



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:39 AM UTC

PDB ID : 3E3K / pdb_00003e3k
Title : Structural characterization of a putative endogenous metal chelator in the periplasmic nickel transporter NikA (butane-1,2,4-tricarboxylate without nickel form)
Authors : Cherrier, M.V.; Cavazza, C.; Bochot, C.; Lemaire, D.; Fontecilla-Camps, J.C.
Deposited on : 2008-08-07
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

<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

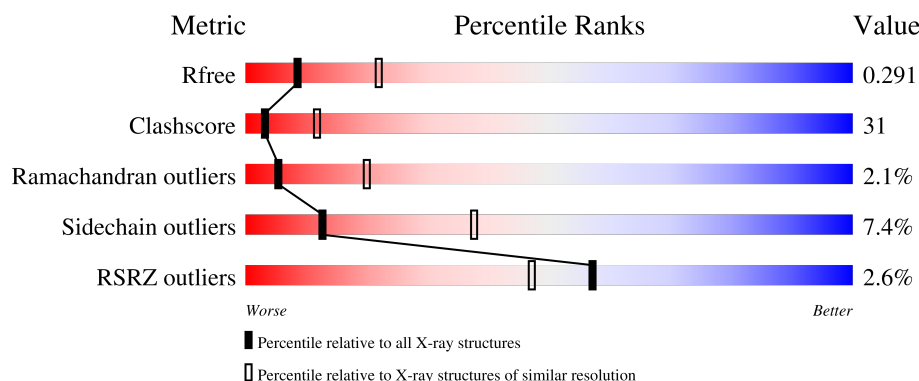
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	502	
1	B	502	
1	C	502	

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
3	ACT	B	505	-	-	X	-
5	HCT	A	507	X	-	-	-
5	HCT	B	508[A]	X	-	-	-
5	HCT	C	508	X	-	X	-

2 Entry composition [i](#)

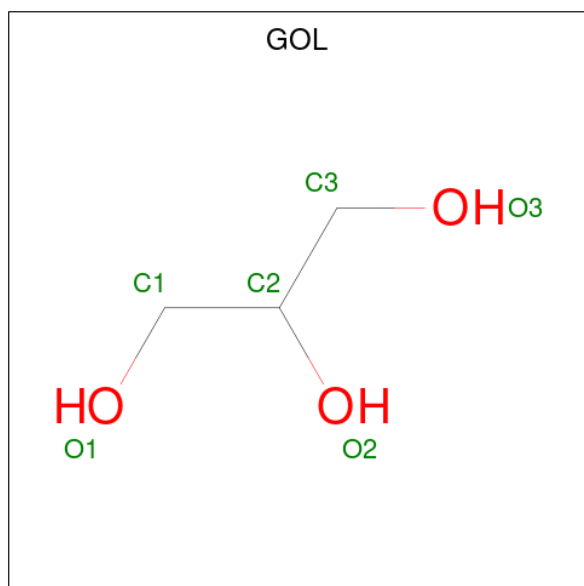
There are 7 unique types of molecules in this entry. The entry contains 12085 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	60	0	0
			3958	2537	668	743	10			
1	B	500	Total	C	N	O	S	48	0	0
			3970	2545	670	745	10			
1	C	498	Total	C	N	O	S	60	0	0
			3951	2532	667	742	10			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



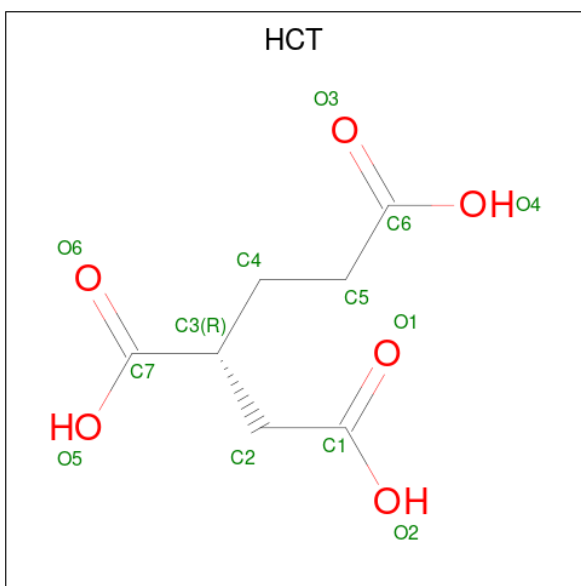
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (2R)-butane-1,2,4-tricarboxylic acid (CCD ID: HCT) (formula: C₇H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		
5	B	1	Total	C	O	0	1
			26	14	12		
5	C	1	Total	C	O	0	0
			13	7	6		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0
6	C	3	Total 3	Cl 3	0	0

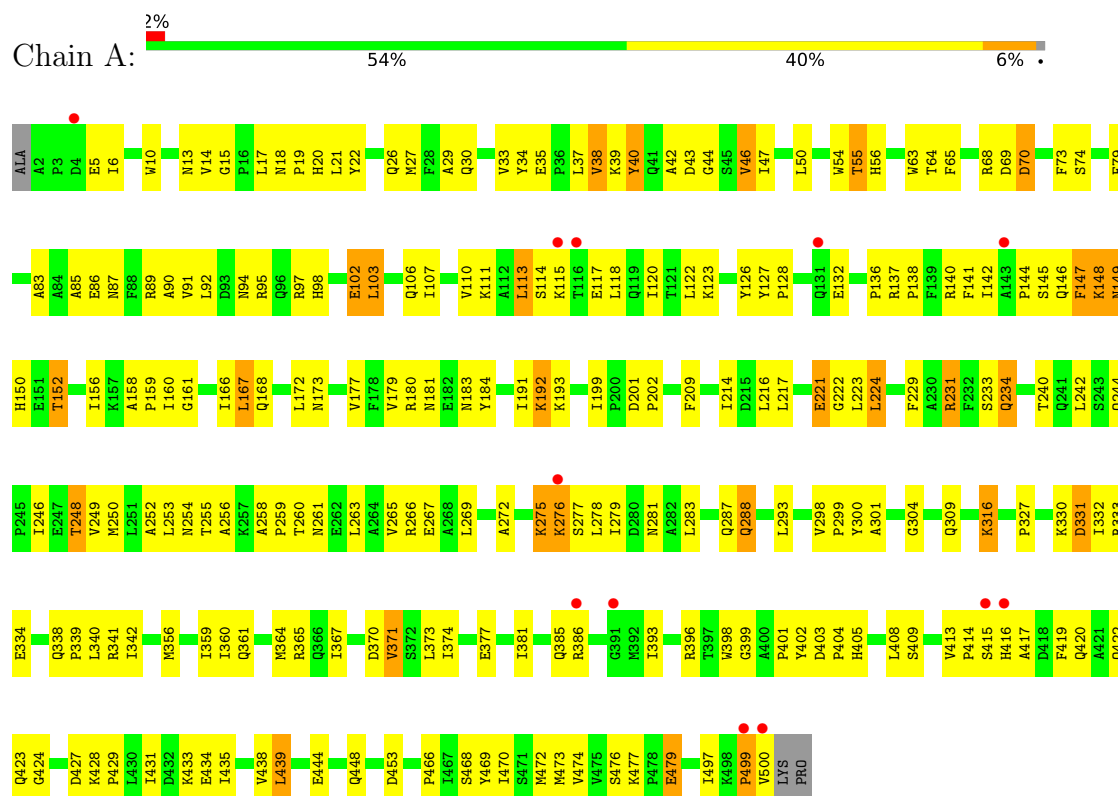
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total 42	O 42	0	0
7	B	35	Total 35	O 35	0	0
7	C	26	Total 26	O 26	0	0

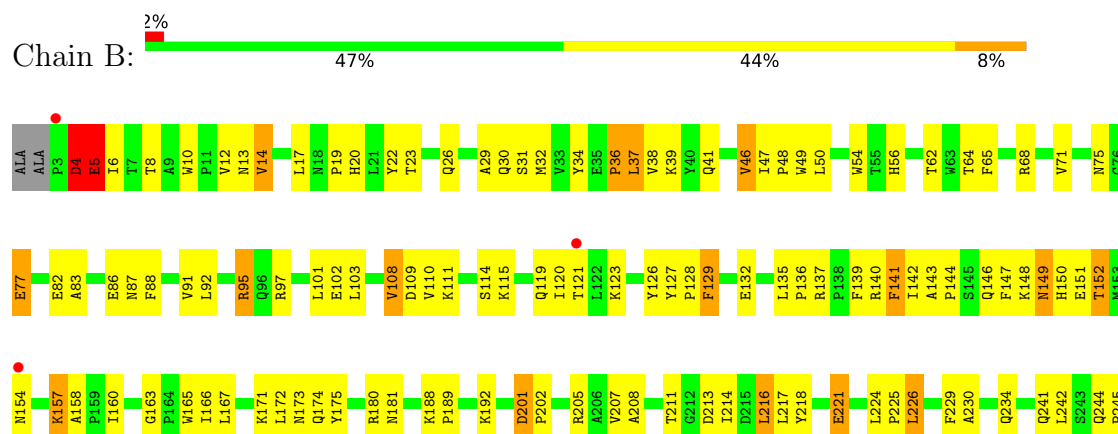
3 Residue-property plots [i](#)

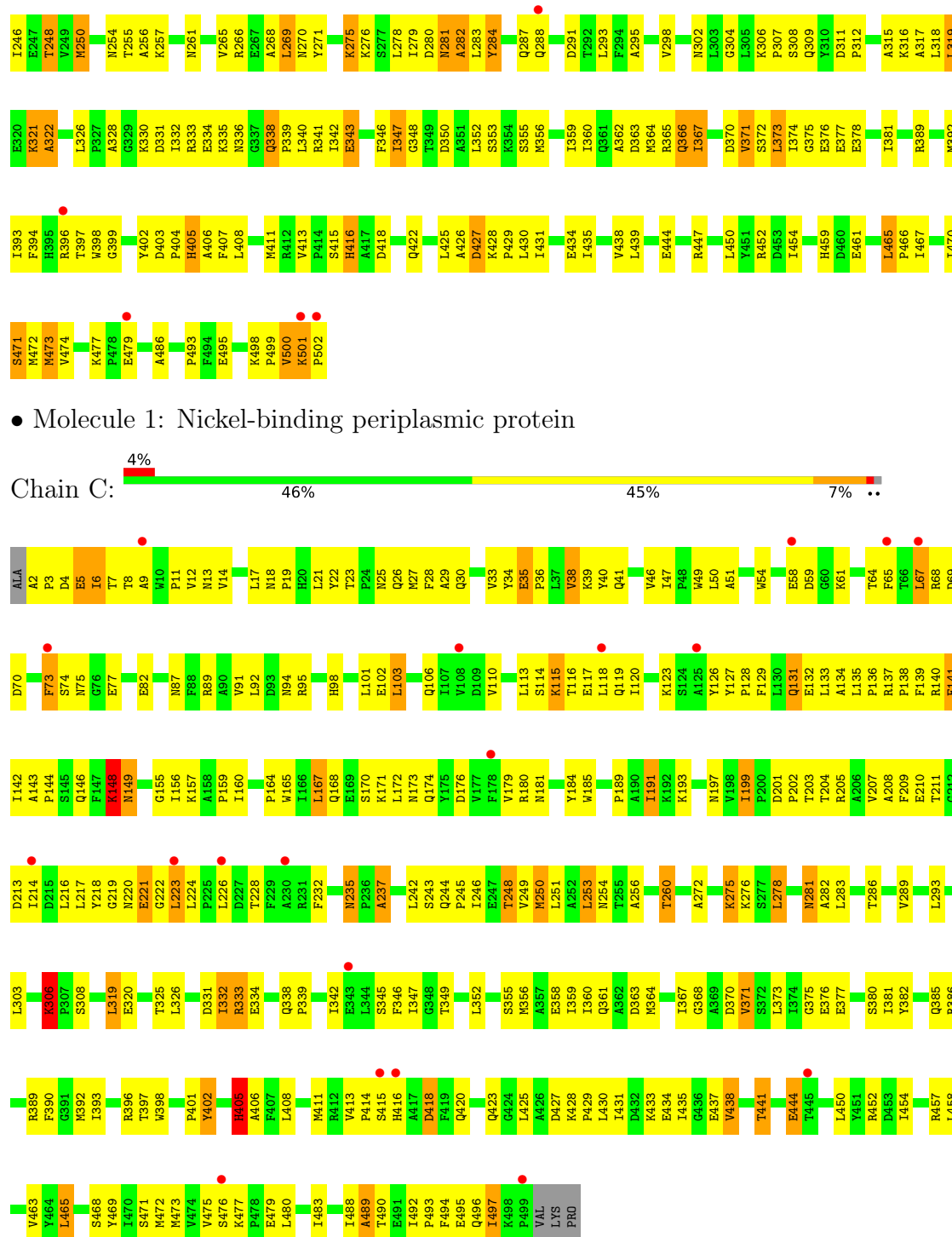
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nickel-binding periplasmic protein



