



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 10:34 PM BST

PDB ID : 6SLH
Title : Conformational flexibility within the small domain of human serine racemase.
Authors : Koulouris, C.R.; Bax, B.; Atack, J.; Roe, S.M.
Deposited on : 2019-08-19
Resolution : 1.89 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

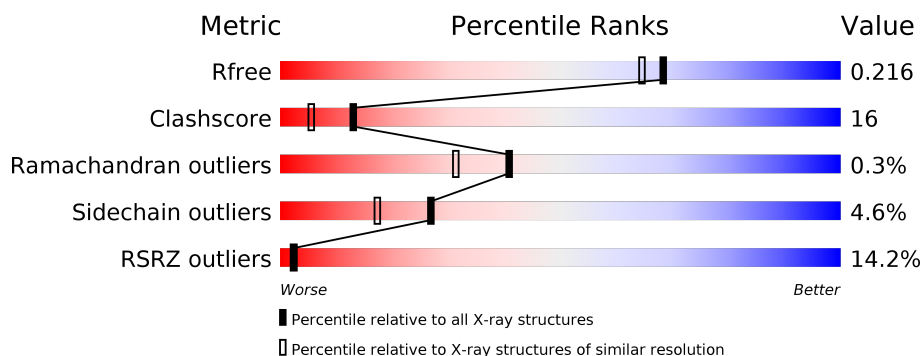
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	346	<div> <div>12%</div> <div>79%</div> <div>12%</div> <div>7%</div> </div>
1	BBB	346	<div> <div>15%</div> <div>73%</div> <div>16%</div> <div>9%</div> </div>
1	CCC	346	<div> <div>18%</div> <div>60%</div> <div>27%</div> <div>5%</div> <div>9%</div> </div>
1	DDD	346	<div> <div>7%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10765 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 Serine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	322	Total	C	N	O	P	S	0	18	0
			2539	1612	428	487	1	11			
1	BBB	314	Total	C	N	O	P	S	0	9	0
			2330	1486	390	443	1	10			
1	CCC	316	Total	C	N	O	P	S	0	85	1
			2842	1801	482	546	1	12			
1	DDD	317	Total	C	N	O	P	S	0	15	0
			2493	1585	418	476	1	13			

There are 32 discrepancies between the modelled and reference sequences:

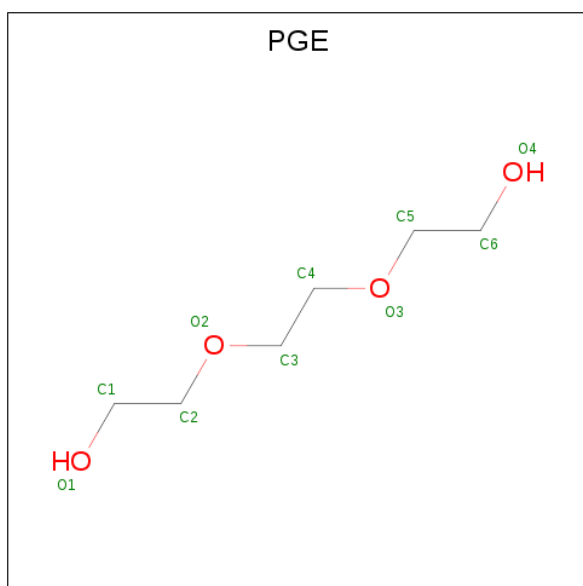
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
CCC	2	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	6	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	341	HIS	-	expression tag	UNP Q9GZT4
CCC	342	HIS	-	expression tag	UNP Q9GZT4
CCC	343	HIS	-	expression tag	UNP Q9GZT4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	344	HIS	-	expression tag	UNP Q9GZT4
CCC	345	HIS	-	expression tag	UNP Q9GZT4
CCC	346	HIS	-	expression tag	UNP Q9GZT4
DDD	2	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	6	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	341	HIS	-	expression tag	UNP Q9GZT4
DDD	342	HIS	-	expression tag	UNP Q9GZT4
DDD	343	HIS	-	expression tag	UNP Q9GZT4
DDD	344	HIS	-	expression tag	UNP Q9GZT4
DDD	345	HIS	-	expression tag	UNP Q9GZT4
DDD	346	HIS	-	expression tag	UNP Q9GZT4

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	AAA	1	Total	C	O	0	0
			3	2	1		
2	BBB	1	Total	C	O	0	0
			4	2	2		
2	CCC	1	Total	C	O	0	0
			5	3	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total Mg 1 1	0	0
3	BBB	1	Total Mg 1 1	0	0
3	DDD	2	Total Mg 2 2	0	0
3	AAA	2	Total Mg 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	2	Total Na 2 2	0	0
4	AAA	4	Total Na 4 4	0	0

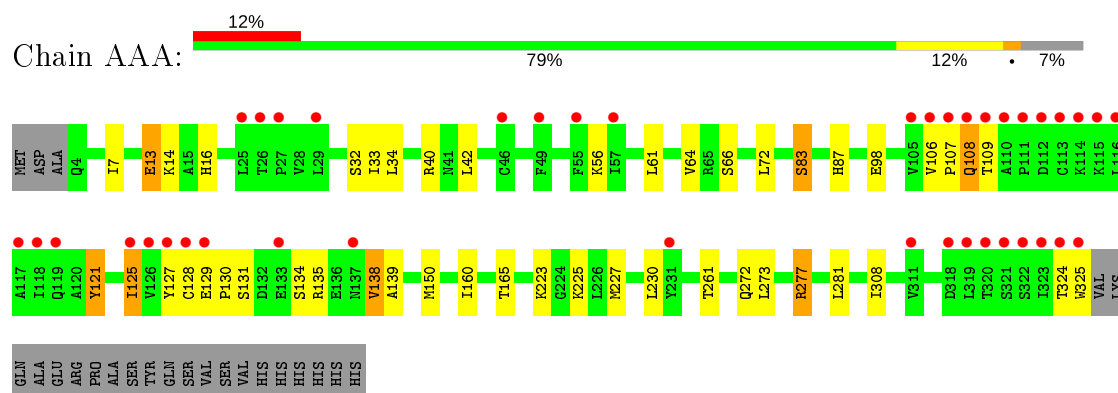
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	222	Total O 223 223	0	1
5	BBB	42	Total O 42 42	0	0
5	CCC	81	Total O 81 81	0	0
5	DDD	187	Total O 187 187	0	0

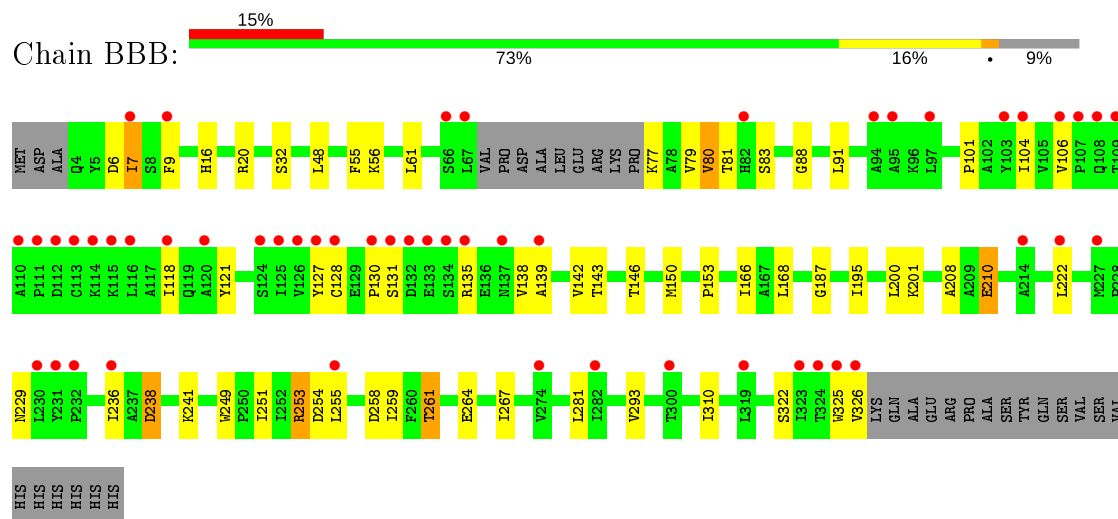
3 Residue-property plots

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.

