



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:22 AM UTC

PDB ID : 8A4R / pdb_00008a4r
Title : Proline Racemase (ProR) from the Gram-positive bacterium *Acetoanaerobium sticklandii* from isotropic orthorhombic data at 3.59 Å
Authors : Najmudin, S.; Pan, X.-S.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2022-06-13
Resolution : 3.59 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

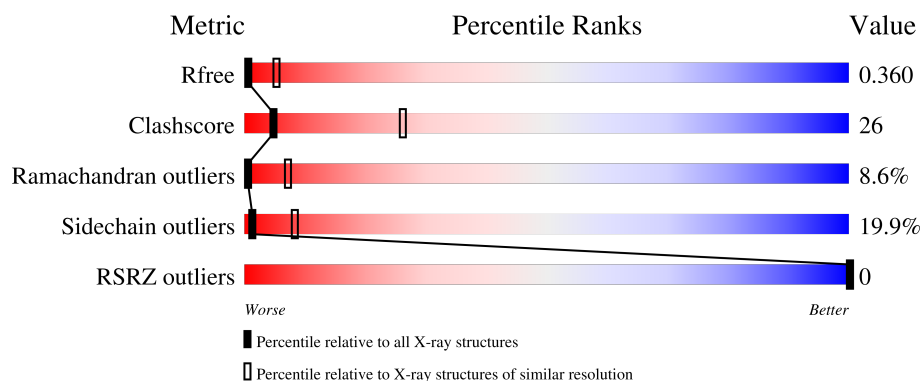
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	AAA	343	 43% 39% 15% ..
1	BBB	343	 45% 37% 14% ..
1	CCC	343	 41% 41% 14% ..
1	DDD	343	 45% 38% 13% ..

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
2	PYC	AAA	401	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20776 atoms, of which 10420 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 Proline racemase A (AsProR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	335	Total	C	H	N	O	S	111	0	0
			5188	1649	2603	421	500	15			
1	BBB	335	Total	C	H	N	O	S	111	0	0
			5188	1649	2603	421	500	15			
1	CCC	335	Total	C	H	N	O	S	111	0	0
			5188	1649	2603	421	500	15			
1	DDD	335	Total	C	H	N	O	S	111	0	0
			5188	1649	2603	421	500	15			

There are 32 discrepancies between the modelled and reference sequences:

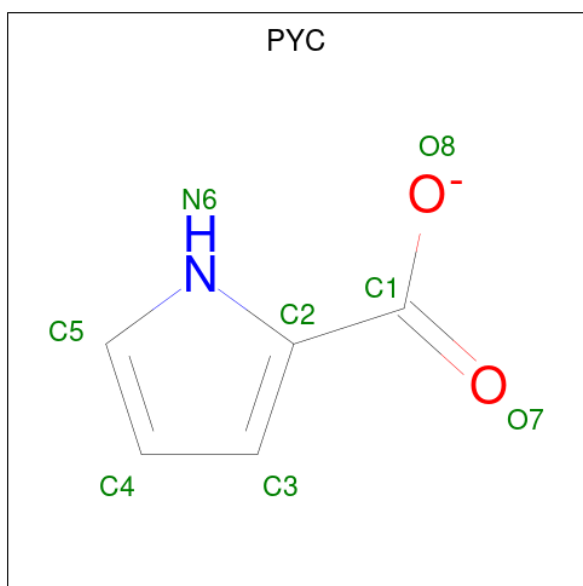
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	336	LEU	-	expression tag	UNP E3PTZ4
AAA	337	GLU	-	expression tag	UNP E3PTZ4
AAA	338	HIS	-	expression tag	UNP E3PTZ4
AAA	339	HIS	-	expression tag	UNP E3PTZ4
AAA	340	HIS	-	expression tag	UNP E3PTZ4
AAA	341	HIS	-	expression tag	UNP E3PTZ4
AAA	342	HIS	-	expression tag	UNP E3PTZ4
AAA	343	HIS	-	expression tag	UNP E3PTZ4
BBB	336	LEU	-	expression tag	UNP E3PTZ4
BBB	337	GLU	-	expression tag	UNP E3PTZ4
BBB	338	HIS	-	expression tag	UNP E3PTZ4
BBB	339	HIS	-	expression tag	UNP E3PTZ4
BBB	340	HIS	-	expression tag	UNP E3PTZ4
BBB	341	HIS	-	expression tag	UNP E3PTZ4
BBB	342	HIS	-	expression tag	UNP E3PTZ4
BBB	343	HIS	-	expression tag	UNP E3PTZ4
CCC	336	LEU	-	expression tag	UNP E3PTZ4
CCC	337	GLU	-	expression tag	UNP E3PTZ4
CCC	338	HIS	-	expression tag	UNP E3PTZ4
CCC	339	HIS	-	expression tag	UNP E3PTZ4
CCC	340	HIS	-	expression tag	UNP E3PTZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	341	HIS	-	expression tag	UNP E3PTZ4
CCC	342	HIS	-	expression tag	UNP E3PTZ4
CCC	343	HIS	-	expression tag	UNP E3PTZ4
DDD	336	LEU	-	expression tag	UNP E3PTZ4
DDD	337	GLU	-	expression tag	UNP E3PTZ4
DDD	338	HIS	-	expression tag	UNP E3PTZ4
DDD	339	HIS	-	expression tag	UNP E3PTZ4
DDD	340	HIS	-	expression tag	UNP E3PTZ4
DDD	341	HIS	-	expression tag	UNP E3PTZ4
DDD	342	HIS	-	expression tag	UNP E3PTZ4
DDD	343	HIS	-	expression tag	UNP E3PTZ4

- Molecule 2 is PYRROLE-2-CARBOXYLATE (CCD ID: PYC) (formula: $C_5H_4NO_2$).

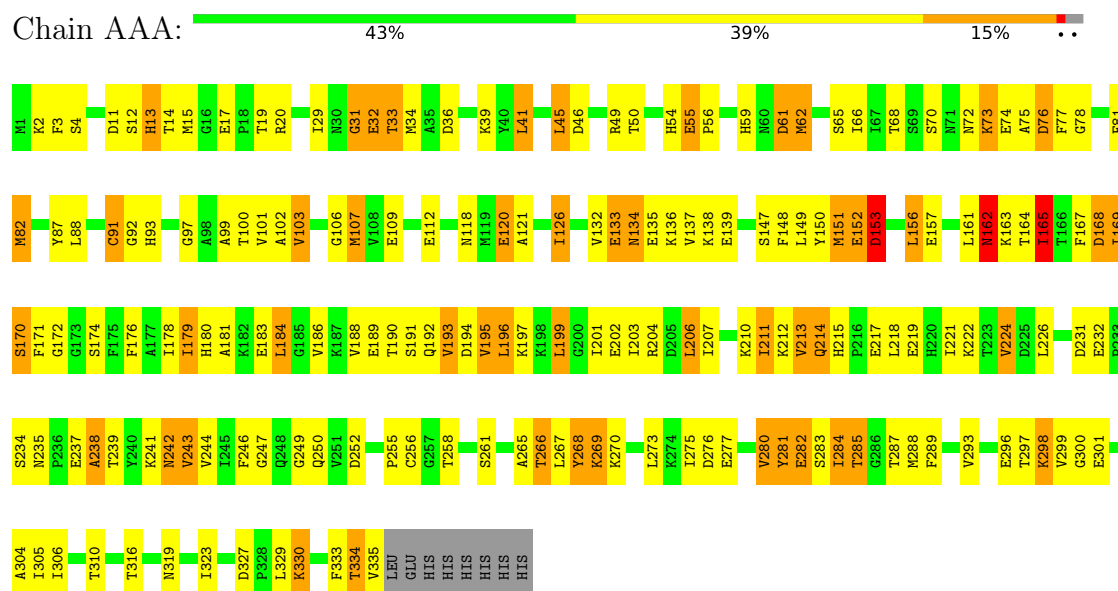


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			12	5	4	1	2		
2	BBB	1	Total	C	H	N	O	0	0
			12	5	4	1	2		

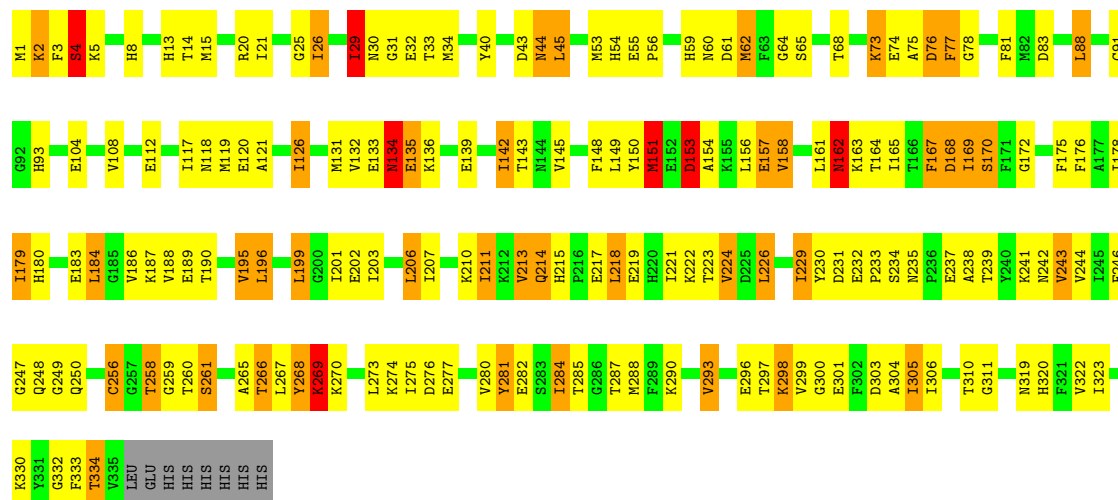
3 Residue-property plots

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

• Molecule 1: Proline racemase A (AsProR)