• Molecule 1: Nickel-binding periplasmic protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	158.70Å 158.70Å 134.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 2.80 48.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-2.80) 99.4 (48.45-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.321 0.218 , 0.291	Depositor DCC
R_{free} test set	2357 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12085	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HCT, CL, ACT, GOL, SO4

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	0.54	0/4062	1.02	16/5535 (0.3%)
1	B	0.51	0/4075	1.05	27/5550 (0.5%)
1	C	0.45	0/4055	0.97	20/5525 (0.4%)
All	All	0.50	0/12192	1.01	63/16610 (0.4%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ILE	N-CA-C	8.23	120.82	109.46
1	A	150	HIS	N-CA-C	-7.97	101.00	110.41
1	B	141	PHE	N-CA-C	7.90	122.27	109.40
1	A	405	HIS	N-CA-C	7.87	119.49	111.07
1	A	141	PHE	N-CA-C	7.82	121.65	108.90
1	C	244	GLN	N-CA-C	-6.80	100.69	110.08
1	B	398	TRP	N-CA-C	6.70	120.88	111.30
1	A	199	ILE	CA-C-N	6.61	125.85	118.97
1	A	199	ILE	C-N-CA	6.61	125.85	118.97
1	A	33	VAL	N-CA-C	6.47	117.47	111.45
1	A	301	ALA	N-CA-C	6.41	121.11	113.16
1	B	201	ASP	CA-C-N	6.41	125.63	118.97
1	B	201	ASP	C-N-CA	6.41	125.63	118.97
1	C	237	ALA	N-CA-C	-6.37	105.33	113.23
1	C	201	ASP	CA-C-N	6.29	125.98	119.56
1	C	201	ASP	C-N-CA	6.29	125.98	119.56
1	C	199	ILE	CA-C-N	6.28	125.69	118.85
1	C	199	ILE	C-N-CA	6.28	125.69	118.85
1	B	163	GLY	CA-C-N	6.25	126.37	119.87
1	B	163	GLY	C-N-CA	6.25	126.37	119.87
1	A	386	ARG	N-CA-C	-6.10	103.37	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	THR	N-CA-C	-6.09	106.49	114.04
1	B	139	PHE	N-CA-C	6.06	120.54	111.81
1	B	317	ALA	N-CA-C	-6.06	104.03	112.45
1	B	281	ASN	N-CA-C	-6.02	101.55	110.46
1	B	221	GLU	N-CA-C	5.83	119.22	111.75
1	C	115	LYS	N-CA-C	-5.81	106.82	114.31
1	B	37	LEU	N-CA-C	-5.75	104.92	111.07
1	B	30	GLN	N-CA-C	-5.72	105.13	111.71
1	B	4	ASP	N-CA-C	-5.62	104.15	111.74
1	B	405	HIS	N-CA-C	5.62	117.85	111.11
1	C	483	ILE	N-CA-C	5.60	113.45	108.63
1	A	152	THR	N-CA-C	-5.56	106.86	113.97
1	A	148	LYS	N-CA-C	-5.54	101.90	109.71
1	B	477	LYS	N-CA-C	-5.52	102.70	109.65
1	C	185	TRP	N-CA-C	5.49	118.19	111.82
1	B	407	PHE	N-CA-C	-5.48	105.22	111.14
1	B	226	LEU	N-CA-C	5.48	118.17	111.82
1	A	40	TYR	N-CA-C	5.47	118.17	109.96
1	C	281	ASN	N-CA-C	-5.41	100.85	109.23
1	B	5	GLU	N-CA-C	-5.33	99.44	110.80
1	C	306	LYS	CA-C-N	5.31	125.78	120.52
1	C	306	LYS	C-N-CA	5.31	125.78	120.52
1	C	141	PHE	N-CA-C	5.30	118.46	109.76
1	B	498	LYS	CA-C-N	5.28	124.73	119.24
1	B	498	LYS	C-N-CA	5.28	124.73	119.24
1	B	372	SER	N-CA-C	-5.26	101.99	110.14
1	A	477	LYS	N-CA-C	-5.24	103.05	109.65
1	C	418	ASP	N-CA-C	5.21	119.92	111.37
1	C	148	LYS	N-CA-C	-5.20	101.94	109.59
1	A	244	GLN	N-CA-C	-5.16	102.65	110.39
1	C	332	ILE	N-CA-C	5.13	115.23	107.80
1	C	106	GLN	N-CA-C	-5.11	106.99	113.43
1	B	39	LYS	N-CA-C	5.11	117.23	108.90
1	C	27	MET	N-CA-C	5.10	117.50	111.33
1	A	288	GLN	N-CA-C	5.09	117.87	109.72
1	A	115	LYS	N-CA-C	-5.09	106.33	112.54
1	A	27	MET	N-CA-C	5.06	116.49	111.07
1	C	402	TYR	N-CA-C	5.04	117.43	111.33
1	C	405	HIS	N-CA-C	5.04	119.68	111.37
1	B	275	LYS	N-CA-C	5.02	117.13	111.11
1	B	326	LEU	CA-C-N	5.02	126.11	119.84
1	B	326	LEU	C-N-CA	5.02	126.11	119.84

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	3958	0	3907	230	0
1	B	3970	0	3923	244	0
1	C	3951	0	3898	255	0
2	A	12	0	16	3	0
2	B	6	0	8	0	0
3	A	4	0	3	0	0
3	B	12	0	9	2	0
3	C	8	0	6	0	0
4	A	5	0	0	0	0
5	A	13	0	7	2	0
5	B	26	0	14	8	0
5	C	13	0	7	6	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
7	A	42	0	0	2	0
7	B	35	0	0	3	0
7	C	26	0	0	1	0
All	All	12085	0	11798	722	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 31.