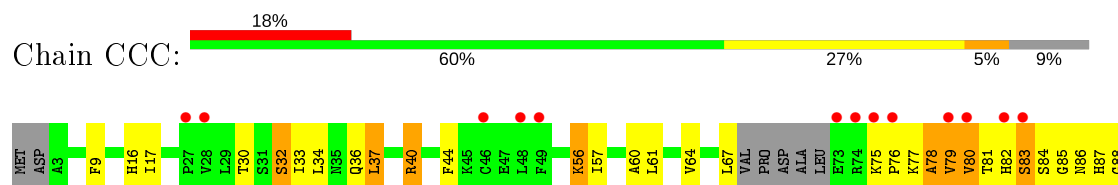
• Molecule 1: Serine racemase

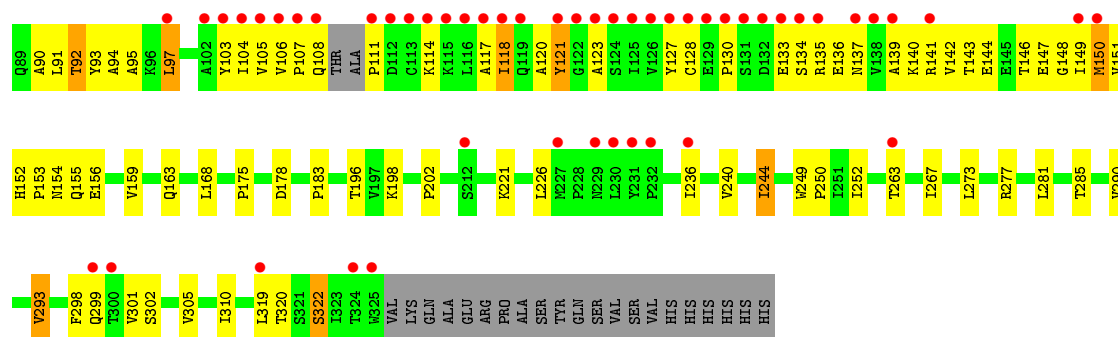


• Molecule 1: Serine racemase

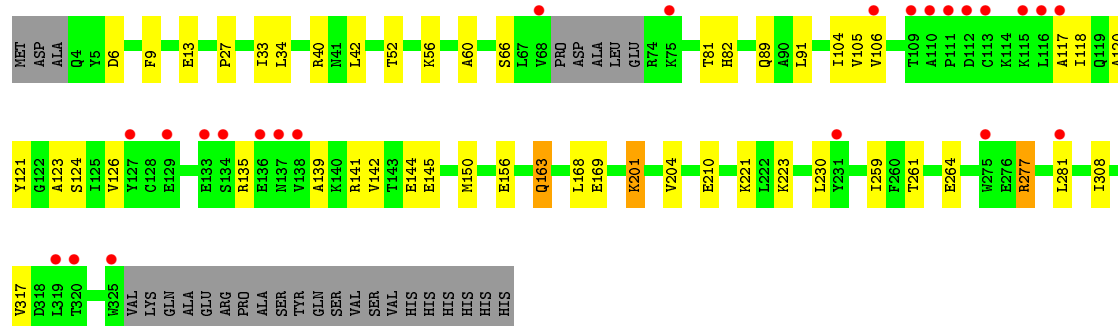
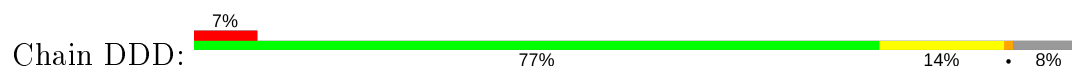


• Molecule 1: Serine racemase





• Molecule 1: Serine racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.20 Å 155.74 Å 85.58 Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	40.87 – 1.89 40.84 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.87-1.89) 99.2 (40.84-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.172 , 0.216 0.172 , 0.216	Depositor DCC
R_{free} test set	4925 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10765	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, PGE, LLP