Chain CCC: 41% 41% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.45Å 107.48Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.55 – 3.59 76.55 – 3.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.55-3.59) 100.0 (76.55-3.59)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.260 , 0.360 0.260 , 0.360	Depositor DCC
R_{free} test set	747 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	119.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 134.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.199 for -h,l,k 0.046 for -l,-k,-h 0.059 for k,h,-l 0.043 for k,l,h 0.043 for l,h,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20776	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: PYC

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	AAA	1.11	0/2634	1.51	7/3556 (0.2%)
1	BBB	1.06	2/2634 (0.1%)	1.47	4/3556 (0.1%)
1	CCC	1.07	1/2634 (0.0%)	1.45	6/3556 (0.2%)
1	DDD	1.06	1/2634 (0.0%)	1.44	2/3556 (0.1%)
All	All	1.08	4/10536 (0.0%)	1.47	19/14224 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1
1	BBB	0	1
1	CCC	0	2
1	DDD	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	158	VAL	N-CA	5.56	1.50	1.45
1	DDD	158	VAL	N-CA	5.48	1.50	1.45
1	BBB	306	ILE	N-CA	5.24	1.50	1.46
1	CCC	158	VAL	N-CA	5.06	1.49	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	168	ASP	CA-CB-CG	-6.40	106.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	109	GLU	CB-CG-CD	6.28	123.27	112.60
1	BBB	109	GLU	CB-CG-CD	6.17	123.09	112.60
1	BBB	162	ASN	CA-CB-CG	6.14	118.74	112.60
1	CCC	41	LEU	CA-C-N	5.82	128.35	120.38
1	CCC	41	LEU	C-N-CA	5.82	128.35	120.38
1	AAA	107	MET	N-CA-C	-5.77	104.91	111.14
1	AAA	103	VAL	N-CA-C	-5.76	105.50	110.74
1	CCC	26	ILE	CB-CA-C	5.70	114.91	109.33
1	CCC	332	GLY	CA-C-O	-5.53	116.83	122.59
1	CCC	17	GLU	CB-CA-C	5.53	116.43	110.08
1	AAA	168	ASP	CA-CB-CG	-5.50	107.10	112.60
1	BBB	107	MET	N-CA-C	-5.49	105.38	111.36
1	DDD	332	GLY	CA-C-O	-5.42	116.95	122.59
1	AAA	298	LYS	CB-CA-C	5.23	118.96	110.22
1	AAA	162	ASN	CA-CB-CG	5.18	117.78	112.60
1	AAA	76	ASP	CA-CB-CG	5.16	117.76	112.60
1	CCC	36	ASP	CA-CB-CG	5.14	117.75	112.60
1	DDD	322	VAL	CA-C-O	-5.13	116.55	121.63