All (722) 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:216:LEU:HD23	1:A:217:LEU:N	1.52	1.24
1:B:308:SER:OG	3:B:505:ACT:H2	1.42	1.15
1:B:13:ASN:ND2	1:B:173:ASN:H	1.54	1.04
1:C:191:ILE:HD12	1:C:191:ILE:H	1.19	1.03
1:C:382:TYR:HB3	1:C:386:ARG:HH12	1.21	1.01
1:A:13:ASN:HD21	1:A:173:ASN:H	1.08	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD23	1:A:217:LEU:H	0.84	1.00
1:B:13:ASN:HD21	1:B:173:ASN:N	1.58	0.99
1:A:216:LEU:CD2	1:A:217:LEU:N	2.24	0.99
1:B:248:THR:HG22	7:B:534:HOH:O	1.64	0.96
1:C:13:ASN:HD21	1:C:173:ASN:H	1.01	0.96
1:A:216:LEU:CD2	1:A:217:LEU:H	1.77	0.96
1:C:223:LEU:HD13	1:C:223:LEU:H	1.32	0.94
1:C:142:ILE:HG12	1:C:143:ALA:H	1.29	0.94
1:A:114:SER:HB3	1:A:117:GLU:HG2	1.50	0.93
1:C:143:ALA:HB3	1:C:146:GLN:HG2	1.51	0.92
1:A:74:SER:HB3	1:A:160:ILE:HG23	1.49	0.92
1:A:30:GLN:HE22	1:A:137:ARG:HD3	1.36	0.91
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.13	0.91
1:A:413:VAL:HG12	1:A:415:SER:H	1.35	0.89
1:B:308:SER:HG	3:B:505:ACT:H2	1.31	0.86
1:C:377:GLU:CD	1:C:377:GLU:H	1.83	0.85
1:B:82:GLU:O	1:B:86:GLU:HG2	1.76	0.85
1:B:216:LEU:HD21	1:B:218:TYR:HB2	1.59	0.84
1:A:5:GLU:HG2	1:A:193:LYS:HB3	1.58	0.84
1:B:87:ASN:HD21	1:B:142:ILE:HG22	1.40	0.84
1:C:254:ASN:O	1:C:260:THR:HB	1.77	0.83
1:A:13:ASN:ND2	1:A:173:ASN:H	1.76	0.83
1:B:373:LEU:HD12	1:B:373:LEU:H	1.44	0.81
1:C:13:ASN:ND2	1:C:173:ASN:H	1.78	0.81
1:A:13:ASN:HD21	1:A:173:ASN:N	1.79	0.80
1:C:332:ILE:HD13	1:C:370:ASP:HB2	1.63	0.80
5:B:508[A]:HCT:O2	5:B:508[A]:HCT:C7	2.29	0.80
1:C:13:ASN:HD21	1:C:173:ASN:N	1.77	0.80
1:B:20:HIS:CE1	1:B:87:ASN:HD22	2.01	0.79
1:A:435:ILE:O	1:A:438:VAL:HG12	1.83	0.78
1:A:107:ILE:HA	1:A:122:LEU:HD23	1.65	0.78
1:B:501:LYS:H	1:B:502:PRO:HD2	1.48	0.78
1:C:19:PRO:HG2	1:C:142:ILE:HB	1.66	0.78
1:C:171:LYS:HB3	1:C:174:GLN:HB2	1.66	0.77
1:A:248:THR:HG21	1:A:293:LEU:O	1.83	0.77
1:C:19:PRO:HG3	1:C:34:TYR:CZ	2.19	0.77
1:C:6:ILE:HG23	1:C:191:ILE:HG21	1.65	0.76
1:C:65:PHE:HE2	1:C:120:ILE:HD12	1.50	0.76
1:C:103:LEU:HD13	1:C:139:PHE:HE1	1.50	0.76
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.33	0.76
1:B:8:THR:HG22	1:B:216:LEU:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:NZ	2:A:503:GOL:H32	2.01	0.76
1:C:278:LEU:HD11	1:C:356:MET:HE2	1.67	0.76
1:C:75:ASN:HD22	1:C:160:ILE:HG21	1.52	0.75
1:B:338:GLN:HG3	1:C:427:ASP:HA	1.68	0.74
1:B:287:GLN:HE21	1:B:470:ILE:HA	1.52	0.73
1:C:13:ASN:ND2	1:C:172:LEU:HD12	2.03	0.73
1:C:248:THR:HG21	1:C:293:LEU:O	1.88	0.73
1:A:14:VAL:HG13	1:A:29:ALA:CB	2.18	0.73
1:B:22:TYR:CD2	5:B:508[B]:HCT:H5	2.23	0.73
1:A:327:PRO:HG2	1:A:330:LYS:HB2	1.69	0.72
1:C:113:LEU:HB3	1:C:117:GLU:HB2	1.70	0.72
1:C:476:SER:HB2	1:C:480:LEU:HD12	1.70	0.72
1:C:437:GLU:O	1:C:441:THR:HG22	1.90	0.72
1:A:246:ILE:HD13	1:A:472:MET:HG2	1.70	0.72
1:C:102:GLU:HB3	1:C:126:TYR:OH	1.90	0.72
1:C:360:ILE:O	1:C:364:MET:HG2	1.89	0.72
1:A:87:ASN:HD21	1:A:142:ILE:H	1.36	0.72
1:B:334:GLU:HA	1:B:338:GLN:O	1.90	0.71
1:B:356:MET:HE2	1:B:467:ILE:HG21	1.72	0.71
1:C:180:ARG:HG3	1:C:189:PRO:HG2	1.72	0.71
1:C:191:ILE:H	1:C:191:ILE:CD1	1.93	0.71
1:C:352:LEU:O	1:C:356:MET:HG3	1.90	0.71
1:B:216:LEU:HD23	1:B:217:LEU:N	2.04	0.71
1:B:13:ASN:HD21	1:B:173:ASN:H	0.78	0.70
1:B:248:THR:CG2	7:B:534:HOH:O	2.29	0.70
1:A:123:LYS:HZ2	2:A:503:GOL:H32	1.55	0.70
1:B:280:ASP:O	1:B:284:TYR:HA	1.92	0.70
1:C:142:ILE:HG12	1:C:143:ALA:N	2.06	0.70
1:B:332:ILE:HD13	1:B:370:ASP:HB2	1.74	0.70
1:A:331:ASP:HB3	1:A:365:ARG:HH12	1.55	0.70
1:B:427:ASP:OD2	1:B:427:ASP:N	2.24	0.70
1:A:148:LYS:O	1:A:149:ASN:HB2	1.92	0.69
1:B:255:THR:HG22	1:B:266:ARG:NH1	2.07	0.69
1:B:352:LEU:O	1:B:356:MET:HG3	1.91	0.69
1:C:221:GLU:HG3	1:C:471:SER:O	1.92	0.69
1:A:192:LYS:HZ2	1:A:192:LYS:HB2	1.58	0.69
1:C:38:VAL:HG12	1:C:134:ALA:HB2	1.73	0.69
1:A:97:ARG:HB2	1:A:97:ARG:CZ	2.22	0.69
1:C:216:LEU:HD13	1:C:217:LEU:N	2.07	0.69
1:B:347:ILE:N	1:B:347:ILE:HD12	2.09	0.68
1:A:107:ILE:HD13	1:A:122:LEU:HD21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:HD22	1:A:184:TYR:HB2	1.56	0.68
1:C:248:THR:HG23	1:C:397:THR:HG23	1.75	0.68
1:B:245:PRO:HG2	1:B:288:GLN:HE22	1.59	0.68
1:B:356:MET:CE	1:B:467:ILE:HG21	2.24	0.68
1:C:38:VAL:HG13	1:C:46:VAL:HG13	1.74	0.68
1:C:87:ASN:ND2	1:C:141:PHE:HB3	2.08	0.68
1:A:30:GLN:NE2	1:A:137:ARG:HD3	2.07	0.68
1:B:281:ASN:O	1:B:283:LEU:N	2.27	0.67
1:C:382:TYR:HB3	1:C:386:ARG:NH1	2.03	0.67
1:A:114:SER:H	1:A:117:GLU:HB2	1.58	0.67
1:B:342:ILE:O	1:B:371:VAL:HA	1.95	0.67
1:A:248:THR:HB	1:A:469:TYR:HD1	1.59	0.67
1:B:255:THR:HG22	1:B:266:ARG:CZ	2.26	0.66
1:A:254:ASN:C	1:A:254:ASN:HD22	2.02	0.66
1:B:501:LYS:N	1:B:502:PRO:HD2	2.10	0.66
1:A:381:ILE:O	1:A:385:GLN:HG3	1.95	0.66
1:B:360:ILE:O	1:B:364:MET:HB2	1.95	0.66
1:C:5:GLU:HG3	1:C:193:LYS:HB3	1.78	0.66
1:C:251:LEU:HB2	1:C:465:LEU:HB3	1.78	0.66
1:A:332:ILE:HD11	1:A:365:ARG:NH2	2.11	0.66
1:C:282:ALA:HB2	1:C:355:SER:OG	1.95	0.66
1:B:22:TYR:HD2	5:B:508[B]:HCT:H5	1.60	0.65
1:B:250:MET:HE2	1:B:396:ARG:HA	1.78	0.65
1:C:332:ILE:CD1	1:C:370:ASP:HB2	2.27	0.65
1:C:420:GLN:HA	1:C:420:GLN:NE2	2.11	0.65
1:A:248:THR:HB	1:A:469:TYR:CD1	2.31	0.65
1:B:339:PRO:HB2	1:B:341:ARG:CD	2.26	0.65
1:A:283:LEU:HD13	1:A:287:GLN:HG3	1.79	0.65
1:A:22:TYR:HH	1:A:98:HIS:HD1	1.45	0.64
1:A:144:PRO:HA	1:A:147:PHE:CE2	2.32	0.64
1:B:158:ALA:HB3	1:B:160:ILE:CD1	2.28	0.64
1:B:312:PRO:O	1:B:316:LYS:HG2	1.98	0.64
1:C:219:GLY:HA3	1:C:223:LEU:HD11	1.79	0.64
1:C:413:VAL:HG13	1:C:414:PRO:HD2	1.80	0.64
1:A:209:PHE:HA	1:A:214:ILE:HB	1.81	0.63
1:C:148:LYS:O	1:C:149:ASN:HB3	1.97	0.63
1:C:191:ILE:HD12	1:C:191:ILE:N	2.04	0.63
1:A:92:LEU:HD22	1:A:95:ARG:HH21	1.62	0.63
1:C:411:MET:HG2	1:C:418:ASP:HB3	1.80	0.63
1:A:180:ARG:HB2	1:A:192:LYS:HA	1.81	0.63
1:B:146:GLN:NE2	1:B:157:LYS:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ALA:HB2	1:C:367:ILE:HD13	1.80	0.63
1:C:202:PRO:HB3	1:C:205:ARG:NH2	2.13	0.63
1:C:226:LEU:HD22	1:C:283:LEU:HA	1.81	0.63
1:B:146:GLN:HE21	1:B:158:ALA:H	1.45	0.62
1:C:22:TYR:HD2	5:C:508:HCT:H4	1.64	0.62
1:C:65:PHE:CE2	1:C:120:ILE:HD12	2.34	0.62
1:A:360:ILE:O	1:A:364:MET:HG2	2.00	0.62
1:B:148:LYS:O	1:B:149:ASN:HB3	2.00	0.62
1:C:34:TYR:OH	1:C:159:PRO:HA	1.98	0.62
1:B:339:PRO:HG2	1:B:341:ARG:HE	1.63	0.62
1:B:102:GLU:HB3	1:B:126:TYR:OH	2.00	0.62
1:C:87:ASN:O	1:C:91:VAL:HG23	1.99	0.62
1:B:101:LEU:HD21	1:B:132:GLU:HB3	1.82	0.61
1:B:158:ALA:HB3	1:B:160:ILE:HD11	1.82	0.61
1:B:346:PHE:O	1:B:375:GLY:HA2	2.00	0.61
1:C:333:ARG:HD2	1:C:368:GLY:HA3	1.82	0.61
1:A:250:MET:HE3	1:A:293:LEU:HD13	1.82	0.61
1:A:221:GLU:HG2	1:A:470:ILE:HB	1.80	0.61
1:A:414:PRO:HA	1:A:419:PHE:CG	2.35	0.61
1:A:38:VAL:CG1	1:A:46:VAL:HG11	2.30	0.61
1:C:49:TRP:C	1:C:51:ALA:H	2.07	0.61
1:C:278:LEU:HD23	1:C:359:ILE:CG2	2.30	0.61
1:A:416:HIS:O	1:A:420:GLN:HG2	2.00	0.61
1:A:246:ILE:O	1:A:399:GLY:HA2	2.00	0.61
1:B:14:VAL:HG13	1:B:17:LEU:HD13	1.82	0.61
1:C:202:PRO:HB3	1:C:205:ARG:HH22	1.65	0.61
1:B:136:PRO:HA	1:B:140:ARG:NE	2.14	0.61
1:C:416:HIS:CD2	5:C:508:HCT:O6	2.53	0.61
1:A:266:ARG:HA	1:A:269:LEU:HD12	1.84	0.60
1:C:14:VAL:HG13	1:C:29:ALA:CB	2.31	0.60
1:C:254:ASN:ND2	1:C:256:ALA:H	1.99	0.60
1:A:18:ASN:ND2	1:A:21:LEU:HD12	2.16	0.60
1:B:166:ILE:HD11	1:B:181:ASN:OD1	2.02	0.60
1:A:137:ARG:NE	5:A:507:HCT:O3	2.33	0.60
1:B:332:ILE:CD1	1:B:370:ASP:HB2	2.31	0.60
1:C:420:GLN:HA	1:C:420:GLN:HE21	1.66	0.60
1:A:146:GLN:HE21	1:A:158:ALA:H	1.50	0.60
1:A:177:VAL:HG11	1:A:193:LYS:HE3	1.83	0.60
1:C:254:ASN:HD22	1:C:256:ALA:H	1.49	0.60
1:C:278:LEU:HD23	1:C:359:ILE:HG21	1.82	0.60
1:A:288:GLN:HB2	7:A:524:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HD13	1:A:191:ILE:HD13	1.82	0.60
1:A:114:SER:HB3	1:A:117:GLU:CG	2.27	0.59
1:A:497:ILE:O	1:A:499:PRO:HD3	2.02	0.59
1:C:17:LEU:HB3	1:C:159:PRO:HB3	1.84	0.59
1:C:254:ASN:HD22	1:C:254:ASN:C	2.10	0.59
1:B:373:LEU:HD12	1:B:373:LEU:N	2.16	0.59
1:B:14:VAL:HG22	1:B:29:ALA:CB	2.33	0.59
1:B:271:TYR:HD1	1:B:309:GLN:O	1.86	0.59
1:A:39:LYS:HB3	1:A:47:ILE:HD11	1.85	0.59
1:B:241:GLN:HB2	1:B:474:VAL:HB	1.83	0.59
1:C:253:LEU:HB2	1:C:463:VAL:O	2.02	0.59
1:C:51:ALA:HA	1:C:67:LEU:HA	1.85	0.59
1:A:216:LEU:CD2	1:A:217:LEU:C	2.76	0.59
1:B:430:LEU:O	1:B:434:GLU:HG3	2.03	0.58
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.86	0.58
1:C:49:TRP:C	1:C:51:ALA:N	2.60	0.58
1:B:282:ALA:HB2	1:B:355:SER:OG	2.04	0.58
1:C:40:TYR:CZ	1:C:401:PRO:HG3	2.38	0.58
1:C:164:PRO:HG3	1:C:184:TYR:CZ	2.39	0.58
1:C:243:SER:OG	1:C:471:SER:HB2	2.03	0.58
1:A:38:VAL:HG13	1:A:46:VAL:HG11	1.83	0.58
1:B:418:ASP:O	1:B:422:GLN:HG3	2.02	0.58
1:C:8:THR:HG22	1:C:9:ALA:H	1.69	0.58
1:A:409:SER:HB2	1:A:439:LEU:HD21	1.84	0.58
1:B:207:VAL:O	1:B:211:THR:HG23	2.04	0.58
1:B:221:GLU:HA	1:B:473:MET:HE3	1.84	0.58
1:B:381:ILE:HG23	1:B:393:ILE:HD11	1.86	0.58
1:A:192:LYS:HB2	1:A:192:LYS:NZ	2.19	0.58
1:B:83:ALA:O	1:B:86:GLU:HB2	2.04	0.58
1:A:64:THR:HA	1:A:118:LEU:O	2.04	0.57
1:B:339:PRO:HB2	1:B:341:ARG:NE	2.19	0.57
1:C:126:TYR:CZ	1:C:128:PRO:HG2	2.38	0.57
1:C:191:ILE:HD11	1:C:497:ILE:O	2.05	0.57
1:C:208:ALA:HB1	1:C:214:ILE:HD13	1.85	0.57
1:A:30:GLN:HE22	1:A:137:ARG:HH11	1.50	0.57
1:C:127:TYR:CG	1:C:128:PRO:HD3	2.40	0.57
1:C:377:GLU:CD	1:C:377:GLU:N	2.58	0.57
1:A:166:ILE:HG13	1:A:181:ASN:HB2	1.87	0.57
1:C:346:PHE:O	1:C:375:GLY:HA2	2.04	0.57
1:B:321:LYS:O	1:B:321:LYS:HG3	2.05	0.57
1:C:477:LYS:HB3	1:C:479:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ALA:O	1:B:213:ASP:HB2	2.04	0.57
1:C:75:ASN:OD1	1:C:77:GLU:HG3	2.04	0.57
1:C:170:SER:HB2	1:C:176:ASP:OD1	2.04	0.57
1:C:197:ASN:O	1:C:199:ILE:HG22	2.04	0.57
1:A:444:GLU:O	1:A:448:GLN:HG3	2.04	0.57
1:B:38:VAL:HG21	1:B:46:VAL:HG13	1.87	0.57
1:B:41:GLN:HG3	1:B:47:ILE:HG23	1.85	0.57
1:A:39:LYS:HB3	1:A:47:ILE:CD1	2.35	0.57
1:A:332:ILE:CD1	1:A:370:ASP:HB2	2.35	0.57
1:A:216:LEU:HD21	1:A:474:VAL:HG13	1.87	0.56
1:B:10:TRP:HE1	1:B:26:GLN:NE2	1.95	0.56
1:C:103:LEU:HD13	1:C:139:PHE:CE1	2.35	0.56
1:A:37:LEU:HA	1:A:50:LEU:HB2	1.86	0.56
1:B:336:ASN:HB3	1:C:457:ARG:HH12	1.70	0.56
1:C:347:ILE:O	1:C:376:GLU:O	2.24	0.56
1:B:189:PRO:HG3	1:B:495:GLU:HB2	1.86	0.56
1:B:389:ARG:HG2	1:B:389:ARG:HH11	1.71	0.56
1:B:330:LYS:HD2	1:B:331:ASP:H	1.69	0.56
1:C:223:LEU:HD13	1:C:223:LEU:N	2.13	0.56
1:A:42:ALA:C	1:A:44:GLY:H	2.13	0.56
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.88	0.56
1:A:373:LEU:N	1:A:373:LEU:HD12	2.21	0.56
1:B:167:LEU:C	1:B:167:LEU:HD13	2.31	0.56
1:B:411:MET:HG2	1:B:418:ASP:HB3	1.88	0.56
1:C:199:ILE:HD11	1:C:204:THR:CB	2.36	0.56
1:A:275:LYS:O	1:A:279:ILE:HG12	2.06	0.56
1:B:144:PRO:HA	1:B:147:PHE:CE2	2.41	0.56
1:A:87:ASN:O	1:A:91:VAL:HG23	2.06	0.56
1:C:216:LEU:HD22	1:C:217:LEU:H	1.71	0.56
