89	112.67
8	A	2009	CLR	C9-C10-C5	2.89	114.16	109.67
8	B	3001	CLR	C12-C13-C14	2.89	112.01	107.31
8	A	2010	CLR	C10-C9-C8	2.90	116.95	112.67
9	A	2011	PC1	O31-C31-C32	2.90	120.73	111.90
9	A	2012	PC1	O21-C21-C22	2.93	117.89	111.53
8	C	2009	CLR	C12-C13-C14	2.93	112.07	107.31
8	B	3001	CLR	C4-C5-C6	2.96	125.59	120.57
6	A	2004	ADP	O2A-PA-O3A	2.97	118.57	105.09
9	C	2013	PC1	O31-C31-C32	2.97	120.96	111.90
8	C	2010	CLR	C10-C9-C8	3.00	117.11	112.67
8	C	2011	CLR	C12-C13-C14	3.14	112.41	107.31
8	C	2010	CLR	C12-C13-C14	3.18	112.48	107.31
9	A	2013	PC1	O31-C3-C2	3.25	117.44	108.69
8	C	2009	CLR	C4-C5-C6	3.25	126.09	120.57
9	D	401	PC1	O21-C21-C22	3.27	118.63	111.53
8	C	2010	CLR	C14-C8-C9	3.33	113.43	109.06
8	A	2009	CLR	C12-C13-C14	3.37	112.79	107.31
9	C	2013	PC1	O21-C21-C22	3.40	118.91	111.53
9	D	401	PC1	C15-N-C13	3.47	117.91	108.98
8	C	2009	CLR	C14-C8-C9	3.56	113.73	109.06
8	C	2009	CLR	C9-C10-C5	3.56	115.21	109.67
9	C	2015	PC1	O31-C3-C2	3.58	118.33	108.69
9	C	2012	PC1	O21-C21-C22	3.58	119.31	111.53
9	A	2014	PC1	C15-N-C13	3.60	118.23	108.98
8	C	2011	CLR	C4-C5-C10	3.60	121.68	116.43
9	A	2012	PC1	O31-C3-C2	3.61	118.40	108.69
9	C	2015	PC1	C15-N-C13	3.63	118.31	108.98
8	B	3001	CLR	C10-C9-C8	3.63	118.03	112.67
9	C	2014	PC1	C15-N-C13	3.63	118.32	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2010	CLR	C9-C10-C5	3.65	115.36	109.67
9	C	2012	PC1	O31-C3-C2	3.67	118.58	108.69
9	C	2013	PC1	O31-C3-C2	3.71	118.68	108.69
9	D	401	PC1	O31-C3-C2	3.74	118.77	108.69
8	C	2009	CLR	C10-C9-C8	3.78	118.25	112.67
9	A	2011	PC1	O21-C21-C22	3.80	119.78	111.53
9	A	2013	PC1	C15-N-C13	3.80	118.75	108.98
8	B	3001	CLR	C9-C10-C5	3.85	115.65	109.67
9	A	2013	PC1	O21-C21-C22	3.85	119.90	111.53
8	C	2011	CLR	C14-C8-C9	3.86	114.13	109.06
9	B	3002	PC1	C15-N-C13	3.88	118.96	108.98
9	B	3002	PC1	O21-C21-C22	3.88	119.97	111.53
9	A	2012	PC1	C15-N-C13	3.90	119.01	108.98
9	C	2014	PC1	O21-C21-C22	4.05	120.32	111.53
9	C	2013	PC1	C15-N-C13	4.06	119.41	108.98
9	A	2014	PC1	O21-C21-C22	4.07	120.37	111.53
9	A	2014	PC1	O31-C3-C2	4.11	119.75	108.69
9	A	2011	PC1	C15-N-C13	4.14	119.63	108.98
8	A	2009	CLR	C10-C9-C8	4.20	118.88	112.67
9	C	2012	PC1	C15-N-C13	4.23	119.86	108.98
8	C	2010	CLR	C13-C14-C8	4.25	121.02	114.37
8	C	2010	CLR	C9-C10-C5	4.33	116.41	109.67
8	B	3001	CLR	C14-C8-C9	4.34	114.76	109.06