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	266	THR	Peptide
1	BBB	266	THR	Peptide
1	CCC	266	THR	Peptide
1	CCC	319	ASN	Peptide
1	DDD	266	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2585	2603	2593	127	1
1	BBB	2585	2603	2593	148	1
1	CCC	2585	2603	2593	138	1
1	DDD	2585	2603	2593	121	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	8	4	4	4	0
2	BBB	8	4	4	2	0
All	All	10356	10420	10380	529	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (529) 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:CCC:91:CYS:SG	1:CCC:93:HIS:HD2	1.58	1.24
1:CCC:91:CYS:SG	1:CCC:93:HIS:CD2	2.51	1.04
1:BBB:70:SER:O	1:BBB:120:GLU:OE1	1.92	0.88
1:AAA:153:ASP:HA	1:AAA:167:PHE:O	1.76	0.86
1:BBB:170:SER:OG	1:BBB:266:THR:HG21	1.76	0.86
1:CCC:93:HIS:CE1	1:CCC:256:CYS:HA	2.13	0.83
1:CCC:244:VAL:HG21	1:CCC:256:CYS:HB2	1.61	0.82
1:CCC:54:HIS:HB3	1:CCC:333:PHE:O	1.80	0.82
1:AAA:226:LEU:HD23	1:AAA:246:PHE:HB3	1.63	0.81
1:CCC:93:HIS:HE1	1:CCC:256:CYS:HA	1.46	0.80
1:BBB:297:THR:O	1:BBB:304:ALA:HB3	1.82	0.79
1:CCC:63:PHE:CD2	1:CCC:83:ASP:HB3	2.18	0.79
1:DDD:217:GLU:O	1:DDD:219:GLU:N	2.16	0.79
1:CCC:126:ILE:HB	1:CCC:142:ILE:HD11	1.67	0.77
1:BBB:33:THR:HG23	1:BBB:36:ASP:CG	2.10	0.76
1:AAA:92:GLY:N	2:AAA:401:PYC:O8	2.20	0.74
1:CCC:226:LEU:HD12	1:CCC:246:PHE:HB3	1.70	0.73
1:DDD:201:ILE:HG21	1:DDD:249:GLY:HA2	1.69	0.73
1:BBB:213:VAL:HG11	1:BBB:224:VAL:HG22	1.69	0.73
1:CCC:243:VAL:HB	1:CCC:284:ILE:HB	1.70	0.73
1:CCC:133:GLU:O	1:CCC:135:GLU:N	2.20	0.73
1:CCC:15:MET:O	1:CCC:287:THR:HG21	1.88	0.73
1:BBB:108:VAL:HG21	1:BBB:117:ILE:HD11	1.68	0.73
1:AAA:133:GLU:O	1:AAA:135:GLU:OE1	2.07	0.72
1:BBB:91:CYS:SG	1:BBB:93:HIS:CE1	2.82	0.72
1:BBB:153:ASP:HA	1:BBB:167:PHE:O	1.90	0.72
1:CCC:226:LEU:CD1	1:CCC:246:PHE:HB3	2.20	0.72
1:BBB:242:ASN:HB3	1:BBB:281:TYR:CE1	2.25	0.72
1:DDD:126:ILE:HB	1:DDD:142:ILE:HD11	1.71	0.72
1:CCC:217:GLU:O	1:CCC:219:GLU:N	2.22	0.71
1:BBB:61:ASP:HA	1:BBB:250:GLN:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:33:THR:HG23	1:AAA:36:ASP:CG	2.15	0.71
1:AAA:235:ASN:ND2	1:AAA:288:MET:SD	2.64	0.70
1:BBB:226:LEU:HD12	1:BBB:246:PHE:HB3	1.73	0.70
1:AAA:176:PHE:CZ	1:AAA:226:LEU:HD13	2.27	0.69
1:CCC:61:ASP:HA	1:CCC:250:GLN:HB2	1.75	0.69
1:AAA:297:THR:O	1:AAA:304:ALA:HB3	1.91	0.69
1:BBB:98:ALA:O	1:BBB:101:VAL:HG12	1.92	0.69
1:AAA:213:VAL:HG11	1:AAA:224:VAL:HG22	1.75	0.69
1:CCC:170:SER:OG	1:CCC:266:THR:HG21	1.93	0.68
1:DDD:91:CYS:SG	1:DDD:93:HIS:ND1	2.66	0.68
1:DDD:133:GLU:O	1:DDD:135:GLU:N	2.26	0.68
1:AAA:241:LYS:HZ2	1:AAA:282:GLU:CD	2.02	0.67
1:DDD:243:VAL:HB	1:DDD:284:ILE:HB	1.76	0.67
1:AAA:267:LEU:O	1:AAA:269:LYS:N	2.27	0.67
1:BBB:61:ASP:O	1:BBB:62:MET:O	2.14	0.66
1:CCC:176:PHE:CZ	1:CCC:259:GLY:HA2	2.31	0.66
1:CCC:213:VAL:HG11	1:CCC:224:VAL:HG22	1.77	0.66
1:AAA:20:ARG:HB2	1:AAA:62:MET:HE1	1.77	0.66
1:BBB:156:LEU:HD11	1:BBB:164:THR:OG1	1.96	0.66
1:DDD:14:THR:HG21	1:DDD:93:HIS:HA	1.77	0.66
1:BBB:172:GLY:O	1:BBB:258:THR:HG22	1.95	0.65
1:DDD:170:SER:OG	1:DDD:266:THR:HG21	1.96	0.65
1:BBB:150:TYR:O	1:BBB:169:ILE:O	2.14	0.65
1:DDD:244:VAL:HG21	1:DDD:256:CYS:HB2	1.77	0.65
1:AAA:319:ASN:OD1	1:BBB:319:ASN:OD1	2.14	0.65
1:CCC:176:PHE:CZ	1:CCC:259:GLY:CA	2.80	0.65
1:CCC:268:TYR:OH	1:CCC:296:GLU:HG2	1.97	0.65
1:BBB:170:SER:HG	1:BBB:266:THR:HG21	1.61	0.64
1:CCC:242:ASN:HB3	1:CCC:281:TYR:CE1	2.33	0.64
1:BBB:267:LEU:O	1:BBB:269:LYS:N	2.31	0.64
1:AAA:327:ASP:OD1	1:BBB:13:HIS:NE2	2.30	0.64
1:DDD:226:LEU:HD12	1:DDD:246:PHE:HB3	1.79	0.64
1:AAA:156:LEU:HB2	1:AAA:165:ILE:O	1.98	0.64
1:DDD:213:VAL:HG11	1:DDD:224:VAL:HG22	1.80	0.63
1:AAA:334:THR:O	1:AAA:335:VAL:HG23	1.98	0.63
1:DDD:150:TYR:O	1:DDD:169:ILE:O	2.15	0.63
1:CCC:297:THR:O	1:CCC:304:ALA:HB3	1.98	0.63
1:DDD:108:VAL:HG11	1:DDD:117:ILE:HD11	1.81	0.63
1:DDD:226:LEU:CD1	1:DDD:246:PHE:HB3	2.29	0.63
1:AAA:242:ASN:HB3	1:AAA:281:TYR:CE1	2.34	0.62
1:AAA:150:TYR:O	1:AAA:169:ILE:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:170:SER:HB3	1:AAA:266:THR:CG2	2.29	0.62
1:AAA:242:ASN:OD1	1:AAA:242:ASN:C	2.42	0.62
1:DDD:268:TYR:OH	1:DDD:296:GLU:HG2	2.00	0.62
1:CCC:283:SER:OG	1:CCC:287:THR:HG22	2.00	0.62
1:DDD:4:SER:OG	1:DDD:5:LYS:N	2.33	0.62
1:BBB:228:GLU:OE2	1:BBB:242:ASN:ND2	2.32	0.61
1:BBB:72:ASN:HB2	1:BBB:120:GLU:OE2	1.98	0.61
1:AAA:13:HIS:CE1	1:BBB:329:LEU:HD22	2.36	0.61
1:DDD:1:MET:HB3	1:DDD:3:PHE:CE2	2.36	0.61
1:AAA:70:SER:O	1:AAA:120:GLU:OE2	2.18	0.61
1:BBB:3:PHE:O	1:BBB:323:ILE:O	2.19	0.61
1:DDD:167:PHE:HB2	1:DDD:179:ILE:HB	1.83	0.61
1:AAA:195:VAL:O	1:AAA:199:LEU:HB2	2.01	0.60
1:BBB:226:LEU:CD1	1:BBB:246:PHE:HB3	2.31	0.60
1:BBB:133:GLU:O	1:BBB:135:GLU:N	2.31	0.60
1:CCC:207:ILE:O	1:CCC:211:ILE:HG23	2.01	0.60
1:DDD:139:GLU:HB2	1:DDD:311:GLY:O	2.02	0.60
1:DDD:25:GLY:C	1:DDD:26:ILE:HD13	2.26	0.60
1:DDD:91:CYS:SG	1:DDD:93:HIS:CE1	2.95	0.60
1:AAA:285:THR:OG1	1:AAA:287:THR:HG22	2.01	0.60
1:CCC:70:SER:O	1:CCC:120:GLU:OE2	2.20	0.59
1:BBB:207:ILE:CG2	1:BBB:224:VAL:HG21	2.32	0.59
1:CCC:167:PHE:HB2	1:CCC:179:ILE:HB	1.84	0.59
1:DDD:242:ASN:HB3	1:DDD:281:TYR:CE1	2.36	0.59
1:AAA:153:ASP:O	1:AAA:167:PHE:O	2.21	0.59
1:BBB:326:GLU:OE1	1:BBB:326:GLU:HA	2.03	0.59
1:DDD:61:ASP:HA	1:DDD:250:GLN:HB2	1.84	0.59
1:CCC:176:PHE:CE2	1:CCC:259:GLY:HA2	2.37	0.59
1:BBB:14:THR:HG21	1:BBB:93:HIS:HA	1.85	0.59
1:BBB:243:VAL:HB	1:BBB:284:ILE:HB	1.84	0.59
1:CCC:108:VAL:HG21	1:CCC:117:ILE:HD11	1.85	0.59
1:CCC:139:GLU:HB2	1:CCC:311:GLY:O	2.03	0.59
1:CCC:144:ASN:HD22	1:CCC:261:SER:CB	2.16	0.58
1:DDD:207:ILE:HG22	1:DDD:224:VAL:HG21	1.85	0.58
1:AAA:15:MET:O	1:AAA:287:THR:HG21	2.04	0.58
1:AAA:170:SER:HB3	1:AAA:266:THR:HG21	1.85	0.58
1:AAA:186:VAL:HG11	1:AAA:196:LEU:HG	1.86	0.58
1:BBB:34:MET:HE3	1:BBB:78:GLY:HA3	1.85	0.58
1:DDD:156:LEU:HD11	1:DDD:164:THR:OG1	2.03	0.58
1:BBB:149:LEU:HD23	1:BBB:266:THR:HG22	1.84	0.57
1:AAA:61:ASP:HA	1:AAA:250:GLN:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:207:ILE:O	1:DDD:211:ILE:HG23	2.04	0.57
1:CCC:244:VAL:HG21	1:CCC:256:CYS:CB	2.33	0.57
1:BBB:20:ARG:HB2	1:BBB:62:MET:HE1	1.86	0.57
1:CCC:108:VAL:HG11	1:CCC:117:ILE:HD11	1.85	0.57
1:BBB:241:LYS:HZ2	1:BBB:282:GLU:HG2	1.68	0.57
1:BBB:96:ILE:CG1	1:BBB:142:ILE:HD12	2.34	0.56
1:CCC:256:CYS:O	1:CCC:256:CYS:SG	2.63	0.56
1:DDD:195:VAL:O	1:DDD:199:LEU:HB2	2.05	0.56
1:DDD:54:HIS:HB3	1:DDD:333:PHE:O	2.06	0.56
1:DDD:108:VAL:HG21	1:DDD:117:ILE:HD11	1.86	0.56
1:DDD:267:LEU:O	1:DDD:269:LYS:N	2.38	0.56
1:BBB:4:SER:OG	1:BBB:5:LYS:N	2.36	0.56
1:AAA:214:GLN:OE1	1:AAA:214:GLN:O	2.24	0.56
1:CCC:186:VAL:HG11	1:CCC:196:LEU:HG	1.86	0.56
1:DDD:241:LYS:HG2	1:DDD:282:GLU:HG2	1.87	0.56
1:CCC:112:GLU:OE2	1:CCC:134:ASN:HA	2.05	0.56
1:BBB:33:THR:HG23	1:BBB:36:ASP:OD1	2.04	0.55
1:DDD:207:ILE:CG2	1:DDD:224:VAL:HG21	2.37	0.55
1:DDD:201:ILE:HG21	1:DDD:249:GLY:CA	2.35	0.55
1:AAA:207:ILE:CG2	1:AAA:224:VAL:HG21	2.36	0.55
1:AAA:149:LEU:HD23	1:AAA:266:THR:HG22	1.89	0.55
1:AAA:201:ILE:HG21	1:AAA:249:GLY:HA2	1.89	0.55
1:DDD:242:ASN:C	1:DDD:242:ASN:OD1	2.50	0.55
1:DDD:256:CYS:O	1:DDD:256:CYS:SG	2.64	0.55
1:CCC:150:TYR:O	1:CCC:169:ILE:O	2.25	0.54
1:CCC:242:ASN:HB3	1:CCC:281:TYR:CZ	2.42	0.54
1:BBB:256:CYS:O	1:BBB:260:THR:HG23	2.07	0.54
1:DDD:44:ASN:C	1:DDD:45:LEU:HD13	2.33	0.54
1:BBB:112:GLU:OE1	1:BBB:112:GLU:HA	2.08	0.54
1:DDD:20:ARG:NH1	1:DDD:62:MET:HE2	2.23	0.54
1:BBB:244:VAL:HG21	1:BBB:256:CYS:CB	2.37	0.54
1:DDD:229:ILE:HG12	1:DDD:243:VAL:HG13	1.90	0.54
1:AAA:327:ASP:O	1:AAA:330:LYS:HB3	2.07	0.54
1:CCC:89:ASN:C	1:CCC:89:ASN:HD22	2.15	0.54
1:DDD:172:GLY:O	1:DDD:258:THR:HG22	2.08	0.54
1:CCC:172:GLY:O	1:CCC:258:THR:HG22	2.08	0.54
1:DDD:73:LYS:O	1:DDD:75:ALA:N	2.40	0.54
1:DDD:201:ILE:CG2	1:DDD:249:GLY:HA2	2.38	0.54
1:DDD:233:PRO:HA	1:DDD:241:LYS:HG3	1.90	0.54
1:DDD:297:THR:O	1:DDD:304:ALA:HB3	2.08	0.54
1:CCC:201:ILE:HG21	1:CCC:249:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:34:MET:HE3	1:DDD:78:GLY:HA3	1.89	0.53
1:DDD:221:ILE:HD12	1:DDD:222:LYS:N	2.23	0.53
1:BBB:207:ILE:HG22	1:BBB:224:VAL:HG21	1.89	0.53
1:AAA:14:THR:HG21	1:AAA:93:HIS:HA	1.89	0.53
1:AAA:242:ASN:HB3	1:AAA:281:TYR:CZ	2.43	0.53
1:AAA:133:GLU:O	1:AAA:135:GLU:N	2.41	0.53
1:AAA:207:ILE:O	1:AAA:211:ILE:HD12	2.08	0.53
1:BBB:265:ALA:HA	1:BBB:305:ILE:HG21	1.91	0.53
1:CCC:176:PHE:CZ	1:CCC:259:GLY:N	2.76	0.53
1:CCC:207:ILE:O	1:CCC:211:ILE:HD12	2.09	0.53
1:CCC:207:ILE:CG2	1:CCC:224:VAL:HG21	2.38	0.53
1:CCC:207:ILE:HG22	1:CCC:224:VAL:HG21	1.90	0.53
1:BBB:240:TYR:O	1:BBB:282:GLU:HB3	2.09	0.53
1:CCC:175:PHE:HB2	1:CCC:223:THR:O	2.08	0.53
1:BBB:65:SER:HB3	1:BBB:79:ILE:HD11	1.89	0.53