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	0.70	1/2561 (0.0%)	0.98	2/3495 (0.1%)
1	BBB	0.44	1/2346 (0.0%)	0.84	0/3213
1	CCC	0.49	0/2864	0.90	5/3910 (0.1%)
1	DDD	0.62	2/2512 (0.1%)	0.95	3/3426 (0.1%)
All	All	0.57	4/10283 (0.0%)	0.92	10/14044 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	169	GLU	CD-OE1	6.07	1.32	1.25
1	BBB	210	GLU	CD-OE2	5.66	1.31	1.25
1	DDD	264	GLU	CD-OE2	5.03	1.31	1.25
1	AAA	13	GLU	CD-OE2	-5.00	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	40	ARG	CG-CD-NE	6.96	126.42	111.80
1	DDD	121	TYR	CB-CA-C	6.42	123.23	110.40
1	DDD	163	GLN	CB-CG-CD	6.09	127.42	111.60
1	CCC	40	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	CCC	121[A]	TYR	CB-CA-C	5.45	121.31	110.40
1	CCC	121[B]	TYR	CB-CA-C	5.45	121.31	110.40
1	AAA	277	ARG	CG-CD-NE	-5.42	100.42	111.80
1	DDD	277	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	CCC	40	ARG	CD-NE-CZ	5.22	130.91	123.60
1	AAA	121	TYR	CB-CA-C	5.06	120.52	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2539	0	2518	63	0
1	BBB	2330	0	2247	54	0
1	CCC	2842	0	2673	194	0
1	DDD	2493	0	2475	28	0
2	AAA	7	0	7	1	0
2	BBB	4	0	5	2	0
2	CCC	5	0	4	2	0
3	AAA	2	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	2	0	0	0	0
4	AAA	4	0	0	1	0
4	DDD	2	0	0	0	0
5	AAA	223	0	0	10	0
5	BBB	42	0	0	3	0
5	CCC	81	0	0	9	0
5	DDD	187	0	0	2	0
All	All	10765	0	9929	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (333) 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:139[B]:ALA:HB1	1:CCC:150[B]:MET:CE	1.27	1.57
1:AAA:107[A]:PRO:CG	1:AAA:135[A]:ARG:NH2	1.80	1.42
1:CCC:141[B]:ARG:C	1:CCC:142[B]:VAL:N	1.71	1.42
1:AAA:107[A]:PRO:HG2	1:AAA:135[A]:ARG:NH2	1.13	1.41
1:CCC:80[B]:VAL:O	1:CCC:150[B]:MET:HA	1.31	1.27
1:CCC:140[A]:LYS:C	1:CCC:141[A]:ARG:C	2.00	1.20
1:AAA:108[B]:GLN:O	1:AAA:108[B]:GLN:NE2	1.77	1.16
1:CCC:139[B]:ALA:CB	1:CCC:150[B]:MET:CE	2.24	1.14
1:CCC:79[B]:VAL:CG1	1:CCC:91[B]:LEU:HD21	1.80	1.11
1:AAA:128:CYS:HB3	1:AAA:138:VAL:HG11	1.18	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:108[B]:GLN:C	1:AAA:108[B]:GLN:HE21	1.54	1.10
1:CCC:140[A]:LYS:O	1:CCC:141[A]:ARG:C	1.90	1.10
1:CCC:111[B]:PRO:HD2	1:CCC:114[B]:LYS:CB	1.82	1.09
1:BBB:80:VAL:CG1	1:BBB:143:THR:HG22	1.82	1.09
1:CCC:83[B]:SER:OG	1:CCC:153:PRO:HB3	1.51	1.08
1:DDD:156:GLU:OE2	5:DDD:501:HOH:O	1.72	1.07
1:CCC:139[B]:ALA:HB1	1:CCC:150[B]:MET:HE2	1.12	1.06
1:CCC:80[B]:VAL:O	1:CCC:150[B]:MET:CA	2.04	1.06
1:CCC:133[B]:GLU:O	1:CCC:137[B]:ASN:ND2	1.89	1.05
1:CCC:107[B]:PRO:HA	1:CCC:128[B]:CYS:SG	1.98	1.03
1:CCC:139[B]:ALA:CB	1:CCC:150[B]:MET:HE1	1.87	1.02
1:AAA:107[A]:PRO:CG	1:AAA:135[A]:ARG:CZ	2.39	1.00
1:AAA:107[A]:PRO:HG3	1:AAA:135[A]:ARG:CZ	1.91	1.00
1:CCC:139[B]:ALA:HB1	1:CCC:150[B]:MET:HE1	1.04	1.00
1:BBB:80:VAL:HG13	1:BBB:143:THR:HG22	1.41	0.99
1:AAA:107[A]:PRO:HG2	1:AAA:135[A]:ARG:HH22	1.23	0.99
1:BBB:7:ILE:HD13	1:BBB:195:ILE:HD13	1.43	0.98
1:CCC:139[B]:ALA:CB	1:CCC:150[B]:MET:HE2	1.88	0.97
1:CCC:80[B]:VAL:HB	1:CCC:150[B]:MET:SD	2.06	0.95
1:CCC:83[B]:SER:OG	1:CCC:153:PRO:CB	2.15	0.95
1:CCC:60:ALA:HB1	1:CCC:91[B]:LEU:HA	1.46	0.94
1:CCC:152[B]:HIS:HD2	1:CCC:155:GLN:H	0.97	0.92
1:AAA:107[A]:PRO:CG	1:AAA:135[A]:ARG:HH21	1.72	0.91
1:AAA:107[A]:PRO:HG3	1:AAA:135[A]:ARG:NH2	1.78	0.90
1:CCC:106[B]:VAL:O	1:CCC:128[B]:CYS:SG	2.29	0.90
1:CCC:107[B]:PRO:CA	1:CCC:128[B]:CYS:SG	2.62	0.88
1:CCC:152[B]:HIS:CD2	1:CCC:155:GLN:H	1.90	0.87
1:CCC:141[B]:ARG:HA	1:CCC:144[B]:GLU:OE1	1.75	0.86
1:CCC:80[B]:VAL:C	1:CCC:150[B]:MET:HA	1.94	0.86
1:CCC:151[B]:VAL:HG12	1:CCC:151[B]:VAL:O	1.74	0.86
1:CCC:83[B]:SER:CB	1:CCC:153:PRO:HB3	2.05	0.86
1:CCC:80[B]:VAL:O	1:CCC:151[B]:VAL:N	2.09	0.85
1:CCC:141[B]:ARG:CA	1:CCC:142[B]:VAL:N	2.39	0.85
1:AAA:108[B]:GLN:CA	1:AAA:108[B]:GLN:HE21	1.87	0.85
1:AAA:107[A]:PRO:HG2	1:AAA:135[A]:ARG:HH21	1.21	0.85
1:BBB:80:VAL:HG11	1:BBB:143:THR:HG22	1.56	0.84
1:AAA:223[B]:LYS:HG2	1:AAA:225:LYS:HG2	1.58	0.84
1:AAA:33:ILE:HD12	1:AAA:33:ILE:H	1.41	0.84
1:CCC:79[B]:VAL:HG11	1:CCC:91[B]:LEU:HD21	1.59	0.83
1:BBB:7:ILE:HD13	1:BBB:195:ILE:CD1	2.08	0.83
1:CCC:301:VAL:CG1	1:CCC:305:VAL:HG11	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:106[B]:VAL:C	1:CCC:128[B]:CYS:SG	2.57	0.82
1:AAA:134:SER:O	1:AAA:138:VAL:HG12	1.79	0.82
1:CCC:143[B]:THR:OG1	1:CCC:149[B]:ILE:HA	1.79	0.81
1:AAA:16[B]:HIS:ND1	5:AAA:501:HOH:O	2.12	0.81
1:BBB:251:ILE:HG23	1:BBB:255:LEU:HD12	1.63	0.81
1:CCC:81[B]:THR:HG22	1:CCC:104[B]:ILE:CD1	2.10	0.81
1:AAA:98:GLU:HG2	5:AAA:567:HOH:O	1.80	0.81
1:AAA:223[B]:LYS:HE2	1:AAA:225:LYS:CD	2.11	0.80
1:AAA:108[B]:GLN:CA	1:AAA:108[B]:GLN:NE2	2.43	0.80
2:BBB:402:PGE:H62	1:DDD:27:PRO:HB3	1.64	0.79
1:CCC:302:SER:O	1:CCC:305:VAL:HG12	1.82	0.79
1:CCC:118[B]:ILE:HG13	5:CCC:506:HOH:O	1.83	0.78
1:CCC:137[B]:ASN:O	1:CCC:141[B]:ARG:HG3	1.84	0.78
1:AAA:128:CYS:HB3	1:AAA:138:VAL:CG1	2.07	0.78
1:CCC:143[B]:THR:OG1	1:CCC:148[B]:GLY:O	2.02	0.78
1:CCC:79[B]:VAL:HG12	1:CCC:91[B]:LEU:HD21	1.65	0.77
1:CCC:152[B]:HIS:HD2	1:CCC:155:GLN:N	1.79	0.77
1:CCC:61:LEU:HA	1:CCC:94[B]:ALA:HB1	1.66	0.77
1:AAA:128:CYS:CB	1:AAA:138:VAL:HG11	2.09	0.77
1:CCC:301:VAL:HG12	1:CCC:305:VAL:HG11	1.67	0.76
1:CCC:79[B]:VAL:HG11	1:CCC:91[B]:LEU:HD11	1.67	0.75
1:CCC:87[B]:HIS:CD2	1:CCC:153:PRO:HA	2.21	0.75
1:CCC:141[B]:ARG:N	1:CCC:142[B]:VAL:N	2.34	0.75
1:CCC:118[B]:ILE:HG12	1:CCC:121[B]:TYR:OH	1.87	0.74
1:CCC:141[B]:ARG:C	1:CCC:142[B]:VAL:CA	2.56	0.73
1:CCC:301:VAL:HG12	1:CCC:305:VAL:CG1	2.18	0.73
1:CCC:107[B]:PRO:HB3	1:CCC:130[B]:PRO:HA	1.71	0.72
1:CCC:141[B]:ARG:O	1:CCC:144[B]:GLU:HB2	1.89	0.72
1:CCC:93[B]:TYR:O	1:CCC:97[B]:LEU:HD23	1.88	0.72
1:CCC:226:LEU:HD13	1:CCC:244:ILE:HG22	1.72	0.71
1:CCC:80[B]:VAL:HG13	1:CCC:103[B]:TYR:HB2	1.72	0.71
1:AAA:107[A]:PRO:HG3	1:AAA:135[A]:ARG:NE	2.04	0.71
1:AAA:125:ILE:H	1:AAA:125:ILE:HD12	1.55	0.71
1:AAA:135[A]:ARG:HD3	5:AAA:579:HOH:O	1.90	0.71
1:DDD:9:PHE:HE1	1:DDD:168[B]:LEU:HD21	1.56	0.70
1:CCC:140[A]:LYS:O	1:CCC:143[A]:THR:HG22	1.92	0.69
1:CCC:107[B]:PRO:N	1:CCC:128[B]:CYS:SG	2.65	0.69
1:CCC:92[B]:THR:O	1:CCC:95[B]:ALA:HB3	1.92	0.69
1:CCC:80[B]:VAL:HG23	1:CCC:150[B]:MET:H	1.55	0.69
1:CCC:84[A]:SER:HB2	5:CCC:506:HOH:O	1.92	0.68
1:CCC:107[B]:PRO:HA	1:CCC:128[B]:CYS:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:175:PRO:HD2	5:CCC:543:HOH:O	1.94	0.68
1:CCC:82[B]:HIS:HB3	1:CCC:153:PRO:HD2	1.74	0.68
1:AAA:16[A]:HIS:HD2	1:AAA:165:THR:HB	1.60	0.67
1:AAA:108[B]:GLN:HA	1:AAA:108[B]:GLN:NE2	2.10	0.67
1:BBB:200:LEU:HD13	1:CCC:17:ILE:CD1	2.26	0.67
1:CCC:140[B]:LYS:O	1:CCC:144[B]:GLU:HG3	1.95	0.67
1:BBB:200:LEU:HD22	1:CCC:17:ILE:HD12	1.76	0.66
1:DDD:81:THR:CG2	1:DDD:104:ILE:HD13	2.26	0.66
1:BBB:80:VAL:HG21	1:BBB:142:VAL:HG23	1.77	0.66
1:BBB:200:LEU:HD13	1:CCC:17:ILE:HD11	1.78	0.66
1:AAA:16[B]:HIS:CG	5:AAA:501:HOH:O	2.48	0.65
1:CCC:80[B]:VAL:CB	1:CCC:150[B]:MET:SD	2.83	0.65
1:CCC:151[B]:VAL:CG1	1:CCC:151[B]:VAL:O	2.45	0.65
1:CCC:80[B]:VAL:HG23	1:CCC:150[B]:MET:N	2.11	0.65
1:CCC:79[B]:VAL:CB	1:CCC:91[B]:LEU:HD21	2.28	0.64
1:CCC:156:GLU:OE2	5:CCC:501:HOH:O	2.14	0.64
1:CCC:32:SER:O	1:CCC:36:GLN:HG2	1.98	0.64
1:CCC:93[B]:TYR:CD1	1:CCC:93[B]:TYR:O	2.51	0.63
1:BBB:79:VAL:CG1	1:BBB:91[B]:LEU:HD13	2.29	0.63
1:AAA:108[A]:GLN:OE1	1:AAA:127:TYR:HB3	1.98	0.63
1:CCC:141[B]:ARG:CZ	1:CCC:141[B]:ARG:HB3	2.28	0.62
1:CCC:141[A]:ARG:C	1:CCC:144[A]:GLU:HB2	2.20	0.62
1:CCC:60:ALA:HB1	1:CCC:91[B]:LEU:CA	2.24	0.62
1:AAA:128:CYS:SG	1:AAA:135[A]:ARG:HG2	2.40	0.62
1:CCC:83[B]:SER:H	1:CCC:153:PRO:HD3	1.64	0.62
1:CCC:77[B]:LYS:O	1:CCC:78[B]:ALA:HB2	1.98	0.61
2:BBB:402:PGE:H62	1:DDD:27:PRO:CB	2.30	0.61
1:AAA:16[B]:HIS:CE1	5:AAA:501:HOH:O	2.51	0.61
1:BBB:200:LEU:HB3	1:CCC:17:ILE:HD13	1.82	0.61
1:BBB:208:ALA:HB3	1:BBB:259:ILE:HG13	1.83	0.61
1:CCC:80[B]:VAL:CG2	1:CCC:150[B]:MET:SD	2.89	0.61
1:CCC:105[B]:VAL:HG11	1:CCC:139[B]:ALA:HB2	1.83	0.61
1:CCC:81[B]:THR:HG23	1:CCC:83[B]:SER:O	2.01	0.60
1:DDD:9:PHE:CE1	1:DDD:168[B]:LEU:HD21	2.37	0.60
1:AAA:108[B]:GLN:HB2	5:AAA:697[B]:HOH:O	2.01	0.60
1:AAA:16[A]:HIS:CD2	1:AAA:165:THR:HB	2.35	0.60
1:CCC:67:LEU:O	1:CCC:76[B]:PRO:HD3	2.01	0.60
1:CCC:103[A]:TYR:CE2	1:CCC:146[A]:THR:HG21	2.36	0.60
1:BBB:77:LYS:O	1:BBB:101:PRO:HD2	2.01	0.60
4:AAA:406:NA:NA	5:AAA:617:HOH:O	1.74	0.59
1:CCC:94[B]:ALA:O	1:CCC:97[B]:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:149[B]:ILE:O	1:CCC:150[B]:MET:O	2.21	0.58
1:CCC:226:LEU:CD1	1:CCC:244:ILE:HG22	2.34	0.58
1:CCC:301:VAL:HG11	1:CCC:305:VAL:HG11	1.85	0.58
1:CCC:80[B]:VAL:O	1:CCC:150[B]:MET:C	2.41	0.58
1:CCC:80[B]:VAL:HA	1:CCC:103[B]:TYR:O	2.03	0.58
1:DDD:223:LYS:HE3	5:DDD:665:HOH:O	2.03	0.58
1:AAA:108[B]:GLN:C	1:AAA:108[B]:GLN:NE2	2.37	0.58
1:BBB:249:TRP:CH2	1:BBB:253:ARG:HB3	2.39	0.57
1:CCC:118[B]:ILE:HG12	1:CCC:121[B]:TYR:CZ	2.39	0.57
1:CCC:16:HIS:ND1	5:CCC:503:HOH:O	2.32	0.57
1:AAA:34:LEU:HD21	1:AAA:273:LEU:HD21	1.86	0.57
1:CCC:152[B]:HIS:CD2	1:CCC:154:ASN:H	2.23	0.57
1:CCC:81[B]:THR:HG22	1:CCC:104[B]:ILE:HD12	1.83	0.57
1:DDD:105:VAL:HG12	1:DDD:126[B]:VAL:HG23	1.86	0.57
1:BBB:258:ASP:C	1:BBB:259:ILE:HD12	2.25	0.56
1:CCC:93[B]:TYR:CD1	1:CCC:93[B]:TYR:C	2.78	0.56
1:CCC:33:ILE:O	1:CCC:37:LEU:HD12	2.06	0.56
1:AAA:131:SER:O	1:AAA:135[A]:ARG:HG3	2.05	0.56
1:BBB:236[A]:ILE:HG12	1:BBB:264:GLU:OE1	2.05	0.56
1:AAA:281[A]:LEU:HD22	1:CCC:281[A]:LEU:HD21	1.87	0.56
2:CCC:401:PGE:H4	5:CCC:574:HOH:O	2.04	0.56