9	C	2015	PC1	O21-C21-C22	4.45	121.21	111.53
8	A	2009	CLR	C14-C8-C9	4.57	115.06	109.06
8	C	2011	CLR	C11-C9-C10	4.64	119.25	113.11
8	C	2011	CLR	C9-C10-C5	4.68	116.95	109.67
8	B	3001	CLR	C11-C9-C10	4.69	119.33	113.11
8	A	2010	CLR	C14-C8-C9	4.69	115.22	109.06
8	A	2009	CLR	C11-C9-C10	4.76	119.42	113.11
8	B	3001	CLR	C13-C14-C8	4.93	122.07	114.37
8	C	2009	CLR	C11-C9-C10	4.94	119.66	113.11
8	C	2010	CLR	C11-C9-C10	4.96	119.68	113.11
8	C	2011	CLR	C13-C14-C8	5.18	122.46	114.37
8	A	2009	CLR	C13-C14-C8	5.18	122.47	114.37
8	A	2010	CLR	C11-C9-C10	5.20	120.01	113.11
8	C	2009	CLR	C13-C14-C8	5.26	122.59	114.37
8	A	2010	CLR	C13-C14-C8	5.41	122.83	114.37
8	A	2010	CLR	C17-C13-C14	5.71	106.81	100.09
8	B	3001	CLR	C17-C13-C14	6.43	107.65	100.09
8	C	2011	CLR	C17-C13-C14	6.58	107.83	100.09
8	A	2009	CLR	C17-C13-C14	6.86	108.16	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2010	CLR	C17-C13-C14	7.02	108.35	100.09
8	C	2009	CLR	C17-C13-C14	7.11	108.45	100.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	2015	PC1	C2-O21-C21-O22
9	C	2015	PC1	C2-O21-C21-C22

There are no ring outliers.

19 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2002	ALF	1	0
6	A	2004	ADP	5	0
8	A	2009	CLR	4	0
8	A	2010	CLR	8	0
9	A	2011	PC1	4	0
9	A	2012	PC1	4	0
9	A	2013	PC1	3	0
9	A	2014	PC1	4	0
8	B	3001	CLR	4	0
5	C	2002	ALF	2	0
6	C	2004	ADP	6	0
8	C	2009	CLR	4	0
8	C	2010	CLR	12	0
8	C	2011	CLR	7	0
9	C	2012	PC1	3	0
9	C	2013	PC1	3	0
9	C	2014	PC1	11	0
9	C	2015	PC1	6	0
9	D	401	PC1	3	0

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	994/1016 (97%)	-0.16	29 (2%)	55	43	25, 73, 140, 201	0
1	C	994/1016 (97%)	0.07	43 (4%)	39	27	47, 84, 159, 204	0
2	B	303/303 (100%)	0.83	46 (15%)	3	1	71, 147, 222, 240	0
2	D	303/303 (100%)	0.84	52 (17%)	2	1	71, 136, 214, 240	0
3	E	35/65 (53%)	0.63	5 (14%)	4	2	76, 95, 189, 199	0
3	G	34/65 (52%)	0.92	4 (11%)	6	3	78, 101, 174, 199	0
All	All	2663/2768 (96%)	0.18	179 (6%)	21	12	25, 89, 176, 240	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	15	ASP	15.1
2	D	218	ASP	14.2
2	D	166	THR	13.0
2	B	1	MET	11.9
1	C	396	THR	10.5
3	E	15	ASP	9.9
2	D	219	GLU	9.8
2	B	217	ARG	9.3
2	D	167	TYR	9.0
3	G	16	VAL	8.9
2	B	218	ASP	8.6
1	A	272	GLY	8.1
2	D	195	SER	8.0
2	B	165	GLU	7.9
2	D	198	THR	7.8
1	A	268	SER	7.8
2	D	2	ALA	7.6