1:AAA:151:MET:O	1:AAA:152:GLU:HB2	2.08	0.53
1:BBB:148:PHE:HA	1:BBB:265:ALA:HB1	1.91	0.53
1:BBB:221:ILE:HD12	1:BBB:222:LYS:N	2.24	0.53
1:AAA:243:VAL:HB	1:AAA:284:ILE:HB	1.90	0.52
1:BBB:298:LYS:HA	1:BBB:303:ASP:HA	1.91	0.52
1:CCC:112:GLU:CD	1:CCC:134:ASN:HA	2.34	0.52
1:CCC:176:PHE:CE2	1:CCC:259:GLY:CA	2.92	0.52
1:DDD:149:LEU:HD23	1:DDD:266:THR:HG22	1.91	0.52
1:CCC:221:ILE:HD12	1:CCC:222:LYS:N	2.24	0.52
1:AAA:147:SER:O	1:AAA:304:ALA:HB1	2.10	0.52
1:BBB:334:THR:O	1:BBB:335:VAL:HG23	2.10	0.52
1:BBB:162:ASN:HD21	1:BBB:164:THR:HG22	1.74	0.52
1:AAA:3:PHE:O	1:AAA:323:ILE:O	2.26	0.52
1:AAA:170:SER:CB	1:AAA:266:THR:HG21	2.40	0.52
1:AAA:210:LYS:O	1:AAA:211:ILE:HG23	2.09	0.52
1:AAA:268:TYR:OH	1:AAA:296:GLU:HG2	2.09	0.52
1:BBB:297:THR:O	1:BBB:304:ALA:CB	2.56	0.52
1:CCC:242:ASN:C	1:CCC:242:ASN:OD1	2.51	0.52
1:BBB:91:CYS:SG	1:BBB:93:HIS:ND1	2.83	0.52
1:BBB:162:ASN:HD21	1:BBB:164:THR:CG2	2.23	0.52
1:BBB:179:ILE:HG12	1:BBB:229:ILE:HG22	1.92	0.52
1:BBB:96:ILE:HG13	1:BBB:142:ILE:HD12	1.92	0.52
1:CCC:195:VAL:O	1:CCC:199:LEU:HB2	2.10	0.52
1:BBB:14:THR:OG1	1:BBB:313:ALA:HB2	2.10	0.52
1:DDD:20:ARG:HB2	1:DDD:62:MET:HE1	1.91	0.52
1:BBB:186:VAL:HG11	1:BBB:196:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:176:PHE:CE2	1:DDD:259:GLY:HA2	2.46	0.51
1:AAA:148:PHE:CE2	1:AAA:299:VAL:HG11	2.45	0.51
1:AAA:283:SER:OG	1:AAA:287:THR:HG22	2.11	0.51
1:DDD:59:HIS:ND1	1:DDD:60:ASN:O	2.38	0.51
1:BBB:150:TYR:O	1:BBB:151:MET:O	2.28	0.51
1:DDD:235:ASN:ND2	1:DDD:288:MET:SD	2.84	0.51
1:AAA:184:LEU:HD13	1:AAA:186:VAL:HG23	1.93	0.51
1:BBB:184:LEU:HD13	1:BBB:186:VAL:HG23	1.92	0.51
1:CCC:148:PHE:HA	1:CCC:265:ALA:HB1	1.93	0.51
1:AAA:203:ILE:HA	1:AAA:206:LEU:CD2	2.41	0.51
1:BBB:207:ILE:O	1:BBB:211:ILE:HG23	2.11	0.51
1:BBB:252:ASP:OD1	1:BBB:254:SER:OG	2.15	0.51
1:AAA:121:ALA:HB2	1:AAA:126:ILE:CD1	2.41	0.50
1:BBB:98:ALA:O	1:BBB:101:VAL:CG1	2.59	0.50
1:CCC:257:GLY:HA2	1:CCC:309:ILE:HG21	1.93	0.50
1:DDD:298:LYS:HB2	1:DDD:303:ASP:HA	1.94	0.50
1:BBB:215:HIS:HB2	1:BBB:221:ILE:HD11	1.94	0.50
1:CCC:184:LEU:HD13	1:CCC:186:VAL:HG23	1.93	0.50
1:AAA:153:ASP:CA	1:AAA:167:PHE:O	2.55	0.50
1:BBB:221:ILE:HD12	1:BBB:222:LYS:H	1.77	0.50
1:CCC:181:ALA:HB1	1:CCC:186:VAL:O	2.12	0.50
1:BBB:90:MET:HE2	1:BBB:126:ILE:CD1	2.42	0.50
1:BBB:242:ASN:HB3	1:BBB:281:TYR:CZ	2.46	0.50
1:CCC:49:ARG:HD2	1:CCC:86:GLY:O	2.11	0.50
1:CCC:241:LYS:HG2	1:CCC:282:GLU:HG2	1.93	0.50
1:DDD:112:GLU:CD	1:DDD:134:ASN:HA	2.37	0.50
1:CCC:55:GLU:HB3	1:CCC:56:PRO:HA	1.93	0.50
1:CCC:63:PHE:CE2	1:CCC:83:ASP:HB3	2.46	0.50
1:AAA:299:VAL:O	1:AAA:301:GLU:N	2.45	0.50
1:CCC:115:THR:HB	1:CCC:130:VAL:HG13	1.94	0.50
1:DDD:176:PHE:CZ	1:DDD:259:GLY:HA2	2.47	0.50
1:AAA:81:PHE:CD1	1:AAA:91:CYS:HB3	2.47	0.49
1:CCC:150:TYR:O	1:CCC:151:MET:O	2.30	0.49
1:DDD:203:ILE:HA	1:DDD:206:LEU:CD2	2.42	0.49
1:AAA:329:LEU:HD22	1:BBB:13:HIS:CE1	2.47	0.49
1:BBB:25:GLY:C	1:BBB:26:ILE:HD13	2.37	0.49
1:BBB:90:MET:CE	1:BBB:126:ILE:CD1	2.89	0.49
1:BBB:90:MET:SD	1:BBB:91:CYS:N	2.85	0.49
1:DDD:207:ILE:O	1:DDD:211:ILE:HD12	2.12	0.49
1:DDD:215:HIS:HB2	1:DDD:221:ILE:HD11	1.94	0.49
1:BBB:207:ILE:O	1:BBB:211:ILE:HD12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:180:HIS:O	1:DDD:183:GLU:HB3	2.13	0.49
1:BBB:31:GLY:HA3	1:BBB:37:LYS:HA	1.94	0.49
1:BBB:299:VAL:O	1:BBB:301:GLU:N	2.45	0.49
1:CCC:203:ILE:HA	1:CCC:206:LEU:CD2	2.43	0.49
1:CCC:76:ASP:OD1	1:CCC:76:ASP:N	2.45	0.49
1:CCC:104:GLU:OE2	1:CCC:136:LYS:HD3	2.12	0.49
1:DDD:176:PHE:CZ	1:DDD:259:GLY:CA	2.95	0.49
1:DDD:248:GLN:HE22	1:DDD:334:THR:HG21	1.77	0.49
1:BBB:218:LEU:HD11	1:BBB:221:ILE:HG12	1.94	0.49
1:BBB:133:GLU:O	1:BBB:135:GLU:OE2	2.31	0.49
1:BBB:256:CYS:SG	2:BBB:401:PYC:N6	2.86	0.49
1:AAA:148:PHE:CD2	1:AAA:299:VAL:HG11	2.48	0.49
1:AAA:171:PHE:CE2	1:AAA:215:HIS:CE1	3.01	0.49
1:CCC:284:ILE:O	1:CCC:284:ILE:HD13	2.12	0.49
1:BBB:219:GLU:O	1:BBB:222:LYS:HE2	2.13	0.48
1:CCC:181:ALA:HB3	1:CCC:231:ASP:HB2	1.95	0.48
1:AAA:66:ILE:HD11	1:AAA:82:MET:HE1	1.95	0.48
1:CCC:267:LEU:O	1:CCC:269:LYS:N	2.46	0.48
1:DDD:187:LYS:O	1:DDD:189:GLU:N	2.46	0.48
1:BBB:176:PHE:CE2	1:BBB:226:LEU:HG	2.48	0.48
1:BBB:233:PRO:HA	1:BBB:241:LYS:HG3	1.95	0.48
1:DDD:241:LYS:CD	1:DDD:282:GLU:HG2	2.43	0.48
1:AAA:149:LEU:HA	1:AAA:266:THR:HG22	1.95	0.48
1:BBB:77:PHE:CE1	1:BBB:119:MET:HG2	2.48	0.48
1:BBB:192:GLN:O	1:BBB:194:ASP:N	2.46	0.48
1:BBB:201:ILE:HG21	1:BBB:249:GLY:HA2	1.95	0.48
1:CCC:229:ILE:HG12	1:CCC:243:VAL:HG13	1.95	0.48
1:DDD:3:PHE:O	1:DDD:323:ILE:O	2.31	0.48
1:AAA:256:CYS:SG	2:AAA:401:PYC:C2	3.02	0.48
1:BBB:96:ILE:HG12	1:BBB:142:ILE:HD12	1.94	0.48
1:DDD:186:VAL:HG11	1:DDD:196:LEU:HG	1.96	0.48
1:BBB:61:ASP:CA	1:BBB:250:GLN:HB2	2.41	0.48
1:CCC:215:HIS:HB2	1:CCC:221:ILE:HD11	1.93	0.48
1:AAA:132:VAL:HA	1:AAA:136:LYS:O	2.14	0.48
1:AAA:138:LYS:O	1:AAA:139:GLU:HB3	2.14	0.48
1:AAA:189:GLU:C	1:AAA:284:ILE:HD11	2.38	0.48
1:BBB:108:VAL:HG21	1:BBB:117:ILE:CD1	2.39	0.48
1:BBB:97:GLY:O	1:BBB:101:VAL:HG12	2.13	0.48
1:BBB:153:ASP:CA	1:BBB:167:PHE:O	2.60	0.48
1:CCC:21:ILE:N	1:CCC:21:ILE:HD12	2.28	0.48
1:DDD:108:VAL:HG21	1:DDD:117:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:170:SER:CB	1:BBB:266:THR:HG21	2.43	0.47
1:DDD:83:ASP:OD1	1:DDD:88:LEU:HD23	2.14	0.47
1:AAA:54:HIS:C	1:AAA:55:GLU:O	2.56	0.47
1:BBB:179:ILE:O	1:BBB:229:ILE:HA	2.14	0.47
1:BBB:268:TYR:OH	1:BBB:296:GLU:HG2	2.13	0.47
1:CCC:20:ARG:HB2	1:CCC:62:MET:HE1	1.95	0.47
1:AAA:180:HIS:O	1:AAA:183:GLU:HB3	2.15	0.47
1:AAA:210:LYS:O	1:AAA:211:ILE:CG2	2.63	0.47
1:BBB:195:VAL:O	1:BBB:199:LEU:HB2	2.15	0.47
1:BBB:244:VAL:HG21	1:BBB:256:CYS:HB3	1.95	0.47
1:CCC:93:HIS:CE1	1:CCC:252:ASP:OD2	2.66	0.47
1:CCC:180:HIS:O	1:CCC:183:GLU:HB3	2.13	0.47
1:DDD:153:ASP:O	1:DDD:154:ALA:HB3	2.15	0.47
1:AAA:192:GLN:O	1:AAA:194:ASP:N	2.47	0.47
1:BBB:62:MET:SD	1:BBB:63:PHE:N	2.87	0.47
1:AAA:244:VAL:HG21	1:AAA:256:CYS:CB	2.44	0.47
1:BBB:285:THR:OG1	1:BBB:287:THR:HG22	2.14	0.47
1:AAA:201:ILE:HG21	1:AAA:249:GLY:CA	2.45	0.47
1:CCC:149:LEU:HD13	1:CCC:149:LEU:C	2.40	0.47
1:CCC:225:ASP:O	1:CCC:226:LEU:HD13	2.15	0.47
1:CCC:299:VAL:O	1:CCC:301:GLU:N	2.48	0.47
1:DDD:121:ALA:HB2	1:DDD:126:ILE:CD1	2.45	0.47
1:CCC:149:LEU:HD23	1:CCC:266:THR:HG22	1.96	0.47
1:DDD:149:LEU:HA	1:DDD:266:THR:HG22	1.97	0.47
1:DDD:176:PHE:CZ	1:DDD:259:GLY:N	2.83	0.47
1:DDD:214:GLN:HA	1:DDD:222:LYS:HG3	1.96	0.47
1:BBB:55:GLU:HB3	1:BBB:56:PRO:HA	1.97	0.46
1:CCC:61:ASP:CA	1:CCC:250:GLN:HB2	2.43	0.46
1:CCC:208:ASN:OD1	1:CCC:224:VAL:HG23	2.15	0.46
1:CCC:298:LYS:HA	1:CCC:303:ASP:HA	1.96	0.46
1:AAA:11:ASP:HB3	1:AAA:316:THR:OG1	2.15	0.46
1:BBB:61:ASP:C	1:BBB:62:MET:O	2.57	0.46
1:BBB:99:ALA:O	1:BBB:100:THR:C	2.58	0.46
1:BBB:218:LEU:HD12	1:BBB:218:LEU:C	2.40	0.46
1:CCC:31:GLY:O	1:CCC:32:GLU:HB2	2.15	0.46
1:CCC:208:ASN:CG	1:CCC:224:VAL:HG23	2.40	0.46
1:DDD:55:GLU:HB3	1:DDD:56:PRO:HA	1.97	0.46
1:AAA:148:PHE:HA	1:AAA:265:ALA:HB1	1.97	0.46
1:AAA:226:LEU:HD23	1:AAA:246:PHE:CB	2.41	0.46
1:AAA:17:GLU:HG3	1:AAA:93:HIS:CE1	2.50	0.46
1:BBB:100:THR:HG21	1:BBB:313:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:298:LYS:HB2	1:CCC:303:ASP:HA	1.96	0.46
1:DDD:242:ASN:HB3	1:DDD:281:TYR:CZ	2.51	0.46
1:CCC:34:MET:HE3	1:CCC:78:GLY:HA3	1.98	0.46
1:CCC:218:LEU:HD12	1:CCC:219:GLU:N	2.30	0.46
1:BBB:246:PHE:CZ	1:BBB:250:GLN:NE2	2.84	0.46
1:DDD:132:VAL:HA	1:DDD:136:LYS:O	2.15	0.46
1:DDD:265:ALA:HA	1:DDD:305:ILE:HG21	1.96	0.46
1:BBB:102:ALA:HA	1:BBB:107:MET:HE2	1.97	0.46
1:DDD:40:TYR:CD1	1:DDD:40:TYR:C	2.94	0.46
1:DDD:153:ASP:N	1:DDD:168:ASP:OD1	2.49	0.46
1:BBB:15:MET:HG3	1:BBB:289:PHE:CE1	2.51	0.46
1:CCC:241:LYS:HZ2	1:CCC:282:GLU:HG2	1.82	0.46
1:AAA:49:ARG:HD3	1:AAA:87:TYR:CE1	2.51	0.45
1:AAA:255:PRO:HD2	1:AAA:289:PHE:CE2	2.51	0.45
1:BBB:256:CYS:SG	2:BBB:401:PYC:C2	3.04	0.45
1:CCC:20:ARG:NH1	1:CCC:62:MET:HE2	2.32	0.45
1:CCC:153:ASP:O	1:CCC:154:ALA:HB3	2.16	0.45
1:DDD:81:PHE:HB2	1:DDD:88:LEU:O	2.15	0.45
1:DDD:148:PHE:HA	1:DDD:265:ALA:HB1	1.99	0.45
1:BBB:102:ALA:HA	1:BBB:107:MET:CE	2.47	0.45
1:DDD:241:LYS:CG	1:DDD:282:GLU:HG2	2.46	0.45
1:DDD:284:ILE:HD13	1:DDD:284:ILE:O	2.16	0.45
1:AAA:91:CYS:HA	2:AAA:401:PYC:O8	2.16	0.45
1:AAA:244:VAL:HG21	1:AAA:256:CYS:HB2	1.97	0.45
1:AAA:256:CYS:SG	2:AAA:401:PYC:N6	2.90	0.45
1:BBB:203:ILE:O	1:BBB:204:ARG:C	2.60	0.45
1:BBB:214:GLN:HA	1:BBB:222:LYS:HG3	1.97	0.45
1:CCC:73:LYS:O	1:CCC:75:ALA:N	2.48	0.45
1:CCC:189:GLU:C	1:CCC:284:ILE:HD11	2.42	0.45
1:CCC:201:ILE:HG21	1:CCC:249:GLY:CA	2.47	0.45
1:AAA:172:GLY:O	1:AAA:258:THR:HG22	2.16	0.45
1:AAA:178:ILE:O	1:AAA:178:ILE:HG22	2.17	0.45