1:CCC:61:LEU:HA	1:CCC:94[B]:ALA:CB	2.36	0.56
1:CCC:79[B]:VAL:HG11	1:CCC:91[B]:LEU:CD2	2.35	0.56
1:CCC:140[A]:LYS:C	1:CCC:141[A]:ARG:CA	2.73	0.55
1:BBB:236[A]:ILE:HD11	1:BBB:267:ILE:HB	1.88	0.55
1:CCC:305:VAL:HG13	1:CCC:305:VAL:O	2.06	0.55
1:BBB:80:VAL:HG13	1:BBB:143:THR:CG2	2.27	0.55
1:CCC:33:ILE:HD12	1:CCC:33:ILE:H	1.72	0.55
1:CCC:83[B]:SER:OG	1:CCC:153:PRO:CG	2.54	0.55
1:CCC:319:LEU:O	1:CCC:322:SER:HB3	2.07	0.54
1:CCC:83[B]:SER:HB3	1:CCC:87[B]:HIS:HB3	1.89	0.54
1:DDD:82[B]:HIS:CD2	1:DDD:135[B]:ARG:HG2	2.42	0.54
1:BBB:128:CYS:HB2	1:BBB:138:VAL:HG21	1.90	0.54
1:AAA:61:LEU:HD11	5:AAA:567:HOH:O	2.07	0.53
1:CCC:141[A]:ARG:O	1:CCC:142[A]:VAL:N	2.41	0.53
1:AAA:64:VAL:HG12	1:AAA:98:GLU:HG3	1.91	0.53
1:CCC:91[B]:LEU:HD13	1:CCC:151[B]:VAL:CG1	2.38	0.53
1:DDD:52:THR:HB	1:DDD:89[A]:GLN:HG2	1.90	0.53
1:AAA:139:ALA:HB1	1:AAA:150:MET:CE	2.39	0.53
1:CCC:91[B]:LEU:CD1	1:CCC:151[B]:VAL:HG11	2.39	0.53
1:BBB:79:VAL:HG13	1:BBB:91[B]:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:57:ILE:HD11	1:CCC:93[B]:TYR:HD1	1.74	0.52
1:CCC:93[B]:TYR:O	1:CCC:97[B]:LEU:CD2	2.57	0.52
1:AAA:261:THR:H	2:AAA:402:PGE:C6	2.22	0.52
1:CCC:83[B]:SER:HB2	1:CCC:153:PRO:HB3	1.86	0.52
1:CCC:9:PHE:CZ	1:CCC:168:LEU:HD21	2.45	0.52
1:CCC:79[B]:VAL:HB	1:CCC:91[B]:LEU:HD21	1.92	0.52
1:CCC:140[B]:LYS:O	1:CCC:143[B]:THR:HG22	2.10	0.52
1:BBB:80:VAL:CG1	1:BBB:143:THR:CG2	2.73	0.51
1:AAA:109[A]:THR:HG23	1:AAA:130:PRO:HG3	1.91	0.51
1:CCC:117[B]:ALA:O	1:CCC:120[B]:ALA:HB3	2.11	0.51
1:BBB:131:SER:O	1:BBB:135:ARG:HB2	2.11	0.51
1:DDD:126[B]:VAL:HG21	1:DDD:142:VAL:HG21	1.92	0.51
1:CCC:57:ILE:HA	1:CCC:90[B]:ALA:HB1	1.92	0.51
1:DDD:106:VAL:HG11	1:DDD:118:ILE:HD13	1.94	0.50
1:BBB:79:VAL:HG13	1:BBB:91[B]:LEU:CD1	2.42	0.50
1:CCC:249:TRP:HB3	1:CCC:250:PRO:HD3	1.92	0.50
1:BBB:258:ASP:O	1:BBB:259:ILE:HD12	2.11	0.50
1:CCC:140[B]:LYS:C	1:CCC:142[B]:VAL:N	2.65	0.50
1:CCC:82[B]:HIS:HB3	1:CCC:153:PRO:CD	2.41	0.50
1:CCC:118[A]:ILE:HG23	1:CCC:123[A]:ALA:HB3	1.93	0.50
1:CCC:178:ASP:HB3	1:CCC:305:VAL:HG23	1.94	0.50
1:CCC:80[A]:VAL:HG13	1:CCC:103[A]:TYR:HB2	1.94	0.50
1:CCC:80[A]:VAL:HA	1:CCC:103[A]:TYR:O	2.12	0.50
1:CCC:107[B]:PRO:HB3	1:CCC:130[B]:PRO:CA	2.40	0.50
1:CCC:108[B]:GLN:N	1:CCC:128[B]:CYS:O	2.41	0.50
1:BBB:79:VAL:HG13	1:BBB:91[A]:LEU:HD11	1.94	0.49
1:BBB:79:VAL:CG1	1:BBB:91[B]:LEU:CD1	2.90	0.49
1:AAA:33:ILE:CD1	1:AAA:33:ILE:H	2.15	0.49
1:BBB:128:CYS:HB3	1:BBB:138:VAL:HG11	1.94	0.49
1:DDD:117:ALA:O	1:DDD:120:ALA:HB3	2.12	0.49
1:CCC:87[B]:HIS:CG	1:CCC:153:PRO:HA	2.47	0.49
1:AAA:7:ILE:HD13	1:AAA:160:ILE:HG22	1.94	0.49
1:CCC:80[B]:VAL:CA	1:CCC:150[B]:MET:HA	2.42	0.49
1:CCC:80[B]:VAL:CG1	1:CCC:103[B]:TYR:HB2	2.43	0.49
1:AAA:66[B]:SER:HB3	5:AAA:557:HOH:O	2.13	0.48
1:CCC:80[B]:VAL:H	1:CCC:150[B]:MET:HA	1.78	0.48
1:CCC:87[B]:HIS:CD2	1:CCC:153:PRO:CA	2.94	0.48
1:CCC:91[B]:LEU:O	1:CCC:92[B]:THR:C	2.51	0.48
1:DDD:82[B]:HIS:CD2	1:DDD:135[B]:ARG:CG	2.96	0.48
1:DDD:210:GLU:O	1:DDD:261:THR:HA	2.14	0.48
1:CCC:149[B]:ILE:O	1:CCC:150[B]:MET:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:277:ARG:NE	5:CCC:507:HOH:O	2.47	0.48
1:CCC:77[B]:LYS:O	1:CCC:78[B]:ALA:CB	2.61	0.48
1:CCC:87[B]:HIS:NE2	1:CCC:153:PRO:HA	2.28	0.47
1:BBB:200:LEU:HB3	1:CCC:17:ILE:CD1	2.44	0.47
1:CCC:149[B]:ILE:C	1:CCC:150[B]:MET:O	2.52	0.47
1:CCC:9:PHE:HE1	1:CCC:196:THR:HG23	1.80	0.47
1:CCC:75[B]:LYS:HB3	1:CCC:76[B]:PRO:HD2	1.96	0.47
1:CCC:81[A]:THR:OG1	1:CCC:82[A]:HIS:N	2.48	0.47
1:CCC:301:VAL:CG1	1:CCC:305:VAL:CG1	2.82	0.47
1:CCC:80[B]:VAL:HG23	1:CCC:150[B]:MET:HG2	1.96	0.47
1:CCC:91[B]:LEU:CD1	1:CCC:151[B]:VAL:CG1	2.92	0.47
1:CCC:136[B]:GLU:O	1:CCC:136[B]:GLU:HG2	2.13	0.47
1:CCC:140[B]:LYS:O	1:CCC:144[B]:GLU:CG	2.62	0.47
1:AAA:13:GLU:OE2	1:DDD:13:GLU:HG2	2.15	0.47
1:BBB:106:VAL:O	1:BBB:127:TYR:HA	2.14	0.47
1:CCC:83[B]:SER:OG	1:CCC:153:PRO:HG3	2.16	0.46
1:BBB:83:SER:O	1:BBB:88:GLY:HA3	2.15	0.46
1:CCC:106[A]:VAL:O	1:CCC:127[A]:TYR:HA	2.15	0.46
1:CCC:198:LYS:O	1:CCC:202:PRO:HG3	2.14	0.46
1:CCC:143[B]:THR:HB	1:CCC:150[B]:MET:HG2	1.98	0.46
1:DDD:40:ARG:HD2	1:DDD:308:ILE:HD12	1.97	0.46
1:BBB:80:VAL:HG11	1:BBB:143:THR:CG2	2.38	0.46
1:DDD:221:LYS:HG3	1:DDD:259:ILE:HD11	1.98	0.46
1:DDD:60:ALA:HB1	1:DDD:91[B]:LEU:HD23	1.98	0.46
1:AAA:109[A]:THR:CG2	1:AAA:130:PRO:HG3	2.46	0.46
1:BBB:142:VAL:O	1:BBB:146:THR:HG23	2.16	0.46
1:BBB:253:ARG:HH21	1:BBB:254:ASP:CG	2.19	0.46
1:CCC:240:VAL:HG13	1:CCC:285:THR:HG23	1.98	0.45
1:DDD:40:ARG:HD2	1:DDD:308:ILE:CD1	2.46	0.45
1:CCC:140[A]:LYS:O	1:CCC:143[A]:THR:CG2	2.61	0.45
1:CCC:139[B]:ALA:O	1:CCC:150[B]:MET:SD	2.75	0.45
1:CCC:56:LLP:HD3	1:CCC:86[B]:ASN:HB2	1.99	0.45
1:DDD:201:LYS:HG2	1:DDD:204:VAL:HG23	1.97	0.45
1:BBB:81:THR:HG22	1:BBB:104:ILE:CD1	2.47	0.45
1:CCC:56:LLP:HD2	1:CCC:87[B]:HIS:HB2	1.99	0.45
1:DDD:104:ILE:HG12	1:DDD:123:ALA:HB1	1.99	0.45
1:AAA:108[B]:GLN:N	5:AAA:697[B]:HOH:O	2.50	0.45
1:CCC:79[B]:VAL:HG11	1:CCC:91[B]:LEU:CD1	2.41	0.45
1:DDD:105:VAL:HG12	1:DDD:126[B]:VAL:CG2	2.46	0.45
1:BBB:9:PHE:HE1	1:BBB:168:LEU:HD21	1.82	0.45
1:AAA:34:LEU:HB3	1:AAA:42:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:81:THR:HB	1:BBB:91[A]:LEU:CD2	2.47	0.44
1:CCC:79[A]:VAL:HG12	1:CCC:91[A]:LEU:HD21	1.99	0.44
1:CCC:82[B]:HIS:C	1:CCC:82[B]:HIS:ND1	2.71	0.44
1:CCC:87[B]:HIS:O	1:CCC:90[B]:ALA:HB3	2.17	0.44
1:CCC:79[A]:VAL:CG1	1:CCC:91[A]:LEU:HD21	2.48	0.44
1:BBB:322:SER:HA	1:BBB:325:TRP:NE1	2.32	0.44
1:BBB:293:VAL:HG21	1:BBB:310:ILE:HD11	2.00	0.44
1:CCC:146[B]:THR:O	1:CCC:147[B]:GLU:C	2.56	0.44
1:DDD:34:LEU:HB3	1:DDD:42:LEU:HD12	2.00	0.44
1:CCC:104[B]:ILE:HG21	1:CCC:118[B]:ILE:HD11	1.99	0.44
1:AAA:139:ALA:HB1	1:AAA:150:MET:HE1	1.99	0.44
1:CCC:290:VAL:O	1:CCC:293[B]:VAL:HG12	2.18	0.44
1:AAA:64:VAL:CG1	1:AAA:98:GLU:HG3	2.47	0.44
1:BBB:55:PHE:HB2	1:BBB:166:ILE:HD11	1.98	0.44
1:CCC:159:VAL:O	1:CCC:163:GLN:HG2	2.17	0.44
1:AAA:34:LEU:HD23	1:AAA:34:LEU:HA	1.86	0.44
1:AAA:14[B]:LYS:HB2	1:AAA:14[B]:LYS:HE2	1.64	0.43
1:BBB:229:ASN:HB2	5:BBB:504:HOH:O	2.18	0.43
1:CCC:293[A]:VAL:HG21	1:CCC:310:ILE:HD11	2.00	0.43
1:AAA:40:ARG:HD2	1:AAA:308:ILE:CD1	2.48	0.43
1:CCC:140[B]:LYS:HA	1:CCC:143[B]:THR:HG22	2.00	0.43
1:BBB:139:ALA:HA	1:BBB:142:VAL:HG22	2.00	0.43
1:CCC:221:LYS:HE2	1:CCC:252:ILE:O	2.18	0.43
1:AAA:129:GLU:HB2	1:AAA:134:SER:CB	2.48	0.43
1:BBB:81:THR:HG22	1:BBB:104:ILE:HD13	2.01	0.43
1:CCC:80[B]:VAL:HG23	1:CCC:150[B]:MET:CG	2.49	0.43
1:CCC:93[B]:TYR:CG	1:CCC:93[B]:TYR:O	2.72	0.43
1:CCC:107[B]:PRO:O	1:CCC:108[B]:GLN:O	2.35	0.43
1:CCC:56:LLP:H2'1	1:CCC:86[B]:ASN:ND2	2.33	0.43
1:CCC:88[B]:GLY:C	1:CCC:90[B]:ALA:N	2.72	0.43
1:AAA:272[B]:GLN:HG3	1:AAA:325:TRP:HZ3	1.84	0.42
1:AAA:223[B]:LYS:HD3	1:AAA:227:MET:SD	2.59	0.42
1:BBB:16:HIS:O	1:BBB:20:ARG:HB2	2.19	0.42
1:CCC:298:PHE:O	1:CCC:301:VAL:HG23	2.20	0.42
1:CCC:79[A]:VAL:HG11	1:CCC:91[A]:LEU:HD11	2.00	0.42
1:CCC:93[B]:TYR:CE1	1:CCC:97[B]:LEU:HD21	2.55	0.42
1:DDD:33:ILE:HG21	1:DDD:277:ARG:HB3	2.02	0.42
1:CCC:34:LEU:HD21	1:CCC:273[A]:LEU:HD23	2.01	0.42
1:CCC:33:ILE:N	1:CCC:33:ILE:HD12	2.34	0.42
1:DDD:141:ARG:O	1:DDD:145:GLU:HG2	2.20	0.42
1:BBB:130:PRO:O	1:BBB:131:SER:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:34:LEU:CD2	1:AAA:273:LEU:HD21	2.48	0.42
1:BBB:153:PRO:HB2	5:BBB:531:HOH:O	2.20	0.42
1:CCC:105[A]:VAL:HG11	1:CCC:139[A]:ALA:HB2	2.02	0.42
1:AAA:34:LEU:HD21	1:AAA:273:LEU:CD2	2.48	0.41
1:CCC:134[B]:SER:O	1:CCC:135[B]:ARG:C	2.58	0.41
1:CCC:64:VAL:HG11	1:CCC:95[B]:ALA:HA	2.02	0.41
1:CCC:64:VAL:HG22	1:CCC:79[B]:VAL:HG21	2.02	0.41
1:CCC:9:PHE:CE1	1:CCC:196:THR:HG23	2.54	0.41
1:AAA:106:VAL:HG21	1:AAA:125:ILE:HG23	2.02	0.41
1:BBB:56:LLP:P	1:BBB:187:GLY:H	2.43	0.41
1:CCC:75[B]:LYS:HB3	1:CCC:76[B]:PRO:CD	2.49	0.41
1:BBB:118:ILE:HG12	1:BBB:121:TYR:OH	2.21	0.41
1:CCC:30:THR:O	2:CCC:401:PGE:H42	2.21	0.41
1:CCC:82[B]:HIS:CE1	5:CCC:534:HOH:O	2.73	0.41
1:CCC:150[B]:MET:HG2	1:CCC:150[B]:MET:H	1.66	0.41
1:BBB:210:GLU:O	1:BBB:261:THR:HA	2.21	0.41
1:AAA:83:SER:OG	1:AAA:87:HIS:HB3	2.21	0.41
1:BBB:7:ILE:HG23	1:BBB:195:ILE:CD1	2.51	0.41
1:BBB:281[A]:LEU:HD21	1:DDD:281[A]:LEU:HD13	2.02	0.41
1:CCC:121[B]:TYR:HB2	5:CCC:553:HOH:O	2.20	0.41
1:CCC:118[B]:ILE:HG23	1:CCC:123[B]:ALA:HB3	2.03	0.41
1:CCC:108[A]:GLN:N	1:CCC:128[A]:CYS:O	2.46	0.41
1:BBB:201:LYS:HE2	5:BBB:502:HOH:O	2.20	0.41
1:CCC:91[B]:LEU:HD11	1:CCC:151[B]:VAL:HB	2.03	0.41
1:AAA:230:LEU:HA	1:AAA:230:LEU:HD23	1.82	0.40
1:AAA:108[A]:GLN:CA	1:AAA:108[A]:GLN:OE1	2.69	0.40
1:CCC:84[B]:SER:HB3	1:CCC:104[B]:ILE:CG2	2.52	0.40
1:BBB:56:LLP:NZ	1:BBB:56:LLP:O3	2.54	0.40
1:CCC:263:THR:O	1:CCC:267:ILE:HG13	2.22	0.40
1:BBB:238:ASP:OD1	1:BBB:241:LYS:NZ	2.43	0.40
1:CCC:107[B]:PRO:C	1:CCC:108[B]:GLN:O	2.60	0.40
1:CCC:9:PHE:HZ	1:CCC:168:LEU:HD21	1.82	0.40
1:CCC:34:LEU:HD13	1:CCC:44:PHE:CZ	2.56	0.40
1:CCC:83[B]:SER:CB	1:CCC:87[B]:HIS:HB3	2.51	0.40
1:AAA:125:ILE:N	1:AAA:125:ILE:HD12	2.30	0.40
1:DDD:139:ALA:HB1	1:DDD:150:MET:HE1	2.03	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	AAA	338/346 (98%)	331 (98%)	7 (2%)	0	100	100
1	BBB	318/346 (92%)	305 (96%)	13 (4%)	0	100	100
1	CCC	392/346 (113%)	353 (90%)	31 (8%)	8 (2%)	7	1
1	DDD	327/346 (94%)	318 (97%)	9 (3%)	0	100	100
All	All	1375/1384 (99%)	1307 (95%)	60 (4%)	8 (1%)	41	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CCC	78[A]	ALA
1	CCC	78[B]	ALA
1	CCC	150[A]	MET
1	CCC	150[B]	MET
1	CCC	85[A]	GLY
1	CCC	85[B]	GLY
1	CCC	92[A]	THR
1	CCC	92[B]	THR