1:B:428:LYS:HB3	1:B:429:PRO:HD3	1.88	0.56
1:B:346:PHE:HB3	1:B:394:PHE:HD1	1.71	0.55
1:A:146:GLN:NE2	1:A:158:ALA:H	2.03	0.55
1:A:279:ILE:CD1	1:A:468:SER:HB2	2.37	0.55
1:B:146:GLN:NE2	1:B:158:ALA:H	2.03	0.55
1:C:127:TYR:CD1	1:C:128:PRO:HD3	2.42	0.55
1:A:74:SER:HB2	1:A:161:GLY:O	2.07	0.55
1:C:199:ILE:HG23	1:C:205:ARG:HG2	1.87	0.55
1:A:265:VAL:O	1:A:269:LEU:HG	2.07	0.55
1:A:342:ILE:O	1:A:371:VAL:HA	2.05	0.55
1:B:135:LEU:HD22	1:B:402:TYR:CZ	2.41	0.55
1:A:85:ALA:O	1:A:89:ARG:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:HA	1:C:135:LEU:HG	1.89	0.55
1:A:223:LEU:HG	1:A:224:LEU:HD12	1.89	0.55
1:B:283:LEU:CD2	1:B:352:LEU:HD11	2.36	0.55
1:C:75:ASN:HD22	1:C:160:ILE:CG2	2.18	0.55
1:C:438:VAL:HG23	1:C:450:LEU:HB2	1.87	0.55
1:C:101:LEU:HD11	1:C:132:GLU:HB3	1.89	0.55
1:B:364:MET:O	1:B:367:ILE:HG13	2.06	0.55
1:C:142:ILE:CG1	1:C:143:ALA:H	2.12	0.55
1:A:377:GLU:CD	1:A:377:GLU:H	2.14	0.54
1:B:283:LEU:HD21	1:B:352:LEU:HD11	1.89	0.54
1:C:245:PRO:HA	1:C:471:SER:HB3	1.88	0.54
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.22	0.54
1:B:431:ILE:O	1:B:435:ILE:HG13	2.08	0.54
1:A:98:HIS:ND1	1:A:138:PRO:HG3	2.22	0.54
1:A:221:GLU:HG2	1:A:470:ILE:CG2	2.37	0.54
1:B:64:THR:HG22	1:B:119:GLN:HG3	1.90	0.54
1:B:426:ALA:O	1:C:338:GLN:HG2	2.07	0.54
1:A:15:GLY:O	1:A:17:LEU:HD12	2.07	0.54
1:A:177:VAL:CG1	1:A:193:LYS:HE3	2.37	0.54
1:B:201:ASP:O	1:B:205:ARG:HG3	2.06	0.54
1:C:199:ILE:HD11	1:C:204:THR:OG1	2.07	0.54
1:C:218:TYR:CD2	1:C:492:ILE:HG12	2.43	0.54
1:A:19:PRO:HB3	1:A:34:TYR:CD1	2.43	0.54
1:A:68:ARG:NH1	1:A:70:ASP:OD2	2.41	0.54
1:A:255:THR:O	1:A:261:ASN:HA	2.07	0.54
1:C:283:LEU:O	1:C:286:THR:HG23	2.08	0.54
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.02	0.54
1:A:279:ILE:HD12	1:A:468:SER:HB2	1.88	0.54
1:B:359:ILE:O	1:B:362:ALA:HB3	2.08	0.54
1:B:180:ARG:HD2	1:B:188:LYS:HG3	1.90	0.53
1:B:224:LEU:O	1:B:224:LEU:HD12	2.08	0.53
1:B:339:PRO:CG	1:B:341:ARG:HE	2.21	0.53
1:C:402:TYR:HA	1:C:406:ALA:HB3	1.91	0.53
1:A:14:VAL:HG13	1:A:29:ALA:HB1	1.89	0.53
1:A:224:LEU:HD21	1:A:229:PHE:HB2	1.91	0.53
1:B:244:GLN:O	1:B:471:SER:HB3	2.07	0.53
1:C:222:GLY:C	1:C:224:LEU:H	2.17	0.53
1:C:95:ARG:HB2	1:C:95:ARG:HH11	1.74	0.53
1:C:250:MET:SD	1:C:293:LEU:HD12	2.49	0.53
1:C:281:ASN:O	1:C:282:ALA:HB3	2.08	0.53
1:B:38:VAL:CG2	1:B:46:VAL:HG13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ASP:C	1:C:214:ILE:HD12	2.33	0.53
1:A:221:GLU:HG2	1:A:470:ILE:CB	2.39	0.53
1:B:425:LEU:HD13	1:B:461:GLU:OE1	2.09	0.53
1:B:146:GLN:HE21	1:B:157:LYS:HB2	1.72	0.52
1:A:217:LEU:HB3	1:A:223:LEU:HD21	1.90	0.52
1:A:256:ALA:HB2	1:A:424:GLY:N	2.24	0.52
1:C:425:LEU:HD11	1:C:463:VAL:HG22	1.92	0.52
1:B:330:LYS:CD	1:B:331:ASP:H	2.22	0.52
1:B:422:GLN:HB2	1:B:428:LYS:HE2	1.92	0.52
1:A:152:THR:HG22	1:A:156:ILE:HG22	1.91	0.52
1:A:332:ILE:HD13	1:A:370:ASP:HB2	1.92	0.52
1:B:246:ILE:HG12	1:B:471:SER:HA	1.90	0.52
1:C:115:LYS:HG2	1:C:116:THR:HG23	1.91	0.52
1:C:143:ALA:O	1:C:146:GLN:N	2.36	0.52
1:B:137:ARG:HH21	5:B:508[B]:HCT:H5A	1.74	0.52
1:C:98:HIS:ND1	1:C:138:PRO:HG3	2.25	0.52
1:B:64:THR:CG2	1:B:119:GLN:HG3	2.40	0.52
1:C:216:LEU:HD23	1:C:476:SER:HB3	1.91	0.52
1:C:235:ASN:C	1:C:235:ASN:HD22	2.18	0.52
1:C:444:GLU:OE1	1:C:444:GLU:HA	2.09	0.52
1:A:253:LEU:HD12	1:A:253:LEU:N	2.25	0.52
1:C:246:ILE:HG12	1:C:471:SER:HA	1.92	0.52
1:C:278:LEU:HD13	1:C:278:LEU:O	2.10	0.52
1:B:444:GLU:OE2	1:B:447:ARG:NH1	2.43	0.52
1:C:131:GLN:HE21	1:C:131:GLN:H	1.58	0.52
1:B:499:PRO:O	1:B:500:VAL:O	2.29	0.51
1:C:199:ILE:CG2	1:C:205:ARG:HG2	2.39	0.51
1:B:92:LEU:O	1:B:95:ARG:HB2	2.10	0.51
1:B:149:ASN:HD22	1:B:150:HIS:H	1.57	0.51
1:B:149:ASN:ND2	1:B:150:HIS:H	2.08	0.51
1:C:18:ASN:HB3	1:C:21:LEU:HB2	1.92	0.51
1:A:107:ILE:HD13	1:A:122:LEU:CD2	2.40	0.51
1:A:253:LEU:N	1:A:253:LEU:CD1	2.74	0.51
1:A:47:ILE:O	1:A:47:ILE:HD12	2.10	0.51
1:A:136:PRO:HA	1:A:140:ARG:CZ	2.39	0.51
1:B:356:MET:O	1:B:360:ILE:HG13	2.10	0.51
1:C:221:GLU:HA	1:C:473:MET:HE3	1.92	0.51
1:A:114:SER:CB	1:A:117:GLU:HG2	2.34	0.51
1:C:405:HIS:CG	1:C:406:ALA:N	2.78	0.51
1:B:87:ASN:O	1:B:91:VAL:HG23	2.11	0.51
1:B:250:MET:CE	1:B:396:ARG:HA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ARG:O	1:C:390:PHE:HB3	2.11	0.51
1:C:450:LEU:O	1:C:454:ILE:HG13	2.10	0.51
1:B:245:PRO:HG2	1:B:288:GLN:NE2	2.23	0.51
1:B:275:LYS:HE2	1:B:466:PRO:O	2.10	0.51
1:C:381:ILE:O	1:C:385:GLN:HG3	2.10	0.51
1:A:259:PRO:HG3	1:A:340:LEU:HD12	1.92	0.51
1:C:282:ALA:CB	1:C:355:SER:OG	2.58	0.51
1:C:168:GLN:OE1	1:C:179:VAL:HG11	2.11	0.51
1:C:272:ALA:O	1:C:363:ASP:HB3	2.10	0.51
1:C:488:ILE:O	1:C:490:THR:N	2.44	0.51
1:A:309:GLN:HE21	1:A:309:GLN:HA	1.76	0.51
1:B:180:ARG:NH2	1:B:192:LYS:HG2	2.26	0.51
1:C:408:LEU:O	1:C:435:ILE:HD13	2.11	0.50
1:C:278:LEU:CD1	1:C:356:MET:HE2	2.40	0.50
1:B:348:GLY:C	1:B:350:ASP:H	2.19	0.50
1:C:219:GLY:CA	1:C:223:LEU:HD11	2.40	0.50
1:A:419:PHE:CD1	1:A:419:PHE:C	2.90	0.50
1:B:244:GLN:C	1:B:471:SER:HB3	2.36	0.50
1:C:34:TYR:HB3	1:C:140:ARG:HB3	1.92	0.50
1:C:411:MET:HE1	1:C:458:LEU:HD11	1.92	0.50
1:A:221:GLU:CG	1:A:470:ILE:HB	2.42	0.50
1:A:234:GLN:NE2	1:B:304:GLY:O	2.35	0.50
1:B:216:LEU:HD23	1:B:216:LEU:C	2.36	0.50
1:B:127:TYR:CG	1:B:128:PRO:HD3	2.46	0.50
1:A:334:GLU:HA	1:A:338:GLN:O	2.12	0.50
1:C:303:LEU:HD22	1:C:452:ARG:HG3	1.94	0.50
1:A:127:TYR:CE1	1:A:128:PRO:HG3	2.47	0.49
1:B:8:THR:HG21	1:B:216:LEU:HD22	1.94	0.49
1:A:278:LEU:HD21	1:A:356:MET:HG2	1.93	0.49
1:A:413:VAL:HG12	1:A:415:SER:N	2.18	0.49
1:A:38:VAL:HG13	1:A:46:VAL:CG1	2.41	0.49
1:A:144:PRO:C	1:A:146:GLN:H	2.21	0.49
1:B:246:ILE:HD13	1:B:472:MET:HG2	1.94	0.49
1:C:131:GLN:H	1:C:131:GLN:NE2	2.10	0.49
1:A:19:PRO:C	1:A:20:HIS:HD1	2.20	0.49
1:A:373:LEU:N	1:A:373:LEU:CD1	2.75	0.49
1:B:75:ASN:OD1	1:B:77:GLU:HB2	2.12	0.49
1:A:216:LEU:HG	1:A:476:SER:HB3	1.95	0.49
1:B:214:ILE:HG22	1:B:216:LEU:H	1.78	0.49
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.95	0.49
1:B:268:ALA:HB2	1:B:318:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD13	1:C:278:LEU:C	2.38	0.49
1:B:346:PHE:HB3	1:B:394:PHE:CD1	2.46	0.49
1:B:365:ARG:O	1:B:365:ARG:HG2	2.13	0.49
1:A:42:ALA:C	1:A:44:GLY:N	2.70	0.49
1:A:281:ASN:HD22	1:A:359:ILE:HD11	1.77	0.49
1:B:316:LYS:HB2	1:B:333:ARG:HH11	1.78	0.49
1:C:361:GLN:HB2	1:C:373:LEU:HD11	1.94	0.49
1:A:148:LYS:O	1:A:149:ASN:CB	2.60	0.48
1:A:181:ASN:HD21	1:A:183:ASN:C	2.21	0.48
1:B:338:GLN:HG2	1:C:430:LEU:HB2	1.95	0.48
1:B:500:VAL:O	1:B:501:LYS:HB2	2.11	0.48
1:C:430:LEU:O	1:C:434:GLU:HG3	2.13	0.48
1:B:347:ILE:N	1:B:347:ILE:CD1	2.76	0.48
1:C:30:GLN:OE1	1:C:137:ARG:HD3	2.13	0.48
1:C:40:TYR:CE2	1:C:401:PRO:HG3	2.48	0.48
1:A:92:LEU:HD22	1:A:95:ARG:NH2	2.27	0.48
1:A:240:THR:OG1	1:B:302:ASN:ND2	2.38	0.48
1:A:428:LYS:HB3	1:A:429:PRO:HD3	1.95	0.48
1:C:36:PRO:HB3	1:C:140:ARG:HE	1.77	0.48
1:A:30:GLN:HE22	1:A:137:ARG:CD	2.15	0.48
1:B:291:ASP:CG	1:B:307:PRO:HB3	2.38	0.48
1:B:377:GLU:CD	1:B:377:GLU:H	2.21	0.48
1:B:435:ILE:HG12	1:B:454:ILE:HD13	1.94	0.48
1:B:20:HIS:CD2	1:B:152:THR:HG21	2.49	0.48
1:B:32:MET:HB3	1:B:165:TRP:HB2	1.95	0.48
1:B:224:LEU:CD1	1:B:229:PHE:HB2	2.44	0.48
1:B:330:LYS:HG3	1:B:332:ILE:H	1.78	0.48
1:C:22:TYR:CE2	5:C:508:HCT:H3	2.49	0.48
1:A:113:LEU:HB2	1:A:117:GLU:HB2	1.96	0.48
1:A:331:ASP:HB3	1:A:365:ARG:NH1	2.27	0.48
1:B:142:ILE:HG12	1:B:143:ALA:N	2.29	0.48
1:A:137:ARG:NH2	5:A:507:HCT:O3	2.47	0.48
1:A:166:ILE:HD11	1:A:181:ASN:OD1	2.14	0.48
1:B:5:GLU:O	1:B:5:GLU:HG2	2.14	0.48
1:C:306:LYS:HB2	1:C:306:LYS:NZ	2.28	0.48
1:A:256:ALA:HB2	1:A:424:GLY:H	1.77	0.48
1:B:147:PHE:HB3	1:B:151:GLU:O	2.14	0.48
1:B:338:GLN:OE1	1:C:429:PRO:HB2	2.14	0.48
1:C:8:THR:HG22	1:C:9:ALA:N	2.28	0.48
1:C:126:TYR:CE2	1:C:128:PRO:HG2	2.49	0.48
1:C:495:GLU:HG2	1:C:496:GLN:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:PHE:CE2	1:C:475:VAL:HG12	2.49	0.48
1:C:253:LEU:HD12	1:C:392:MET:HG2	1.96	0.48
1:A:240:THR:HA	1:A:474:VAL:O	2.13	0.48
1:A:250:MET:HE3	1:A:293:LEU:CD1	2.44	0.48
1:B:56:HIS:HA	1:B:62:THR:O	2.14	0.48
1:B:341:ARG:HA	1:B:370:ASP:O	2.14	0.48
1:B:427:ASP:O	1:B:428:LYS:C	2.57	0.47
1:B:501:LYS:N	1:B:502:PRO:CD	2.77	0.47
1:C:135:LEU:HD13	1:C:402:TYR:CE2	2.49	0.47
1:C:209:PHE:CZ	1:C:475:VAL:HG12	2.48	0.47
1:C:223:LEU:H	1:C:223:LEU:CD1	2.15	0.47
1:C:338:GLN:NE2	1:C:339:PRO:HD2	2.29	0.47
1:A:341:ARG:C	1:A:342:ILE:HG13	2.39	0.47
1:A:438:VAL:HG13	1:A:439:LEU:HD13	1.94	0.47
1:B:230:ALA:O	1:B:234:GLN:HG3	2.14	0.47
1:B:257:LYS:O	1:B:261:ASN:HB3	2.13	0.47
1:C:202:PRO:HA	1:C:205:ARG:CZ	2.44	0.47
1:B:339:PRO:HB2	1:B:341:ARG:HD2	1.94	0.47
1:C:17:LEU:HD22	1:C:167:LEU:HD12	1.96	0.47
1:C:137:ARG:HB2	1:C:138:PRO:HA	1.96	0.47
1:A:263:LEU:O	1:A:267:GLU:HG3	2.14	0.47
1:B:435:ILE:O	1:B:438:VAL:HG12	2.14	0.47
1:A:222:GLY:O	1:A:223:LEU:C	2.57	0.47
1:A:192:LYS:NZ	1:A:192:LYS:CB	2.77	0.47
1:A:258:ALA:HA	1:A:261:ASN:OD1	2.13	0.47
1:B:10:TRP:NE1	1:B:26:GLN:HE21	1.96	0.47
1:B:41:GLN:CG	1:B:47:ILE:HG23	2.44	0.47
1:B:355:SER:O	1:B:359:ILE:HG13	2.15	0.47
1:C:17:LEU:HD21	1:C:33:VAL:HG21	1.95	0.47
1:C:249:VAL:HG12	1:C:468:SER:O	2.13	0.47
1:C:472:MET:HE2	1:C:489:ALA:O	2.13	0.47
1:A:30:GLN:NE2	1:A:137:ARG:HH11	2.13	0.47
1:A:127:TYR:CG	1:A:128:PRO:HD3	2.49	0.47
1:C:35:GLU:C	1:C:140:ARG:HD2	2.39	0.47
1:C:148:LYS:HB2	1:C:155:GLY:O	2.14	0.47
1:C:281:ASN:C	1:C:283:LEU:H	2.23	0.47
1:A:136:PRO:HA	1:A:140:ARG:NH2	2.29	0.47
1:B:248:THR:HG21	1:B:293:LEU:O	2.15	0.47
1:C:136:PRO:HD2	1:C:402:TYR:OH	2.15	0.47
1:A:19:PRO:HB3	1:A:34:TYR:CE1	2.51	0.46
1:A:233:SER:O	1:B:452:ARG:NH2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASN:HD21	1:B:256:ALA:HB3	1.78	0.46
1:C:8:THR:HG23	1:C:216:LEU:O	2.15	0.46
1:C:207:VAL:HA	1:C:210:GLU:HG2	1.97	0.46
1:B:226:LEU:HB2	1:B:282:ALA:O	2.15	0.46
1:B:413:VAL:O	1:B:415:SER:N	2.47	0.46
1:A:56:HIS:HB3	1:A:63:TRP:CE3	2.51	0.46
1:A:102:GLU:HB3	1:A:126:TYR:OH	2.15	0.46
1:A:299:PRO:O	1:A:300:TYR:HB2	2.15	0.46
1:B:265:VAL:O	1:B:269:LEU:HB2	2.16	0.46
1:B:322:ALA:O	1:B:335:LYS:HE2	2.15	0.46
1:A:147:PHE:N	1:A:147:PHE:CD2	2.84	0.46
1:B:224:LEU:HD11	1:B:229:PHE:HB2	1.96	0.46
1:B:330:LYS:HG3	1:B:331:ASP:N	2.30	0.46
1:C:376:GLU:HB3	1:C:380:SER:HB2	1.96	0.46
1:C:428:LYS:N	1:C:429:PRO:CD	2.78	0.46
1:A:434:GLU:OE2	1:A:453:ASP:OD2	2.34	0.46
1:B:330:LYS:CG	1:B:331:ASP:N	2.79	0.46
1:B:311:ASP:C	1:B:311:ASP:OD1	2.59	0.46
1:C:38:VAL:HG13	1:C:46:VAL:CG1	2.44	0.46
1:B:87:ASN:ND2	1:B:142:ILE:HG22	2.21	0.46
1:B:180:ARG:NH1	1:B:188:LYS:HD3	2.31	0.46
1:B:332:ILE:HD13	1:B:370:ASP:CB	2.43	0.46
1:A:74:SER:CB	1:A:160:ILE:HG23	2.35	0.46
1:B:486:ALA:HB2	1:B:493:PRO:HD3	1.96	0.46
1:C:199:ILE:HD11	1:C:204:THR:HB	1.98	0.46
1:B:254:ASN:C	1:B:254:ASN:HD22	2.22	0.46