1:CCC:156:LEU:HD23	1:CCC:165:ILE:O	2.17	0.45
1:BBB:59:HIS:O	1:BBB:62:MET:HB3	2.17	0.45
1:BBB:241:LYS:HG2	1:BBB:282:GLU:HG2	1.99	0.45
1:CCC:162:ASN:HD21	1:CCC:164:THR:CG2	2.29	0.45
1:AAA:167:PHE:HB2	1:AAA:179:ILE:HB	1.98	0.45
1:BBB:148:PHE:HB3	1:BBB:304:ALA:CB	2.47	0.45
1:BBB:153:ASP:N	1:BBB:168:ASP:OD1	2.49	0.45
1:AAA:237:GLU:O	1:AAA:238:ALA:HB3	2.17	0.45
1:BBB:12:SER:HA	1:BBB:314:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:131:MET:SD	1:CCC:131:MET:N	2.90	0.45
1:AAA:282:GLU:HG3	1:AAA:283:SER:O	2.16	0.45
1:DDD:53:MET:HE1	1:DDD:64:GLY:HA3	1.98	0.45
1:AAA:103:VAL:O	1:AAA:106:GLY:N	2.46	0.45
1:AAA:170:SER:CB	1:AAA:266:THR:CG2	2.95	0.45
1:DDD:150:TYR:O	1:DDD:151:MET:O	2.35	0.45
1:DDD:184:LEU:HD13	1:DDD:186:VAL:HG23	1.98	0.45
1:CCC:230:TYR:HA	1:CCC:241:LYS:O	2.15	0.45
1:DDD:20:ARG:CZ	1:DDD:62:MET:HE2	2.46	0.45
1:AAA:31:GLY:O	1:AAA:32:GLU:HB2	2.17	0.44
1:AAA:174:SER:CB	1:AAA:226:LEU:HD12	2.48	0.44
1:BBB:112:GLU:CD	1:BBB:134:ASN:HA	2.42	0.44
1:AAA:207:ILE:HG22	1:AAA:224:VAL:HG21	1.99	0.44
1:CCC:244:VAL:HG11	1:CCC:256:CYS:SG	2.58	0.44
1:BBB:131:MET:SD	1:BBB:131:MET:N	2.90	0.44
1:BBB:90:MET:SD	1:BBB:126:ILE:HD12	2.57	0.44
1:DDD:230:TYR:HA	1:DDD:241:LYS:O	2.17	0.44
1:AAA:13:HIS:O	1:AAA:13:HIS:CG	2.70	0.44
1:BBB:112:GLU:OE2	1:BBB:134:ASN:ND2	2.51	0.44
1:BBB:184:LEU:HD13	1:BBB:186:VAL:CG2	2.47	0.44
1:DDD:104:GLU:OE2	1:DDD:136:LYS:HD3	2.18	0.44
1:DDD:218:LEU:HD11	1:DDD:221:ILE:HG12	2.00	0.44
1:AAA:151:MET:HB2	1:AAA:169:ILE:CG2	2.48	0.44
1:AAA:194:ASP:O	1:AAA:197:LYS:HB3	2.17	0.44
1:BBB:297:THR:O	1:BBB:304:ALA:CA	2.65	0.44
1:CCC:108:VAL:HG21	1:CCC:117:ILE:CD1	2.47	0.44
1:BBB:229:ILE:HG12	1:BBB:243:VAL:HG13	1.98	0.44
1:CCC:117:ILE:HG22	1:CCC:119:MET:HG3	2.00	0.44
1:CCC:121:ALA:HB2	1:CCC:126:ILE:CD1	2.48	0.44
1:DDD:176:PHE:CE2	1:DDD:226:LEU:HG	2.53	0.44
1:DDD:218:LEU:HD12	1:DDD:219:GLU:N	2.32	0.44
1:DDD:285:THR:OG1	1:DDD:287:THR:HG22	2.17	0.44
1:AAA:97:GLY:O	1:AAA:101:VAL:HG12	2.18	0.44
1:CCC:149:LEU:HA	1:CCC:266:THR:HG22	2.00	0.44
1:AAA:112:GLU:CD	1:AAA:134:ASN:HA	2.43	0.44
1:CCC:170:SER:HG	1:CCC:266:THR:HG21	1.80	0.44
1:DDD:15:MET:O	1:DDD:287:THR:HG21	2.18	0.44
1:DDD:176:PHE:CE2	1:DDD:259:GLY:CA	3.01	0.44
1:AAA:75:ALA:HA	1:AAA:118:ASN:O	2.18	0.43
1:BBB:241:LYS:NZ	1:BBB:282:GLU:HG2	2.32	0.43
1:CCC:89:ASN:C	1:CCC:89:ASN:ND2	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:255:PRO:HD2	1:AAA:289:PHE:CD2	2.53	0.43
1:BBB:205:ASP:O	1:BBB:208:ASN:N	2.50	0.43
1:CCC:233:PRO:HA	1:CCC:241:LYS:HG3	1.99	0.43
1:CCC:325:PRO:O	1:CCC:330:LYS:NZ	2.52	0.43
1:AAA:50:THR:O	1:AAA:54:HIS:HB2	2.17	0.43
1:CCC:152:GLU:O	1:CCC:153:ASP:C	2.61	0.43
1:BBB:153:ASP:O	1:BBB:154:ALA:HB3	2.18	0.43
1:BBB:298:LYS:HB2	1:BBB:303:ASP:HA	2.01	0.43
1:DDD:75:ALA:HA	1:DDD:118:ASN:HB2	2.00	0.43
1:AAA:73:LYS:O	1:AAA:75:ALA:N	2.49	0.43
1:CCC:93:HIS:CE1	1:CCC:252:ASP:CG	2.96	0.43
1:DDD:167:PHE:O	1:DDD:167:PHE:CG	2.70	0.43
1:CCC:40:TYR:O	1:CCC:44:ASN:HB2	2.17	0.43
1:BBB:15:MET:O	1:BBB:287:THR:HG21	2.19	0.43
1:CCC:281:TYR:O	1:CCC:288:MET:HA	2.19	0.43
1:DDD:21:ILE:HD12	1:DDD:21:ILE:N	2.34	0.43
1:DDD:299:VAL:O	1:DDD:301:GLU:N	2.52	0.43
1:BBB:215:HIS:CD2	1:BBB:218:LEU:HG	2.54	0.43
1:AAA:284:ILE:HD13	1:AAA:284:ILE:O	2.19	0.43
1:CCC:14:THR:HG21	1:CCC:93:HIS:HA	2.00	0.43
1:CCC:48:VAL:O	1:CCC:49:ARG:C	2.61	0.43
1:CCC:260:THR:HG22	1:CCC:281:TYR:CD2	2.54	0.43
1:CCC:279:PHE:O	1:CCC:291:GLY:O	2.36	0.43
1:DDD:167:PHE:HB2	1:DDD:179:ILE:CB	2.49	0.43
1:AAA:156:LEU:CB	1:AAA:165:ILE:O	2.66	0.42
1:CCC:293:VAL:HG23	1:CCC:305:ILE:CG1	2.50	0.42
1:CCC:334:THR:O	1:CCC:335:VAL:HG23	2.19	0.42
1:DDD:43:ASP:O	1:DDD:44:ASN:CG	2.62	0.42
1:DDD:237:GLU:O	1:DDD:238:ALA:HB3	2.18	0.42
1:BBB:81:PHE:CD1	1:BBB:91:CYS:HB3	2.54	0.42
1:BBB:120:GLU:O	1:BBB:121:ALA:HB3	2.20	0.42
1:BBB:192:GLN:O	1:BBB:193:VAL:C	2.61	0.42
1:CCC:142:ILE:HD13	1:CCC:143:THR:N	2.34	0.42
1:DDD:175:PHE:HB2	1:DDD:223:THR:O	2.19	0.42
1:BBB:180:HIS:O	1:BBB:183:GLU:HB3	2.20	0.42
1:CCC:214:GLN:HA	1:CCC:222:LYS:HG3	2.02	0.42
1:DDD:149:LEU:HD13	1:DDD:149:LEU:C	2.44	0.42
1:DDD:258:THR:HA	1:DDD:261:SER:OG	2.20	0.42
1:AAA:242:ASN:OD1	1:AAA:242:ASN:O	2.37	0.42
1:AAA:299:VAL:O	1:AAA:299:VAL:HG13	2.19	0.42
1:CCC:17:GLU:HG2	1:CCC:93:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:29:ILE:HD12	1:CCC:29:ILE:C	2.44	0.42
1:DDD:168:ASP:O	1:DDD:178:ILE:O	2.37	0.42
1:AAA:54:HIS:HB3	1:AAA:333:PHE:O	2.19	0.42
1:AAA:99:ALA:O	1:AAA:100:THR:C	2.62	0.42
1:AAA:238:ALA:HA	1:AAA:280:VAL:HB	2.01	0.42
1:BBB:218:LEU:HD12	1:BBB:219:GLU:N	2.35	0.42
1:DDD:231:ASP:OD1	1:DDD:232:GLU:N	2.51	0.42
1:DDD:293:VAL:HG23	1:DDD:305:ILE:CG1	2.50	0.42
1:BBB:17:GLU:OE1	1:BBB:252:ASP:HA	2.20	0.42
1:BBB:244:VAL:HG21	1:BBB:256:CYS:HB2	2.01	0.42
1:DDD:142:ILE:HD13	1:DDD:143:THR:N	2.35	0.42
1:AAA:190:THR:O	1:AAA:191:SER:C	2.62	0.42
1:BBB:158:VAL:O	1:BBB:159:PRO:C	2.61	0.42
1:BBB:260:THR:HG22	1:BBB:281:TYR:CD2	2.55	0.42
1:CCC:167:PHE:O	1:CCC:167:PHE:CG	2.71	0.42
1:DDD:44:ASN:O	1:DDD:45:LEU:HD13	2.19	0.42
1:AAA:54:HIS:O	1:AAA:55:GLU:O	2.36	0.42
1:AAA:190:THR:HA	1:AAA:193:VAL:HG13	2.02	0.42
1:AAA:192:GLN:O	1:AAA:193:VAL:C	2.63	0.42
1:AAA:217:GLU:O	1:AAA:219:GLU:N	2.43	0.42
1:CCC:274:LYS:O	1:CCC:275:ILE:C	2.63	0.42
1:AAA:179:ILE:HD11	1:AAA:184:LEU:CD2	2.50	0.41
1:BBB:21:ILE:N	1:BBB:21:ILE:HD12	2.34	0.41
1:CCC:93:HIS:CE1	1:CCC:252:ASP:OD1	2.73	0.41
1:AAA:34:MET:HE3	1:AAA:78:GLY:HA3	2.01	0.41
1:AAA:50:THR:HG22	1:AAA:54:HIS:CE1	2.55	0.41
1:BBB:33:THR:CG2	1:BBB:36:ASP:CG	2.89	0.41
1:BBB:112:GLU:O	1:BBB:113:PRO:C	2.63	0.41
1:BBB:149:LEU:HA	1:BBB:266:THR:HG22	2.01	0.41
1:BBB:261:SER:HB3	1:BBB:307:PRO:HG2	2.02	0.41
1:AAA:41:LEU:HB3	1:AAA:87:TYR:CE2	2.55	0.41
1:BBB:29:ILE:HD12	1:BBB:30:ASN:N	2.35	0.41
1:BBB:96:ILE:O	1:BBB:100:THR:OG1	2.36	0.41
1:BBB:295:GLU:O	1:BBB:305:ILE:HG12	2.19	0.41
1:CCC:187:LYS:O	1:CCC:189:GLU:N	2.53	0.41
1:CCC:265:ALA:HA	1:CCC:305:ILE:HG21	2.00	0.41
1:AAA:59:HIS:CE1	1:AAA:62:MET:HB2	2.55	0.41
1:AAA:213:VAL:CG1	1:AAA:224:VAL:HG22	2.49	0.41
1:CCC:115:THR:HB	1:CCC:130:VAL:CG1	2.50	0.41
1:CCC:255:PRO:HD2	1:CCC:289:PHE:CD2	2.56	0.41
1:DDD:29:ILE:HD12	1:DDD:30:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:45:LEU:O	1:AAA:46:ASP:C	2.63	0.41
1:AAA:181:ALA:HB3	1:AAA:231:ASP:HB2	2.03	0.41
1:AAA:258:THR:HA	1:AAA:261:SER:OG	2.21	0.41
1:CCC:207:ILE:O	1:CCC:211:ILE:CG2	2.69	0.41
1:DDD:1:MET:HB3	1:DDD:3:PHE:HE2	1.83	0.41
1:DDD:298:LYS:HA	1:DDD:303:ASP:HA	2.01	0.41
1:AAA:179:ILE:HD11	1:AAA:184:LEU:HD23	2.02	0.41
1:BBB:156:LEU:HD12	1:BBB:157:GLU:N	2.35	0.41
1:AAA:203:ILE:O	1:AAA:207:ILE:HB	2.21	0.41
1:CCC:17:GLU:HA	1:CCC:18:PRO:HD3	1.86	0.41
1:CCC:20:ARG:CZ	1:CCC:62:MET:HE2	2.50	0.41
1:DDD:25:GLY:O	1:DDD:26:ILE:HD13	2.20	0.41
1:AAA:17:GLU:HG2	1:AAA:252:ASP:OD1	2.20	0.41
1:BBB:75:ALA:HA	1:BBB:118:ASN:HB2	2.02	0.41
1:BBB:217:GLU:C	1:BBB:219:GLU:H	2.25	0.41
1:BBB:234:SER:OG	1:BBB:241:LYS:HE2	2.21	0.41
1:CCC:82:MET:O	1:CCC:82:MET:HG2	2.21	0.41
1:CCC:155:LYS:HE2	1:CCC:164:THR:O	2.21	0.41
1:CCC:237:GLU:O	1:CCC:238:ALA:HB3	2.21	0.41
1:DDD:8:HIS:CE1	1:DDD:320:HIS:CD2	3.09	0.41
1:DDD:156:LEU:HD13	1:DDD:158:VAL:HG23	2.03	0.41
1:DDD:221:ILE:HD12	1:DDD:222:LYS:H	1.86	0.41
1:AAA:135:GLU:H	1:AAA:135:GLU:CD	2.29	0.41
1:DDD:162:ASN:HD21	1:DDD:164:THR:CG2	2.33	0.41
1:DDD:274:LYS:O	1:DDD:275:ILE:C	2.64	0.41
1:AAA:102:ALA:HA	1:AAA:107:MET:HE3	2.02	0.40
1:AAA:170:SER:OG	1:AAA:178:ILE:HD13	2.21	0.40
1:AAA:275:ILE:HG22	1:AAA:276:ASP:OD1	2.21	0.40
1:BBB:201:ILE:HG21	1:BBB:249:GLY:CA	2.51	0.40
1:BBB:210:LYS:HB3	1:CCC:274:LYS:HD2	2.03	0.40
1:DDD:76:ASP:O	1:DDD:77:PHE:O	2.39	0.40
1:DDD:117:ILE:HG22	1:DDD:119:MET:HG3	2.01	0.40
1:AAA:55:GLU:HB3	1:AAA:56:PRO:HA	2.02	0.40
1:CCC:133:GLU:HG3	1:CCC:138:LYS:HB2	2.03	0.40
1:CCC:148:PHE:HB3	1:CCC:304:ALA:CB	2.50	0.40
1:CCC:255:PRO:HD2	1:CCC:289:PHE:CE2	2.56	0.40
1:DDD:112:GLU:OE1	1:DDD:134:ASN:HA	2.21	0.40
1:BBB:267:LEU:HD13	1:BBB:267:LEU:N	2.37	0.40
1:CCC:95:SER:O	1:CCC:119:MET:HE1	2.21	0.40
1:CCC:96:ILE:O	1:CCC:97:GLY:C	2.64	0.40
1:CCC:217:GLU:C	1:CCC:219:GLU:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:136:LYS:HG3	1:AAA:137:VAL:O	2.22	0.40
1:DDD:156:LEU:HD12	1:DDD:157:GLU:N	2.35	0.40
1:AAA:184:LEU:HD13	1:AAA:186:VAL:CG2	2.50	0.40
1:BBB:217:GLU:O	1:BBB:219:GLU:N	2.39	0.40
1:CCC:40:TYR:CD1	1:CCC:40:TYR:C	2.99	0.40
1:DDD:260:THR:HG22	1:DDD:281:TYR:CD2	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:39:LYS:HZ2	1:BBB:153:ASP:OD2[2_555]	1.59	0.01
1:CCC:319:ASN:OD1	1:DDD:319:ASN:OD1[2_454]	2.19	0.01