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	271/290 (93%)	261 (96%)	10 (4%)	34	25
1	BBB	232/290 (80%)	220 (95%)	12 (5%)	23	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	273/290 (94%)	252 (92%)	21 (8%)	13	5
1	DDD	266/290 (92%)	258 (97%)	8 (3%)	41	33
All	All	1042/1160 (90%)	991 (95%)	51 (5%)	27	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	32	SER
1	AAA	72	LEU
1	AAA	83	SER
1	AAA	108[A]	GLN
1	AAA	108[B]	GLN
1	AAA	121	TYR
1	AAA	125	ILE
1	AAA	138	VAL
1	AAA	277	ARG
1	AAA	324	THR
1	BBB	6	ASP
1	BBB	7	ILE
1	BBB	32	SER
1	BBB	48	LEU
1	BBB	61	LEU
1	BBB	80	VAL
1	BBB	150	MET
1	BBB	222	LEU
1	BBB	238	ASP
1	BBB	253	ARG
1	BBB	261	THR
1	BBB	326	VAL
1	CCC	32	SER
1	CCC	37	LEU
1	CCC	40	ARG
1	CCC	79[A]	VAL
1	CCC	79[B]	VAL
1	CCC	80[A]	VAL
1	CCC	80[B]	VAL
1	CCC	83[A]	SER
1	CCC	83[B]	SER
1	CCC	97[A]	LEU
1	CCC	97[B]	LEU
1	CCC	118[A]	ILE