1	A	271	GLU	7.4
2	B	220	ASP	7.4

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Mol	Chain	Res	Type	RSRZ
2	D	16	ILE	7.3
2	B	198	THR	7.2
2	B	202	MET	7.0
3	G	17	ASP	6.9
2	B	15	PHE	6.9
2	D	165	GLU	6.8
2	B	166	THR	6.7
2	D	15	PHE	6.6
1	C	397	GLU	6.6
1	C	268	SER	6.5
2	B	6	ALA	6.4
2	D	9	GLU	6.4
2	D	1	MET	6.2
1	C	395	THR	6.1
3	E	16	VAL	6.1
1	C	78	THR	5.9
2	D	6	ALA	5.9
2	B	9	GLU	5.9
1	A	23	ARG	5.8
2	D	203	LYS	5.8
2	D	217	ARG	5.8
2	D	196	LEU	5.7
2	D	194	GLU	5.7
3	E	18	PRO	5.6
1	A	265	THR	5.6
1	C	265	THR	5.6
2	B	219	GLU	5.5
2	D	162	LEU	5.3
2	D	24	PHE	5.3
1	C	398	ASN	5.2
2	D	23	GLU	5.1
2	D	11	SER	4.9
2	D	17	TRP	4.9
2	D	164	ASP	4.9
2	B	17	TRP	4.9
1	C	24	ASP	4.9
2	D	202	MET	4.9
2	B	23	GLU	4.8
1	A	273	GLY	4.8
1	A	401	GLY	4.8
2	B	163	ASN	4.8
2	B	164	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	395	THR	4.7
1	C	645	VAL	4.6
1	A	400	SER	4.6
2	B	196	LEU	4.6
1	A	24	ASP	4.6
1	C	117	GLU	4.5
2	B	194	GLU	4.4
2	D	201	VAL	4.4
3	E	17	ASP	4.4
1	C	23	ARG	4.3
2	B	3	ARG	4.3
2	B	7	LYS	4.2
1	A	267	ALA	4.1
1	A	396	THR	4.1
2	D	10	GLY	4.0
1	A	78	THR	4.0
1	C	266	LEU	4.0
1	C	116	GLU	4.0
1	C	642	ASN	4.0
2	B	10	GLY	3.9
2	D	220	ASP	3.8
1	A	117	GLU	3.8
2	B	4	GLY	3.8
2	B	201	VAL	3.8
2	B	227	MET	3.7
2	B	167	TYR	3.7
2	D	7	LYS	3.6
1	A	264	ALA	3.6
1	C	82	TRP	3.5
1	C	79	THR	3.5
1	C	273	GLY	3.5
2	B	193	ASN	3.4
2	D	197	GLU	3.4
1	C	495	ARG	3.4
1	C	270	LEU	3.3
2	D	163	ASN	3.3
1	A	266	LEU	3.2
1	C	377	ASN	3.2
2	D	200	PRO	3.1
1	C	85	PHE	3.1
2	B	142	GLU	3.1
1	A	888	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	5	LYS	3.1
2	D	118	LYS	3.1
2	B	195	SER	3.1
2	B	16	ILE	3.1
2	D	273	ARG	3.0
2	D	193	ASN	3.0
2	B	203	LYS	3.0
2	D	89	SER	3.0
1	C	269	GLY	3.0
2	D	19	SER	3.0
1	C	115	GLU	2.9
2	D	82	GLN	2.9
2	D	8	GLU	2.9
1	A	397	GLU	2.9
2	B	262	GLN	2.9
2	B	235	TYR	2.9
2	B	12	TRP	2.9
2	D	33	PHE	2.8
2	B	158	ASN	2.8
1	A	974	TYR	2.8
1	C	631	ASN	2.8
2	B	162	LEU	2.8
1	A	120	ASN	2.8
1	A	119	GLN	2.7
1	C	151	MET	2.7
1	A	399	GLN	2.7
3	G	20	TYR	2.6
2	B	118	LYS	2.6
2	B	302	LYS	2.6
2	B	2	ALA	2.6
1	A	82	TRP	2.6
1	A	270	LEU	2.6
2	D	3	ARG	2.6
2	B	200	PRO	2.6
1	C	700	ARG	2.6
2	B	5	LYS	2.6
1	C	124	TYR	2.6
2	B	120	ASP	2.5
1	C	133	VAL	2.5
1	A	269	GLY	2.5
1	C	120	ASN	2.5
1	C	650	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	49	ARG	2.5
2	D	21	LYS	2.5
2	D	228	GLU	2.5
2	B	21	LYS	2.5