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	AAA	333/343 (97%)	247 (74%)	57 (17%)	29 (9%)	0	7
1	BBB	333/343 (97%)	252 (76%)	54 (16%)	27 (8%)	1	8
1	CCC	333/343 (97%)	251 (75%)	53 (16%)	29 (9%)	0	7
1	DDD	333/343 (97%)	247 (74%)	57 (17%)	29 (9%)	0	7
All	All	1332/1372 (97%)	997 (75%)	221 (17%)	114 (9%)	0	7

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	32	GLU
1	AAA	134	ASN
1	AAA	153	ASP

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Mol	Chain	Res	Type
1	AAA	163	LYS
1	AAA	218	LEU
1	AAA	270	LYS
1	AAA	285	THR
1	AAA	300	GLY
1	BBB	32	GLU
1	BBB	62	MET
1	BBB	134	ASN
1	BBB	151	MET
1	BBB	153	ASP
1	BBB	162	ASN
1	BBB	163	LYS
1	BBB	218	LEU
1	BBB	221	ILE
1	BBB	268	TYR
1	BBB	270	LYS
1	BBB	300	GLY
1	CCC	32	GLU
1	CCC	77	PHE
1	CCC	134	ASN
1	CCC	151	MET
1	CCC	153	ASP
1	CCC	162	ASN
1	CCC	163	LYS
1	CCC	218	LEU
1	CCC	256	CYS
1	CCC	270	LYS
1	CCC	300	GLY
1	DDD	32	GLU
1	DDD	77	PHE
1	DDD	134	ASN
1	DDD	151	MET
1	DDD	153	ASP
1	DDD	163	LYS
1	DDD	188	VAL
1	DDD	218	LEU
1	DDD	270	LYS
1	DDD	300	GLY
1	AAA	31	GLY
1	AAA	77	PHE
1	AAA	152	GLU
1	AAA	157	GLU