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Mol	Chain	Res	Type
1	CCC	118[B]	ILE
1	CCC	183	PRO
1	CCC	236	ILE
1	CCC	244	ILE
1	CCC	293[A]	VAL
1	CCC	293[B]	VAL
1	CCC	299	GLN
1	CCC	320	THR
1	CCC	322	SER
1	DDD	6	ASP
1	DDD	66	SER
1	DDD	124	SER
1	DDD	144	GLU
1	DDD	163	GLN
1	DDD	201	LYS
1	DDD	230	LEU
1	DDD	317	VAL

Some 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 ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	DDD	56	1	23,24,25	0.55	0	25,32,34	1.04	1 (4%)
1	LLP	AAA	56	1	23,24,25	0.83	1 (4%)	25,32,34	1.21	3 (12%)
1	LLP	BBB	56	1	23,24,25	0.47	0	25,32,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	CCC	56	1	23,24,25	0.85	1 (4%)	25,32,34	1.09	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	DDD	56	1	-	4/16/17/19	0/1/1/1
1	LLP	AAA	56	1	-	5/16/17/19	0/1/1/1
1	LLP	BBB	56	1	-	3/16/17/19	0/1/1/1
1	LLP	CCC	56	1	-	4/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	56	LLP	P-OP4	3.16	1.70	1.60
1	AAA	56	LLP	P-OP4	2.06	1.66	1.60