1:C:19:PRO:HG3	1:C:34:TYR:CE1	2.50	0.46
1:A:427:ASP:HB3	1:A:431:ILE:HD11	1.97	0.46
1:B:148:LYS:O	1:B:149:ASN:CB	2.63	0.46
1:B:306:LYS:O	1:B:459:HIS:HE1	1.99	0.46
1:C:143:ALA:HB3	1:C:146:GLN:CG	2.35	0.46
1:A:40:TYR:CZ	1:A:401:PRO:HB3	2.50	0.45
1:B:20:HIS:HD2	1:B:152:THR:OG1	1.99	0.45
1:C:133:LEU:HA	1:C:139:PHE:HD1	1.81	0.45
1:C:345:SER:OG	1:C:393:ILE:HD12	2.15	0.45
1:C:492:ILE:O	1:C:494:PHE:N	2.39	0.45
1:A:14:VAL:CG1	1:A:29:ALA:HB1	2.46	0.45
1:A:103:LEU:HB2	1:A:132:GLU:OE2	2.15	0.45
1:B:14:VAL:HG13	1:B:17:LEU:CD1	2.46	0.45
1:B:338:GLN:NE2	1:B:339:PRO:HD2	2.32	0.45
1:B:342:ILE:CG2	1:B:392:MET:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:LYS:HD2	1:C:428:LYS:O	2.17	0.45
1:A:168:GLN:OE1	1:A:179:VAL:HG11	2.16	0.45
1:A:221:GLU:HG2	1:A:470:ILE:HG21	1.97	0.45
1:A:254:ASN:O	1:A:260:THR:OG1	2.24	0.45
1:A:413:VAL:O	1:A:419:PHE:HB2	2.17	0.45
1:B:180:ARG:HD2	1:B:188:LYS:CG	2.46	0.45
1:B:416:HIS:ND1	5:B:508[A]:HCT:O5	2.49	0.45
1:C:68:ARG:C	1:C:70:ASP:H	2.23	0.45
1:A:259:PRO:C	1:A:261:ASN:H	2.25	0.45
1:B:218:TYR:HE2	1:B:472:MET:HE3	1.80	0.45
1:A:147:PHE:N	1:A:147:PHE:HD2	2.13	0.45
1:A:479:GLU:O	1:A:500:VAL:HG23	2.17	0.45
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.81	0.45
1:B:270:ASN:OD1	1:B:465:LEU:HA	2.17	0.45
1:A:127:TYR:N	1:A:128:PRO:CD	2.79	0.45
1:B:146:GLN:CD	1:B:160:ILE:HD13	2.42	0.45
1:B:350:ASP:OD2	1:B:353:SER:N	2.45	0.45
1:C:12:VAL:HG23	1:C:26:GLN:OE1	2.17	0.45
1:C:220:ASN:O	1:C:222:GLY:N	2.50	0.45
1:A:17:LEU:HD13	1:A:167:LEU:HD12	1.98	0.45
1:A:126:TYR:CD1	1:A:128:PRO:HD2	2.52	0.45
1:B:8:THR:CG2	1:B:216:LEU:HD22	2.47	0.45
1:A:103:LEU:O	1:A:106:GLN:HB3	2.16	0.45
1:C:110:VAL:HA	1:C:119:GLN:O	2.17	0.45
1:C:420:GLN:HE21	1:C:420:GLN:CA	2.25	0.45
1:A:287:GLN:HA	7:A:537:HOH:O	2.16	0.45
1:A:356:MET:O	1:A:360:ILE:HG13	2.17	0.45
1:B:343:GLU:C	1:B:343:GLU:OE1	2.60	0.45
1:C:17:LEU:HD12	1:C:17:LEU:HA	1.85	0.45
1:B:8:THR:HA	1:B:214:ILE:HG23	1.99	0.44
1:C:165:TRP:HZ2	1:C:495:GLU:HA	1.82	0.44
1:A:55:THR:HG22	1:A:64:THR:HB	1.98	0.44
1:A:327:PRO:HG2	1:A:330:LYS:CB	2.42	0.44
1:A:361:GLN:HG3	1:A:371:VAL:HG22	1.98	0.44
1:B:148:LYS:O	1:B:154:ASN:ND2	2.43	0.44
1:B:226:LEU:HD22	1:B:226:LEU:N	2.31	0.44
1:B:282:ALA:C	1:B:283:LEU:HD22	2.42	0.44
1:C:49:TRP:O	1:C:51:ALA:N	2.50	0.44
5:B:508[A]:HCT:O2	5:B:508[A]:HCT:O6	2.34	0.44
1:C:248:THR:HG23	1:C:397:THR:CG2	2.46	0.44
1:C:251:LEU:HD11	1:C:360:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:CG2	1:A:364:MET:HE2	2.48	0.44
1:B:12:VAL:HG23	1:B:13:ASN:O	2.17	0.44
1:C:89:ARG:HG2	1:C:89:ARG:HH11	1.82	0.44
1:A:20:HIS:HE1	1:A:140:ARG:O	2.00	0.44
1:B:14:VAL:HG22	1:B:29:ALA:HB2	1.99	0.44
1:B:108:VAL:CG2	1:B:121:THR:O	2.65	0.44
1:C:34:TYR:OH	1:C:159:PRO:CA	2.64	0.44
1:C:224:LEU:CD2	1:C:475:VAL:HG21	2.47	0.44
1:C:413:VAL:CG1	1:C:414:PRO:HD2	2.46	0.44
1:A:14:VAL:CG1	1:A:17:LEU:HD11	2.47	0.44
1:A:92:LEU:C	1:A:94:ASN:N	2.74	0.44
1:A:180:ARG:N	1:A:192:LYS:O	2.45	0.44
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.18	0.44
1:C:275:LYS:HB3	1:C:289:VAL:HG22	1.99	0.44
1:C:319:LEU:HB3	1:C:333:ARG:HE	1.83	0.44
1:C:39:LYS:HD3	1:C:49:TRP:CZ3	2.53	0.44
1:C:275:LYS:HG2	1:C:289:VAL:HG13	1.98	0.44
1:C:334:GLU:HG2	1:C:339:PRO:HA	2.00	0.44
1:C:6:ILE:HG23	1:C:191:ILE:CG2	2.43	0.44
1:C:171:LYS:HG2	1:C:174:GLN:HG3	2.00	0.44
1:C:411:MET:HG2	1:C:418:ASP:CB	2.45	0.44
1:A:172:LEU:O	1:A:173:ASN:HB2	2.18	0.43
1:A:180:ARG:NH2	1:A:192:LYS:HZ2	2.16	0.43
1:A:254:ASN:C	1:A:254:ASN:ND2	2.72	0.43
1:B:143:ALA:HB3	1:B:146:GLN:HG2	2.00	0.43
1:B:359:ILE:O	1:B:363:ASP:OD2	2.36	0.43
1:B:86:GLU:OE2	1:B:86:GLU:HA	2.17	0.43
1:C:207:VAL:O	1:C:211:THR:HG23	2.18	0.43
1:C:250:MET:HE2	1:C:396:ARG:HA	2.00	0.43
1:A:17:LEU:HD12	1:A:17:LEU:N	2.33	0.43
1:A:92:LEU:C	1:A:94:ASN:H	2.26	0.43
1:A:231:ARG:HD3	1:A:231:ARG:HA	1.72	0.43
1:B:174:GLN:HB3	1:B:175:TYR:CD1	2.53	0.43
1:B:408:LEU:HD23	1:B:408:LEU:HA	1.88	0.43
1:C:431:ILE:HG23	1:C:454:ILE:HG23	2.00	0.43
1:A:10:TRP:NE1	1:A:26:GLN:HE21	2.09	0.43
1:A:250:MET:HB3	1:A:466:PRO:HA	2.01	0.43
1:B:224:LEU:O	1:B:225:PRO:C	2.62	0.43
1:C:75:ASN:ND2	1:C:160:ILE:HG21	2.26	0.43
1:A:87:ASN:ND2	1:A:142:ILE:H	2.10	0.43
1:C:171:LYS:HB3	1:C:174:GLN:CB	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ASN:C	1:C:235:ASN:ND2	2.76	0.43
1:B:295:ALA:HB3	1:B:298:VAL:HG23	2.01	0.43
1:A:276:LYS:O	1:A:277:SER:C	2.61	0.43
1:B:147:PHE:N	1:B:147:PHE:CD2	2.86	0.43
1:C:59:ASP:OD2	1:C:61:LYS:HG2	2.19	0.43
1:C:172:LEU:HG	1:C:173:ASN:ND2	2.34	0.43
1:A:298:VAL:O	1:A:299:PRO:C	2.62	0.43
1:B:339:PRO:HB2	1:B:341:ARG:HE	1.84	0.43
1:C:2:ALA:HB3	1:C:3:PRO:HD3	2.00	0.43
1:C:477:LYS:HE2	1:C:479:GLU:CD	2.44	0.43
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.93	0.43
1:B:65:PHE:HE2	1:B:120:ILE:HD12	1.84	0.43
1:B:126:TYR:O	1:B:129:PHE:HB2	2.19	0.43
1:B:142:ILE:HG13	1:B:160:ILE:O	2.19	0.43
1:B:158:ALA:C	1:B:160:ILE:HD12	2.44	0.43
1:C:92:LEU:C	1:C:94:ASN:H	2.25	0.43
1:A:404:PRO:O	1:A:408:LEU:HG	2.18	0.42
1:C:123:LYS:O	1:C:123:LYS:HG3	2.19	0.42
1:C:228:THR:HG23	1:C:232:PHE:CE1	2.54	0.42
1:C:433:LYS:O	1:C:437:GLU:HG3	2.19	0.42
1:A:38:VAL:HG22	1:A:46:VAL:CG1	2.49	0.42
1:B:144:PRO:C	1:B:146:GLN:H	2.27	0.42
1:B:403:ASP:HA	1:B:404:PRO:HA	1.79	0.42
1:C:4:ASP:O	1:C:5:GLU:HB2	2.19	0.42
1:C:22:TYR:CD2	5:C:508:HCT:H4	2.48	0.42
1:B:22:TYR:CE2	5:B:508[B]:HCT:H5	2.53	0.42
1:B:114:SER:OG	1:B:115:LYS:N	2.52	0.42
1:B:356:MET:HE1	1:B:467:ILE:HG21	2.01	0.42
1:B:254:ASN:ND2	1:B:256:ALA:H	2.17	0.42
1:B:315:ALA:O	1:B:319:LEU:HD22	2.19	0.42
1:C:189:PRO:HB3	1:C:495:GLU:HB2	2.01	0.42
1:B:50:LEU:O	1:B:68:ARG:HG2	2.19	0.42
1:C:11:PRO:HB3	1:C:349:THR:HB	2.00	0.42
1:C:28:PHE:CG	1:C:29:ALA:N	2.88	0.42
1:C:54:TRP:CB	1:C:65:PHE:HD1	2.32	0.42
1:C:95:ARG:HB2	1:C:95:ARG:NH1	2.34	0.42
1:A:217:LEU:HD23	1:A:217:LEU:HA	1.92	0.42
1:A:278:LEU:C	1:A:278:LEU:HD23	2.44	0.42
1:B:31:SER:OG	1:B:136:PRO:HB3	2.19	0.42
1:C:12:VAL:CG2	1:C:26:GLN:OE1	2.67	0.42
1:C:38:VAL:CG1	1:C:46:VAL:CG1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:PHE:O	1:C:495:GLU:C	2.62	0.42
1:A:201:ASP:HA	1:A:202:PRO:HD3	1.90	0.42
1:B:416:HIS:CE1	5:B:508[B]:HCT:O6	2.73	0.42
1:C:248:THR:HB	1:C:469:TYR:CD1	2.55	0.42
1:C:326:LEU:HG	1:C:333:ARG:NH2	2.34	0.42
5:C:508:HCT:O5	5:C:508:HCT:H5A	2.20	0.42
1:A:168:GLN:O	1:A:168:GLN:HG2	2.19	0.42
1:A:327:PRO:HG2	1:A:330:LYS:HG3	2.00	0.42
1:B:136:PRO:HA	1:B:140:ARG:CZ	2.50	0.42
1:A:50:LEU:HD13	1:A:79:PHE:CZ	2.55	0.42
1:B:49:TRP:HB3	1:B:50:LEU:H	1.64	0.42
1:B:339:PRO:CB	1:B:341:ARG:HE	2.33	0.42
1:C:143:ALA:O	1:C:144:PRO:C	2.62	0.42
1:C:205:ARG:HH21	1:C:223:LEU:HA	1.85	0.42
1:A:70:ASP:OD2	1:A:70:ASP:C	2.62	0.42
1:A:123:LYS:NZ	2:A:503:GOL:C3	2.79	0.42
1:A:216:LEU:CD2	1:A:216:LEU:C	2.88	0.42
1:A:221:GLU:H	1:A:221:GLU:HG3	1.50	0.42
1:A:419:PHE:CE1	1:A:423:GLN:OE1	2.73	0.42
1:A:427:ASP:HB3	1:A:431:ILE:CD1	2.49	0.42
1:B:450:LEU:O	1:B:454:ILE:HG13	2.19	0.42
1:C:308:SER:HB3	7:C:518:HOH:O	2.20	0.42
1:C:415:SER:HB3	5:C:508:HCT:O1	2.19	0.42
1:B:48:PRO:HG3	1:B:54:TRP:CZ3	2.55	0.41
1:B:68:ARG:HD3	1:B:71:VAL:CG2	2.50	0.41
1:B:20:HIS:HD2	1:B:152:THR:HG21	1.85	0.41
1:C:41:GLN:HG3	1:C:47:ILE:HG23	2.01	0.41
1:C:110:VAL:CG1	1:C:118:LEU:HD21	2.50	0.41
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.86	0.41
1:A:309:GLN:HA	1:A:309:GLN:NE2	2.34	0.41
1:A:422:GLN:HB2	1:A:428:LYS:HE2	2.02	0.41
1:B:88:PHE:CD2	1:B:110:VAL:HG11	2.55	0.41
1:C:397:THR:C	1:C:398:TRP:CD1	2.98	0.41
1:A:17:LEU:CD1	1:A:167:LEU:HD12	2.50	0.41
1:B:109:ASP:OD1	1:B:111:LYS:HG3	2.20	0.41
1:C:331:ASP:O	1:C:368:GLY:HA2	2.21	0.41
1:A:246:ILE:HD13	1:A:472:MET:CG	2.47	0.41
1:A:374:ILE:O	1:A:374:ILE:HG22	2.20	0.41
1:B:160:ILE:HD12	1:B:160:ILE:N	2.35	0.41
1:B:429:PRO:HB2	1:C:338:GLN:OE1	2.21	0.41
1:C:22:TYR:O	1:C:25:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLY:C	1:C:223:LEU:HD11	2.45	0.41
1:C:242:LEU:HD23	1:C:242:LEU:HA	1.81	0.41
1:A:252:ALA:HB3	1:A:393:ILE:HG22	2.01	0.41
1:A:416:HIS:ND1	1:A:417:ALA:N	2.62	0.41
1:B:279:ILE:HG23	1:B:283:LEU:HB2	2.03	0.41
1:A:69:ASP:OD2	1:A:70:ASP:N	2.54	0.41
1:A:181:ASN:HD22	1:A:184:TYR:CB	2.30	0.41
1:A:333:ARG:O	1:A:339:PRO:HA	2.20	0.41
1:B:363:ASP:HA	1:B:366:GLN:HE21	1.84	0.41
1:C:73:PHE:HE2	1:C:142:ILE:O	2.04	0.41
1:C:164:PRO:HG3	1:C:184:TYR:CE1	2.55	0.41
1:C:203:THR:O	1:C:207:VAL:HG23	2.21	0.41
1:C:216:LEU:HD11	1:C:218:TYR:HB2	2.02	0.41
1:A:35:GLU:OE2	1:A:184:TYR:OH	2.32	0.41
1:A:54:TRP:HB3	1:A:65:PHE:CD1	2.55	0.41
1:B:4:ASP:OD2	1:B:4:ASP:N	2.53	0.41
1:B:37:LEU:HG	1:B:141:PHE:HZ	1.85	0.41
1:B:393:ILE:O	1:B:393:ILE:HG23	2.20	0.41
1:B:431:ILE:HG23	1:B:454:ILE:HG23	2.02	0.41
1:C:411:MET:HE2	1:C:435:ILE:HD11	2.02	0.41
1:A:83:ALA:HA	1:A:144:PRO:HG2	2.03	0.41
1:A:221:GLU:OE1	1:A:396:ARG:NH2	2.50	0.41
1:B:34:TYR:HD2	1:B:141:PHE:O	2.04	0.41
1:B:180:ARG:HH11	1:B:188:LYS:HG2	1.86	0.41
1:B:201:ASP:HA	1:B:202:PRO:HD3	1.83	0.41
1:B:278:LEU:O	1:B:281:ASN:O	2.39	0.41
1:B:283:LEU:O	1:B:284:TYR:C	2.63	0.41
1:B:405:HIS:CG	1:B:406:ALA:N	2.89	0.41
1:C:22:TYR:CD1	1:C:22:TYR:N	2.89	0.41
1:C:103:LEU:HD11	1:C:129:PHE:CD2	2.56	0.41
1:C:180:ARG:HG2	1:C:181:ASN:N	2.35	0.41
1:C:207:VAL:HA	1:C:210:GLU:CG	2.50	0.41
1:C:326:LEU:HG	1:C:333:ARG:HH21	1.85	0.41
1:A:128:PRO:O	1:A:132:GLU:HG3	2.21	0.41
1:B:171:LYS:O	1:B:172:LEU:C	2.64	0.41
1:B:459:HIS:HD2	7:B:538:HOH:O	2.04	0.41
1:A:304:GLY:HA3	1:B:234:GLN:HG2	2.02	0.40
1:B:330:LYS:CG	1:B:331:ASP:H	2.34	0.40
1:A:47:ILE:HD12	1:A:47:ILE:C	2.45	0.40
1:A:398:TRP:HB2	1:A:402:TYR:HB2	2.02	0.40
1:C:347:ILE:HD13	1:C:381:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:GLY:O	1:C:376:GLU:HG3	2.21	0.40
1:A:180:ARG:HH21	1:A:192:LYS:HB2	1.87	0.40
1:B:218:TYR:CE2	1:B:472:MET:HE3	2.56	0.40
1:C:17:LEU:HB3	1:C:159:PRO:CB	2.51	0.40
1:C:235:ASN:ND2	1:C:237:ALA:H	2.19	0.40
1:A:87:ASN:O	1:A:90:ALA:HB3	2.21	0.40
1:A:110:VAL:HG13	1:A:120:ILE:HG12	2.03	0.40
1:A:403:ASP:HA	1:A:404:PRO:HA	1.78	0.40
1:A:473:MET:HE2	1:A:473:MET:HB3	1.92	0.40
1:B:22:TYR:HA	1:B:137:ARG:NH1	2.36	0.40
1:B:316:LYS:HB2	1:B:333:ARG:NH1	2.35	0.40
1:B:374:ILE:HG22	1:B:376:GLU:HG3	2.03	0.40
1:B:396:ARG:NH2	1:B:397:THR:O	2.54	0.40
1:C:3:PRO:O	1:C:4:ASP:C	2.63	0.40
1:C:36:PRO:HB3	1:C:140:ARG:NE	2.35	0.40
1:C:342:ILE:O	1:C:371:VAL:HA	2.21	0.40
1:A:316:LYS:HB2	1:A:333:ARG:NH1	2.36	0.40
1:B:411:MET:HG2	1:B:418:ASP:CB	2.50	0.40
1:C:73:PHE:HB3	1:C:74:SER:H	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/502 (99%)	435 (88%)	54 (11%)	8 (2%)	7	27
1	B	498/502 (99%)	446 (90%)	38 (8%)	14 (3%)	4	14
1	C	496/502 (99%)	430 (87%)	56 (11%)	10 (2%)	6	21
All	All	1491/1506 (99%)	1311 (88%)	148 (10%)	32 (2%)	5	20