2	B	192	LYS	2.5
1	C	406	LYS	2.4
2	D	18	ASN	2.4
2	B	230	PHE	2.4
1	C	87	ARG	2.4
1	A	30	LYS	2.4
1	C	123	LEU	2.3
2	D	236	PRO	2.3
2	D	141	ASN	2.3
2	D	290	ARG	2.3
2	B	207	TYR	2.3
1	A	123	LEU	2.3
2	D	4	GLY	2.3
1	C	1004	ARG	2.3
1	C	122	ASN	2.3
2	D	128	ASN	2.3
1	A	308	TYR	2.2
1	C	90	PHE	2.2
1	C	141	TYR	2.2
1	C	80	PRO	2.1
2	D	115	LEU	2.1
1	A	495	ARG	2.1
1	C	300	PHE	2.1
1	C	492	ALA	2.1
2	D	30	GLY	2.1
2	D	95	PRO	2.1
2	B	107	ARG	2.0
1	C	935	ASN	2.0
1	C	267	ALA	2.0
1	C	646	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
7	NA	A	2005	1/1	0.93	0.44	13.00	159,159,159,159	0
7	NA	A	2007	1/1	0.84	0.43	5.41	127,127,127,127	0
7	NA	C	2007	1/1	0.92	0.35	5.26	179,179,179,179	0
9	PC1	C	2015	54/54	0.75	0.45	4.83	119,145,185,228	0
8	CLR	A	2009	28/28	0.87	0.40	4.69	115,125,157,163	0
9	PC1	C	2014	54/54	0.77	0.51	3.41	93,138,188,199	0
7	NA	A	2006	1/1	0.72	0.27	3.38	86,86,86,86	0
9	PC1	A	2012	54/54	0.81	0.40	3.30	70,138,173,177	0
8	CLR	A	2010	28/28	0.91	0.26	2.78	91,115,123,156	0
9	PC1	C	2013	54/54	0.79	0.36	2.67	76,124,159,196	0
8	CLR	B	3001	28/28	0.85	0.29	2.32	55,124,129,156	0
8	CLR	C	2010	28/28	0.88	0.29	2.28	42,104,166,180	0
9	PC1	A	2013	54/54	0.87	0.33	2.25	88,124,142,168	0
9	PC1	B	3002	54/54	0.80	0.29	2.13	76,116,145,193	0
5	ALF	A	2002	5/5	0.98	0.24	2.02	9,16,42,141	0
7	NA	C	2006	1/1	0.89	0.27	1.96	113,113,113,113	0
9	PC1	D	401	54/54	0.87	0.26	1.60	68,94,169,191	0
9	PC1	A	2011	54/54	0.90	0.30	0.80	81,119,150,155	0
8	CLR	C	2009	28/28	0.89	0.24	0.73	56,113,136,137	0
9	PC1	C	2012	54/54	0.89	0.30	0.63	93,118,156,159	0
7	NA	C	2005	1/1	0.91	0.20	0.53	84,84,84,84	0
9	PC1	A	2014	54/54	0.81	0.38	0.49	105,138,172,233	0
4	MG	A	2003	1/1	0.94	0.18	0.46	24,24,24,24	0
5	ALF	C	2002	5/5	0.95	0.16	-0.58	38,48,56,67	0
6	ADP	C	2004	27/27	0.95	0.15	-0.69	8,62,69,86	0
8	CLR	C	2011	28/28	0.94	0.12	-0.97	45,98,125,139	0
6	ADP	A	2004	27/27	0.97	0.11	-1.05	6,35,51,60	0
4	MG	C	2003	1/1	0.99	0.08	-2.50	48,48,48,48	0
10	NAG	B	3003	14/15	0.80	0.51	-	145,151,160,164	0
7	NA	A	2008	1/1	0.76	0.26	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NA	C	2008	1/1	0.88	0.39	-	62,62,62,62	0
4	MG	C	2001	1/1	0.85	0.28	-	96,96,96,96	0
10	NAG	D	402	14/15	0.84	0.26	-	114,138,143,143	0
4	MG	A	2001	1/1	0.88	0.41	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.