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Mol	Chain	Res	Type
1	AAA	162	ASN
1	AAA	165	ILE
1	AAA	188	VAL
1	AAA	247	GLY
1	AAA	268	TYR
1	BBB	31	GLY
1	BBB	77	PHE
1	BBB	120	GLU
1	BBB	157	GLU
1	BBB	188	VAL
1	BBB	193	VAL
1	BBB	247	GLY
1	BBB	285	THR
1	CCC	31	GLY
1	CCC	120	GLU
1	CCC	188	VAL
1	CCC	247	GLY
1	DDD	31	GLY
1	DDD	247	GLY
1	DDD	256	CYS
1	DDD	268	TYR
1	AAA	4	SER
1	AAA	62	MET
1	AAA	74	GLU
1	AAA	193	VAL
1	AAA	221	ILE
1	BBB	165	ILE
1	CCC	29	ILE
1	CCC	62	MET
1	CCC	157	GLU
1	CCC	268	TYR
1	CCC	277	GLU
1	DDD	2	LYS
1	DDD	4	SER
1	DDD	74	GLU
1	DDD	157	GLU
1	DDD	167	PHE
1	DDD	269	LYS
1	DDD	277	GLU
1	AAA	61	ASP
1	BBB	61	ASP
1	BBB	121	ALA