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	56	LLP	OP4-C5'-C5	2.63	114.37	109.35
1	AAA	56	LLP	C3-C4-C4'	-2.26	116.19	120.41
1	CCC	56	LLP	OP3-P-OP2	2.22	116.10	107.64
1	AAA	56	LLP	OP3-P-OP1	2.13	119.03	110.68
1	AAA	56	LLP	CG-CD-CE	-2.06	106.41	113.57

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	DDD	56	LLP	C4-C4'-NZ-CE
1	DDD	56	LLP	C-CA-CB-CG
1	AAA	56	LLP	C4-C4'-NZ-CE
1	BBB	56	LLP	C4-C4'-NZ-CE
1	BBB	56	LLP	C-CA-CB-CG
1	CCC	56	LLP	C4-C4'-NZ-CE
1	CCC	56	LLP	C-CA-CB-CG
1	AAA	56	LLP	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	BBB	56	LLP	CG-CD-CE-NZ
1	DDD	56	LLP	CD-CE-NZ-C4'
1	DDD	56	LLP	C3-C4-C4'-NZ
1	AAA	56	LLP	CD-CE-NZ-C4'
1	CCC	56	LLP	CD-CE-NZ-C4'
1	AAA	56	LLP	C3-C4-C4'-NZ
1	CCC	56	LLP	C3-C4-C4'-NZ
1	AAA	56	LLP	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BBB	56	LLP	2	0
1	CCC	56	LLP	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z > 2$
2	PGE	BBB	402	-	3,3,9	0.13	0	2,2,8	0.23	0
2	PGE	AAA	401	-	3,3,9	0.14	0	2,2,8	0.23	0
2	PGE	AAA	402	-	2,2,9	0.46	0	1,1,8	0.30	0
2	PGE	CCC	401	-	4,4,9	0.21	0	3,3,8	0.32	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	PGE	BBB	402	-	-	1/1/1/7	-
2	PGE	AAA	401	-	-	1/1/1/7	-
2	PGE	CCC	401	-	-	1/2/2/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	402	PGE	O3-C5-C6-O4
2	CCC	401	PGE	O2-C3-C4-O3
2	AAA	401	PGE	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	402	PGE	2	0
2	AAA	402	PGE	1	0
2	CCC	401	PGE	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	CCC	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CCC	141[A]:ARG	C	142[A]:VAL	N	3.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CCC	140[A]:LYS	C	141[A]:ARG	N	2.86
1	CCC	141[B]:ARG	C	142[B]:VAL	N	1.71
1	CCC	140[B]:LYS	C	141[B]:ARG	N	1.17