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	B	501	LYS
1	C	5	GLU
1	C	67	LEU
1	C	73	PHE
1	C	489	ALA
1	A	102	GLU
1	A	499	PRO
1	B	95	ARG
1	B	500	VAL
1	A	113	LEU
1	B	149	ASN
1	C	149	ASN
1	C	221	GLU
1	A	159	PRO
1	B	36	PRO
1	B	129	PHE
1	B	282	ALA
1	B	321	LYS
1	B	322	ALA
1	C	114	SER
1	C	423	GLN
1	C	493	PRO
1	A	43	ASP
1	A	145	SER
1	B	157	LYS
1	C	69	ASP
1	A	70	ASP
1	B	284	TYR
1	B	328	ALA
1	B	340	LEU
1	B	399	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	423/425 (100%)	399 (94%)	24 (6%)	18	49
1	B	425/425 (100%)	393 (92%)	32 (8%)	12	37
1	C	422/425 (99%)	384 (91%)	38 (9%)	9	28
All	All	1270/1275 (100%)	1176 (93%)	94 (7%)	13	37

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	46	VAL
1	A	55	THR
1	A	73	PHE
1	A	86	GLU
1	A	103	LEU
1	A	111	LYS
1	A	147	PHE
1	A	167	LEU
1	A	192	LYS
1	A	221	GLU
1	A	224	LEU
1	A	231	ARG
1	A	234	GLN
1	A	248	THR
1	A	249	VAL
1	A	275	LYS
1	A	276	LYS
1	A	316	LYS
1	A	331	ASP
1	A	371	VAL
1	A	433	LYS
1	A	439	LEU
1	A	479	GLU
1	B	4	ASP
1	B	5	GLU
1	B	14	VAL
1	B	23	THR
1	B	36	PRO
1	B	46	VAL
1	B	77	GLU
1	B	103	LEU
1	B	108	VAL
1	B	123	LYS