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Mol	Chain	Res	Type
1	BBB	164	THR
1	BBB	283	SER
1	CCC	2	LYS
1	CCC	167	PHE
1	CCC	222	LYS
1	CCC	262	ALA
1	DDD	44	ASN
1	DDD	62	MET
1	DDD	120	GLU
1	DDD	162	ASN
1	DDD	190	THR
1	AAA	72	ASN
1	AAA	238	ALA
1	AAA	277	GLU
1	BBB	197	LYS
1	CCC	146	PRO
1	DDD	165	ILE
1	AAA	120	GLU
1	AAA	164	THR
1	BBB	267	LEU
1	CCC	74	GLU
1	CCC	154	ALA
1	CCC	165	ILE
1	CCC	257	GLY
1	DDD	29	ILE
1	DDD	145	VAL
1	AAA	55	GLU

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	AAA	285/293 (97%)	227 (80%)	58 (20%)	1	8
1	BBB	285/293 (97%)	233 (82%)	52 (18%)	2	11
1	CCC	285/293 (97%)	225 (79%)	60 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DDD	285/293 (97%)	228 (80%)	57 (20%)	1	8
All	All	1140/1172 (97%)	913 (80%)	227 (20%)	1	8

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	2	LYS
1	AAA	12	SER
1	AAA	13	HIS
1	AAA	19	THR
1	AAA	29	ILE
1	AAA	33	THR
1	AAA	41	LEU
1	AAA	45	LEU
1	AAA	65	SER
1	AAA	68	THR
1	AAA	73	LYS
1	AAA	76	ASP
1	AAA	82	MET
1	AAA	88	LEU
1	AAA	91	CYS
1	AAA	126	ILE
1	AAA	133	GLU
1	AAA	151	MET
1	AAA	153	ASP
1	AAA	156	LEU
1	AAA	161	LEU
1	AAA	162	ASN
1	AAA	165	ILE
1	AAA	168	ASP
1	AAA	169	ILE
1	AAA	170	SER
1	AAA	179	ILE
1	AAA	184	LEU
1	AAA	195	VAL
1	AAA	196	LEU
1	AAA	199	LEU
1	AAA	202	GLU
1	AAA	204	ARG
1	AAA	206	LEU
1	AAA	211	ILE
1	AAA	212	LYS

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Mol	Chain	Res	Type
1	AAA	213	VAL
1	AAA	214	GLN
1	AAA	222	LYS
1	AAA	224	VAL
1	AAA	232	GLU
1	AAA	234	SER
1	AAA	239	THR
1	AAA	242	ASN
1	AAA	243	VAL
1	AAA	269	LYS
1	AAA	273	LEU
1	AAA	280	VAL
1	AAA	281	TYR
1	AAA	282	GLU
1	AAA	284	ILE
1	AAA	293	VAL
1	AAA	298	LYS
1	AAA	305	ILE
1	AAA	306	ILE
1	AAA	310	THR
1	AAA	330	LYS
1	AAA	334	THR
1	BBB	2	LYS
1	BBB	13	HIS
1	BBB	19	THR
1	BBB	26	ILE
1	BBB	29	ILE
1	BBB	33	THR
1	BBB	45	LEU
1	BBB	65	SER
1	BBB	68	THR
1	BBB	73	LYS
1	BBB	76	ASP
1	BBB	88	LEU
1	BBB	131	MET
1	BBB	133	GLU
1	BBB	151	MET
1	BBB	153	ASP
1	BBB	161	LEU
1	BBB	162	ASN
1	BBB	169	ILE
1	BBB	170	SER

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Mol	Chain	Res	Type
1	BBB	174	SER
1	BBB	179	ILE
1	BBB	184	LEU
1	BBB	195	VAL
1	BBB	196	LEU
1	BBB	199	LEU
1	BBB	202	GLU
1	BBB	206	LEU
1	BBB	210	LYS
1	BBB	211	ILE
1	BBB	212	LYS
1	BBB	213	VAL
1	BBB	224	VAL
1	BBB	226	LEU
1	BBB	229	ILE
1	BBB	234	SER
1	BBB	239	THR
1	BBB	243	VAL
1	BBB	258	THR
1	BBB	261	SER
1	BBB	267	LEU
1	BBB	269	LYS
1	BBB	273	LEU
1	BBB	280	VAL
1	BBB	281	TYR
1	BBB	284	ILE
1	BBB	293	VAL
1	BBB	298	LYS
1	BBB	305	ILE
1	BBB	306	ILE
1	BBB	330	LYS
1	BBB	334	THR
1	CCC	4	SER
1	CCC	13	HIS
1	CCC	17	GLU
1	CCC	26	ILE
1	CCC	29	ILE
1	CCC	33	THR
1	CCC	43	ASP
1	CCC	45	LEU
1	CCC	65	SER
1	CCC	68	THR

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Mol	Chain	Res	Type
1	CCC	73	LYS
1	CCC	76	ASP
1	CCC	88	LEU
1	CCC	89	ASN
1	CCC	93	HIS
1	CCC	126	ILE
1	CCC	127	LYS
1	CCC	130	VAL
1	CCC	135	GLU
1	CCC	142	ILE
1	CCC	151	MET
1	CCC	153	ASP
1	CCC	161	LEU
1	CCC	162	ASN
1	CCC	168	ASP
1	CCC	169	ILE
1	CCC	170	SER
1	CCC	174	SER
1	CCC	179	ILE
1	CCC	184	LEU
1	CCC	195	VAL
1	CCC	196	LEU
1	CCC	199	LEU
1	CCC	202	GLU
1	CCC	206	LEU
1	CCC	210	LYS
1	CCC	211	ILE
1	CCC	212	LYS
1	CCC	213	VAL
1	CCC	214	GLN
1	CCC	224	VAL
1	CCC	225	ASP
1	CCC	226	LEU
1	CCC	229	ILE
1	CCC	234	SER
1	CCC	239	THR
1	CCC	243	VAL
1	CCC	258	THR
1	CCC	261	SER
1	CCC	269	LYS
1	CCC	273	LEU
1	CCC	276	ASP

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Mol	Chain	Res	Type
1	CCC	280	VAL
1	CCC	281	TYR
1	CCC	284	ILE
1	CCC	293	VAL
1	CCC	305	ILE
1	CCC	306	ILE
1	CCC	310	THR
1	CCC	330	LYS
1	DDD	2	LYS
1	DDD	4	SER
1	DDD	13	HIS
1	DDD	26	ILE
1	DDD	29	ILE
1	DDD	33	THR
1	DDD	45	LEU
1	DDD	65	SER
1	DDD	68	THR
1	DDD	73	LYS
1	DDD	76	ASP
1	DDD	88	LEU
1	DDD	126	ILE
1	DDD	131	MET
1	DDD	134	ASN
1	DDD	135	GLU
1	DDD	142	ILE
1	DDD	151	MET
1	DDD	153	ASP
1	DDD	161	LEU
1	DDD	162	ASN
1	DDD	168	ASP
1	DDD	169	ILE
1	DDD	170	SER
1	DDD	179	ILE
1	DDD	184	LEU
1	DDD	195	VAL
1	DDD	196	LEU
1	DDD	199	LEU
1	DDD	202	GLU
1	DDD	206	LEU
1	DDD	210	LYS
1	DDD	211	ILE
1	DDD	213	VAL

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Mol	Chain	Res	Type
1	DDD	214	GLN
1	DDD	224	VAL
1	DDD	226	LEU
1	DDD	229	ILE
1	DDD	234	SER
1	DDD	239	THR
1	DDD	243	VAL
1	DDD	258	THR
1	DDD	261	SER
1	DDD	269	LYS
1	DDD	273	LEU
1	DDD	276	ASP
1	DDD	280	VAL
1	DDD	281	TYR
1	DDD	284	ILE
1	DDD	290	LYS
1	DDD	293	VAL
1	DDD	298	LYS
1	DDD	305	ILE
1	DDD	306	ILE
1	DDD	310	THR
1	DDD	330	LYS
1	DDD	334	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PYC	AAA	401	-	8,8,8	1.26	1 (12%)	10,10,10	1.45	1 (10%)
2	PYC	BBB	401	-	8,8,8	1.31	2 (25%)	10,10,10	1.20	1 (10%)

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	PYC	AAA	401	-	-	0/4/4/4	0/1/1/1
2	PYC	BBB	401	-	-	4/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	401	PYC	C2-N6	-2.52	1.34	1.37
2	AAA	401	PYC	O8-C1	-2.26	1.24	1.30
2	BBB	401	PYC	O8-C1	-2.05	1.25	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	401	PYC	O8-C1-C2	2.54	119.74	114.27
2	AAA	401	PYC	C3-C2-N6	2.45	109.34	106.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	401	PYC	O7-C1-C2-C3
2	BBB	401	PYC	O7-C1-C2-N6
2	BBB	401	PYC	O8-C1-C2-C3
2	BBB	401	PYC	O8-C1-C2-N6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	PYC	4	0
2	BBB	401	PYC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	335/343 (97%)	-0.77	0 100 100	72, 116, 166, 187	0
1	BBB	335/343 (97%)	-0.75	0 100 100	78, 127, 184, 218	0
1	CCC	335/343 (97%)	-0.60	0 100 100	92, 170, 243, 273	0
1	DDD	335/343 (97%)	-0.66	0 100 100	97, 176, 240, 266	0
All	All	1340/1372 (97%)	-0.69	0 100 100	72, 141, 226, 273	0

There are no RSRZ outliers to report.

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	PYC	BBB	401	8/8	0.97	0.06	116,155,163,163	0
2	PYC	AAA	401	8/8	0.98	0.06	95,120,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.