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	AAA	321/346 (92%)	0.56	40 (12%) 3 4	26, 35, 82, 117	0
1	BBB	313/346 (90%)	0.91	52 (16%) 1 1	37, 63, 125, 166	0
1	CCC	315/346 (91%)	0.94	64 (20%) 1 1	33, 57, 100, 121	0
1	DDD	316/346 (91%)	0.18	24 (7%) 13 15	27, 39, 95, 125	0
All	All	1265/1384 (91%)	0.64	180 (14%) 2 2	26, 48, 103, 166	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	109	THR	10.6
1	CCC	106[A]	VAL	9.6
1	BBB	130	PRO	8.3
1	BBB	113	CYS	8.3
1	CCC	113[A]	CYS	8.1
1	DDD	113	CYS	7.6
1	CCC	128[A]	CYS	7.5
1	CCC	127[A]	TYR	7.5
1	BBB	116	LEU	7.5
1	BBB	132	ASP	7.1
1	BBB	110	ALA	6.8
1	AAA	116	LEU	6.8
1	AAA	118	ILE	6.6
1	BBB	131	SER	6.5
1	BBB	106	VAL	6.3
1	AAA	324	THR	6.3
1	CCC	130[A]	PRO	6.2
1	CCC	76[A]	PRO	6.2
1	CCC	104[A]	ILE	6.2
1	CCC	126[A]	VAL	6.1
1	CCC	134[A]	SER	6.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	110	ALA	6.0
1	AAA	126	VAL	5.9
1	BBB	227	MET	5.9
1	CCC	107[A]	PRO	5.8
1	BBB	112	ASP	5.7
1	CCC	230	LEU	5.6
1	BBB	125	ILE	5.5
1	CCC	325	TRP	5.5
1	AAA	110	ALA	5.4
1	BBB	107	PRO	5.3
1	AAA	127	TYR	5.2
1	DDD	109	THR	5.2
1	AAA	109[A]	THR	5.1
1	CCC	105[A]	VAL	5.0
1	AAA	137	ASN	4.9
1	CCC	116[A]	LEU	4.9
1	BBB	222	LEU	4.9
1	CCC	112[A]	ASP	4.8
1	CCC	82[A]	HIS	4.8
1	CCC	115[A]	LYS	4.8
1	AAA	323	ILE	4.5
1	BBB	124	SER	4.4
1	BBB	133	GLU	4.4
1	BBB	134	SER	4.3
1	CCC	73	GLU	4.3
1	DDD	320	THR	4.3
1	CCC	133[A]	GLU	4.3
1	DDD	68	VAL	4.3
1	AAA	113	CYS	4.2
1	BBB	324	THR	4.2
1	BBB	111	PRO	4.2
1	BBB	7	ILE	4.1
1	CCC	122[A]	GLY	4.1
1	DDD	106	VAL	4.1
1	BBB	115	LYS	4.0
1	CCC	141[A]	ARG	4.0
1	DDD	111	PRO	3.9
1	BBB	95	ALA	3.8
1	AAA	105	VAL	3.8
1	CCC	118[A]	ILE	3.7
1	CCC	135[A]	ARG	3.7
1	AAA	320	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	120	ALA	3.6
1	BBB	323	ILE	3.6
1	BBB	103	TYR	3.5
1	BBB	127	TYR	3.5
1	BBB	128	CYS	3.5
1	CCC	132[A]	ASP	3.5
1	CCC	125[A]	ILE	3.4
1	DDD	116	LEU	3.4
1	AAA	321	SER	3.4
1	BBB	108	GLN	3.4
1	AAA	231	TYR	3.4
1	AAA	133	GLU	3.4
1	DDD	112	ASP	3.4
1	AAA	129	GLU	3.4
1	AAA	319	LEU	3.3
1	AAA	46	CYS	3.3
1	AAA	114	LYS	3.3
1	CCC	131[A]	SER	3.3
1	CCC	97[A]	LEU	3.2
1	DDD	133[A]	GLU	3.2
1	BBB	139	ALA	3.2
1	BBB	135	ARG	3.2
1	CCC	227	MET	3.2
1	CCC	138[A]	VAL	3.2
1	CCC	83[A]	SER	3.1
1	CCC	324	THR	3.1
1	BBB	114	LYS	3.1
1	BBB	230	LEU	3.1
1	BBB	325	TRP	3.0
1	CCC	129[A]	GLU	3.0
1	CCC	80[A]	VAL	3.0
1	AAA	325	TRP	3.0
1	CCC	319	LEU	3.0
1	BBB	326	VAL	3.0
1	CCC	74[A]	ARG	2.9
1	CCC	212	SER	2.9
1	BBB	300	THR	2.9
1	DDD	127	TYR	2.9
1	BBB	231	TYR	2.9
1	CCC	263	THR	2.9
1	AAA	106	VAL	2.9
1	CCC	108[A]	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	CCC	28	VAL	2.9
1	AAA	29	LEU	2.9
1	AAA	27	PRO	2.8
1	AAA	57	ILE	2.8
1	BBB	66	SER	2.8
1	CCC	137[A]	ASN	2.8
1	BBB	82	HIS	2.8
1	CCC	111[A]	PRO	2.8
1	DDD	138	VAL	2.8
1	CCC	119[A]	GLN	2.8
1	CCC	121[A]	TYR	2.8
1	BBB	97	LEU	2.7
1	AAA	112	ASP	2.7
1	BBB	118	ILE	2.7
1	DDD	325	TRP	2.7
1	AAA	26	THR	2.7
1	CCC	102[A]	ALA	2.7
1	CCC	75[A]	LYS	2.7
1	AAA	322	SER	2.7
1	BBB	319	LEU	2.6
1	BBB	9	PHE	2.6
1	DDD	129	GLU	2.6
1	AAA	115	LYS	2.6
1	CCC	139[A]	ALA	2.6
1	AAA	318	ASP	2.6
1	AAA	55	PHE	2.5
1	BBB	94	ALA	2.5
1	CCC	149[A]	ILE	2.5
1	CCC	27[A]	PRO	2.5
1	BBB	126	VAL	2.5
1	CCC	124[A]	SER	2.5
1	AAA	117	ALA	2.5
1	CCC	229	ASN	2.5
1	CCC	117[A]	ALA	2.5
1	DDD	117	ALA	2.5
1	DDD	275	TRP	2.5
1	BBB	67	LEU	2.5
1	BBB	104	ILE	2.4
1	AAA	49	PHE	2.4
1	CCC	103[A]	TYR	2.4
1	AAA	108[A]	GLN	2.4
1	CCC	231	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	255	LEU	2.4
1	BBB	137	ASN	2.4
1	DDD	136	GLU	2.4
1	AAA	25[A]	LEU	2.4
1	CCC	114[A]	LYS	2.4
1	AAA	111	PRO	2.4
1	DDD	231	TYR	2.3
1	AAA	119	GLN	2.3
1	CCC	299	GLN	2.3
1	CCC	232	PRO	2.3
1	CCC	236	ILE	2.3
1	AAA	128	CYS	2.3
1	CCC	46	CYS	2.3
1	BBB	274	VAL	2.2
1	DDD	115	LYS	2.2
1	BBB	232	PRO	2.2
1	AAA	125	ILE	2.2
1	CCC	49	PHE	2.2
1	DDD	75	LYS	2.2
1	DDD	134	SER	2.1
1	BBB	236[A]	ILE	2.1
1	CCC	300	THR	2.1
1	AAA	107[A]	PRO	2.1
1	CCC	123[A]	ALA	2.1
1	CCC	150[A]	MET	2.1
1	DDD	281[A]	LEU	2.1
1	DDD	319	LEU	2.1
1	AAA	311	VAL	2.1
1	BBB	282	ILE	2.1
1	CCC	48	LEU	2.1
1	BBB	214	ALA	2.0
1	CCC	79[A]	VAL	2.0
1	DDD	137	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
1	LLP	BBB	56	24/25	0.96	0.11	43,50,58,63	0
1	LLP	AAA	56	24/25	0.98	0.14	21,28,36,38	0
1	LLP	DDD	56	24/25	0.98	0.14	23,30,38,43	0
1	LLP	CCC	56	24/25	0.98	0.11	29,38,44,49	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
4	NA	DDD	403	1/1	0.79	0.15	78,78,78,78	0
2	PGE	BBB	402	4/10	0.81	0.15	66,69,73,73	0
2	PGE	CCC	401	5/10	0.82	0.47	74,82,84,88	0
4	NA	DDD	404	1/1	0.87	0.07	84,84,84,84	0
3	MG	BBB	401	1/1	0.88	0.06	57,57,57,57	0
4	NA	AAA	408	1/1	0.90	0.15	79,79,79,79	0
2	PGE	AAA	401	4/10	0.91	0.20	59,63,71,79	0
3	MG	DDD	401	1/1	0.92	0.17	58,58,58,58	0
4	NA	AAA	405	1/1	0.93	0.23	76,76,76,76	0
2	PGE	AAA	402	3/10	0.93	0.13	25,25,46,48	0
3	MG	AAA	403	1/1	0.93	0.13	62,62,62,62	0
4	NA	AAA	407	1/1	0.96	0.46	82,82,82,82	0
3	MG	CCC	402	1/1	0.96	0.04	50,50,50,50	0
4	NA	AAA	406	1/1	0.97	0.15	64,64,64,64	0
3	MG	AAA	404	1/1	0.97	0.05	29,29,29,29	0
3	MG	DDD	402	1/1	0.98	0.09	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.