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Mol	Chain	Res	Type
1	B	216	LEU
1	B	242	LEU
1	B	248	THR
1	B	250	MET
1	B	269	LEU
1	B	276	LYS
1	B	319	LEU
1	B	338	GLN
1	B	343	GLU
1	B	347	ILE
1	B	366	GLN
1	B	367	ILE
1	B	371	VAL
1	B	373	LEU
1	B	378	GLU
1	B	416	HIS
1	B	427	ASP
1	B	439	LEU
1	B	465	LEU
1	B	471	SER
1	B	473	MET
1	B	479	GLU
1	C	6	ILE
1	C	7	THR
1	C	23	THR
1	C	35	GLU
1	C	38	VAL
1	C	50	LEU
1	C	58	GLU
1	C	64	THR
1	C	82	GLU
1	C	103	LEU
1	C	131	GLN
1	C	148	LYS
1	C	156	ILE
1	C	157	LYS
1	C	167	LEU
1	C	191	ILE
1	C	223	LEU
1	C	235	ASN
1	C	248	THR
1	C	250	MET

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Mol	Chain	Res	Type
1	C	253	LEU
1	C	260	THR
1	C	275	LYS
1	C	276	LYS
1	C	278	LEU
1	C	306	LYS
1	C	319	LEU
1	C	320	GLU
1	C	325	THR
1	C	333	ARG
1	C	358	GLU
1	C	371	VAL
1	C	405	HIS
1	C	438	VAL
1	C	441	THR
1	C	444	GLU
1	C	465	LEU
1	C	497	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	26	GLN
1	A	30	GLN
1	A	41	GLN
1	A	87	ASN
1	A	94	ASN
1	A	96	GLN
1	A	106	GLN
1	A	131	GLN
1	A	146	GLN
1	A	150	HIS
1	A	154	ASN
1	A	173	ASN
1	A	174	GLN
1	A	181	ASN
1	A	254	ASN
1	A	274	ASN
1	A	281	ASN
1	A	288	GLN
1	A	309	GLN

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Mol	Chain	Res	Type
1	A	361	GLN
1	A	385	GLN
1	A	442	HIS
1	A	448	GLN
1	A	459	HIS
1	B	13	ASN
1	B	20	HIS
1	B	26	GLN
1	B	87	ASN
1	B	94	ASN
1	B	106	GLN
1	B	146	GLN
1	B	149	ASN
1	B	173	ASN
1	B	197	ASN
1	B	244	GLN
1	B	254	ASN
1	B	302	ASN
1	B	361	GLN
1	B	366	GLN
1	B	420	GLN
1	B	423	GLN
1	B	442	HIS
1	B	459	HIS
1	C	13	ASN
1	C	26	GLN
1	C	131	GLN
1	C	154	ASN
1	C	173	ASN
1	C	235	ASN
1	C	239	HIS
1	C	254	ASN
1	C	281	ASN
1	C	288	GLN
1	C	338	GLN
1	C	361	GLN
1	C	385	GLN
1	C	395	HIS
1	C	416	HIS
1	C	420	GLN
1	C	442	HIS
1	C	459	HIS

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Mol	Chain	Res	Type
1	C	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
3	ACT	C	506	-	3,3,3	0.82	0	3,3,3	1.31	0
2	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.29	0
5	HCT	B	508[B]	-	12,12,12	1.47	3 (25%)	14,15,15	2.00	4 (28%)
5	HCT	B	508[A]	-	12,12,12	1.10	1 (8%)	14,15,15	1.90	4 (28%)
5	HCT	C	508	-	12,12,12	1.32	1 (8%)	14,15,15	1.02	0
3	ACT	A	505	-	3,3,3	0.83	0	3,3,3	1.36	0
2	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.23	0
3	ACT	B	505	-	3,3,3	0.77	0	3,3,3	1.34	0
3	ACT	C	507	-	3,3,3	0.85	0	3,3,3	1.31	0
4	SO4	A	506	-	4,4,4	0.24	0	6,6,6	0.08	0
5	HCT	A	507	-	12,12,12	1.39	1 (8%)	14,15,15	1.25	1 (7%)
3	ACT	B	506	-	3,3,3	0.83	0	3,3,3	1.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	504	-	5,5,5	0.37	0	5,5,5	0.29	0
3	ACT	B	507	-	3,3,3	0.84	0	3,3,3	1.29	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
2	GOL	A	503	-	-	4/4/4/4	-
5	HCT	B	508[B]	-	-	6/13/13/13	-
5	HCT	B	508[A]	-	1/1/4/4	5/13/13/13	-
5	HCT	C	508	-	1/1/4/4	1/13/13/13	-
2	GOL	A	504	-	-	1/4/4/4	-
5	HCT	A	507	-	1/1/4/4	4/13/13/13	-
2	GOL	B	504	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	508[B]	HCT	O4-C6	-2.63	1.22	1.30
5	A	507	HCT	C3-C7	2.53	1.56	1.51
5	B	508[A]	HCT	O2-C1	-2.44	1.22	1.30
5	B	508[B]	HCT	O2-C1	-2.43	1.22	1.30
5	B	508[B]	HCT	O5-C7	-2.16	1.23	1.30
5	C	508	HCT	C3-C7	2.08	1.55	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	508[B]	HCT	C4-C5-C6	-5.09	98.90	112.49
5	B	508[A]	HCT	C4-C5-C6	-4.01	101.80	112.49
5	B	508[B]	HCT	C3-C2-C1	-3.86	105.20	113.92
5	B	508[A]	HCT	O3-C6-C5	-3.42	112.25	123.09
5	B	508[A]	HCT	O6-C7-C3	-2.88	115.20	122.86
5	B	508[B]	HCT	O5-C7-C3	2.30	120.12	114.16
5	B	508[B]	HCT	O6-C7-C3	-2.27	116.84	122.86
5	B	508[A]	HCT	O4-C6-C5	2.18	120.89	114.00
5	A	507	HCT	O3-C6-C5	-2.15	116.26	123.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	507	HCT	C3
5	B	508[A]	HCT	C3
5	C	508	HCT	C3

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	C1-C2-C3-O3
5	A	507	HCT	C7-C3-C4-C5
5	A	507	HCT	C2-C3-C7-O5
5	A	507	HCT	C2-C3-C7-O6
5	B	508[A]	HCT	C1-C2-C3-C4
5	B	508[A]	HCT	C1-C2-C3-C7
5	B	508[B]	HCT	C2-C3-C7-O5
5	B	508[B]	HCT	C2-C3-C7-O6
5	C	508	HCT	C3-C4-C5-C6
2	A	503	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	B	504	GOL	C1-C2-C3-O3
2	A	503	GOL	O2-C2-C3-O3
5	B	508[A]	HCT	C2-C3-C4-C5
5	B	508[B]	HCT	C2-C3-C4-C5
5	B	508[A]	HCT	C7-C3-C4-C5
5	B	508[B]	HCT	C7-C3-C4-C5
5	B	508[A]	HCT	C3-C4-C5-C6
5	A	507	HCT	C2-C3-C4-C5
2	A	503	GOL	O1-C1-C2-O2
2	B	504	GOL	O1-C1-C2-O2
2	B	504	GOL	O2-C2-C3-O3
5	B	508[B]	HCT	O1-C1-C2-C3
2	A	504	GOL	C1-C2-C3-O3
5	B	508[B]	HCT	O2-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	3	0
5	B	508[B]	HCT	5	0
5	B	508[A]	HCT	3	0
5	C	508	HCT	6	0
3	B	505	ACT	2	0
5	A	507	HCT	2	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	499/502 (99%)	0.03	12 (2%) 59 49	17, 54, 89, 150	18 (3%)
1	B	500/502 (99%)	0.01	8 (1%) 70 61	8, 52, 89, 166	22 (4%)
1	C	498/502 (99%)	0.31	19 (3%) 44 35	10, 69, 111, 151	20 (4%)
All	All	1497/1506 (99%)	0.12	39 (2%) 57 47	8, 57, 101, 166	60 (4%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	GLN	5.9
1	B	154	ASN	5.1
1	C	108	VAL	4.6
1	B	121	THR	4.5
1	C	343	GLU	4.3
1	B	288	GLN	4.2
1	B	479	GLU	4.1
1	A	416	HIS	3.7
1	C	445	THR	3.7
1	A	415	SER	3.3
1	C	416	HIS	3.3
1	C	226	LEU	3.3
1	B	396	ARG	3.2
1	C	214	ILE	2.8
1	C	178	PHE	2.7
1	C	118	LEU	2.7
1	A	386	ARG	2.7
1	C	73	PHE	2.6
1	B	3	PRO	2.6
1	C	476	SER	2.6
1	C	223	LEU	2.6
1	A	4	ASP	2.6
1	A	115	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	9	ALA	2.5
1	B	501	LYS	2.4
1	C	415	SER	2.4
1	A	116	THR	2.4
1	C	499	PRO	2.3
1	C	125	ALA	2.3
1	A	500	VAL	2.2
1	C	65	PHE	2.2
1	A	499	PRO	2.2
1	B	502	PRO	2.2
1	A	143	ALA	2.2
1	C	58	GLU	2.2
1	C	230	ALA	2.2
1	A	391	GLY	2.1
1	C	67	LEU	2.0
1	A	276	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	GOL	A	503	6/6	0.30	0.30	44,46,46,46	6
3	ACT	C	506	4/4	0.49	0.26	94,94,94,94	0
5	HCT	C	508	13/13	0.63	0.20	90,94,95,95	0
3	ACT	B	507	4/4	0.66	0.17	84,84,84,84	0
3	ACT	A	505	4/4	0.66	0.28	34,34,34,34	4
3	ACT	B	506	4/4	0.66	0.18	85,85,85,85	0
5	HCT	A	507	13/13	0.67	0.19	72,75,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	504	6/6	0.67	0.14	96,96,96,96	0
6	CL	B	503	1/1	0.68	0.32	60,60,60,60	1
3	ACT	C	507	4/4	0.69	0.26	23,24,24,24	4
3	ACT	B	505	4/4	0.75	0.18	69,69,69,69	0
4	SO4	A	506	5/5	0.77	0.16	52,52,52,52	5
2	GOL	A	504	6/6	0.84	0.15	60,60,61,62	0
5	HCT	B	508[A]	13/13	0.85	0.15	43,45,45,45	13
5	HCT	B	508[B]	13/13	0.85	0.15	44,44,45,45	13
6	CL	C	505	1/1	0.91	0.11	77,77,77,77	0
6	CL	C	503	1/1	0.93	0.08	65,65,65,65	0
6	CL	C	504	1/1	0.94	0.12	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.