



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:17 PM BST

PDB ID : 6SX4
Title : Structure of *C. glutamicum* mycoloyltransferase A
Authors : Li de la Sierra-Gallay, I.; Van tilbeurgh, H.; Bayan, N.
Deposited on : 2019-09-24
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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)
Xtrriage (Phenix) : 1.13
EDS : 2.13.1
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

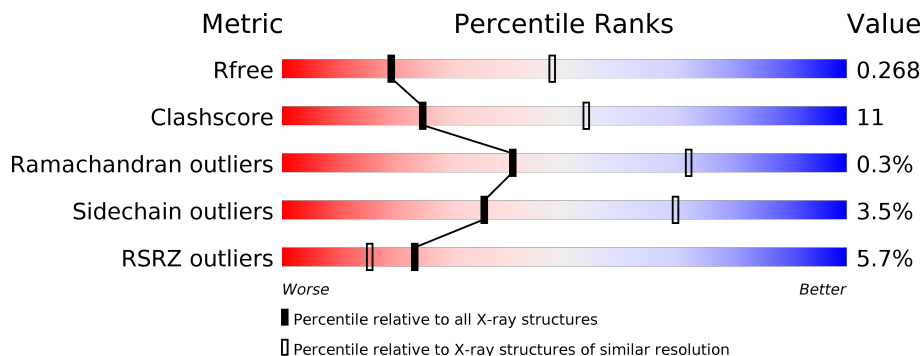
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	620	 5% 75% 19% • 5%
1	BBB	620	 4% 75% 19% • 5%
1	CCC	620	 3% 73% 20% • 5%
1	DDD	620	 10% 75% 19% • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	AAA	707	-	-	X	-
2	ACT	BBB	705	-	-	X	-
2	ACT	CCC	702	-	-	X	-
2	ACT	CCC	706	-	-	X	-
2	ACT	DDD	707	-	-	X	-

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 35499 atoms, of which 17134 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 Protein PS1.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se				
1	AAA	589	8777	2850	4264	764	887	2	10	223	0	0	
1	BBB	590	8784	2852	4267	765	888	2	10	223	0	0	
1	CCC	589	8777	2850	4264	764	887	2	10	223	0	0	
1	DDD	589	8777	2850	4264	764	887	2	10	223	0	0	

There are 24 discrepancies between the modelled and reference sequences:

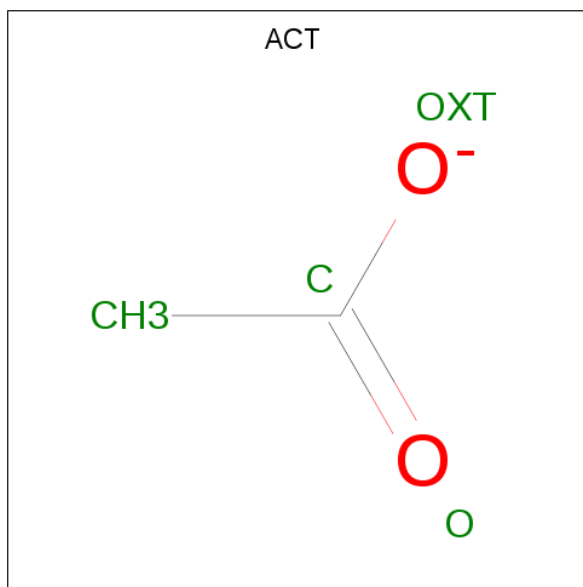
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	658	HIS	-	expression tag	UNP P0C1D6
AAA	659	HIS	-	expression tag	UNP P0C1D6
AAA	660	HIS	-	expression tag	UNP P0C1D6
AAA	661	HIS	-	expression tag	UNP P0C1D6
AAA	662	HIS	-	expression tag	UNP P0C1D6
AAA	663	HIS	-	expression tag	UNP P0C1D6
BBB	658	HIS	-	expression tag	UNP P0C1D6
BBB	659	HIS	-	expression tag	UNP P0C1D6
BBB	660	HIS	-	expression tag	UNP P0C1D6
BBB	661	HIS	-	expression tag	UNP P0C1D6
BBB	662	HIS	-	expression tag	UNP P0C1D6
BBB	663	HIS	-	expression tag	UNP P0C1D6
CCC	658	HIS	-	expression tag	UNP P0C1D6
CCC	659	HIS	-	expression tag	UNP P0C1D6
CCC	660	HIS	-	expression tag	UNP P0C1D6
CCC	661	HIS	-	expression tag	UNP P0C1D6
CCC	662	HIS	-	expression tag	UNP P0C1D6
CCC	663	HIS	-	expression tag	UNP P0C1D6
DDD	658	HIS	-	expression tag	UNP P0C1D6
DDD	659	HIS	-	expression tag	UNP P0C1D6
DDD	660	HIS	-	expression tag	UNP P0C1D6

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	661	HIS	-	expression tag	UNP P0C1D6
DDD	662	HIS	-	expression tag	UNP P0C1D6
DDD	663	HIS	-	expression tag	UNP P0C1D6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	AAA	1	7	2	3	2	0	0
2	BBB	1	7	2	3	2	0	0
2	BBB	1	7	2	3	2	0	0
2	BBB	1	7	2	3	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	BBB	1	Total	C	H	O	0	0
			7	2	3	2		
2	BBB	1	Total	C	H	O	0	0
			7	2	3	2		
2	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
2	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
2	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
2	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
2	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
2	DDD	1	Total	C	H	O	0	0
			7	2	3	2		

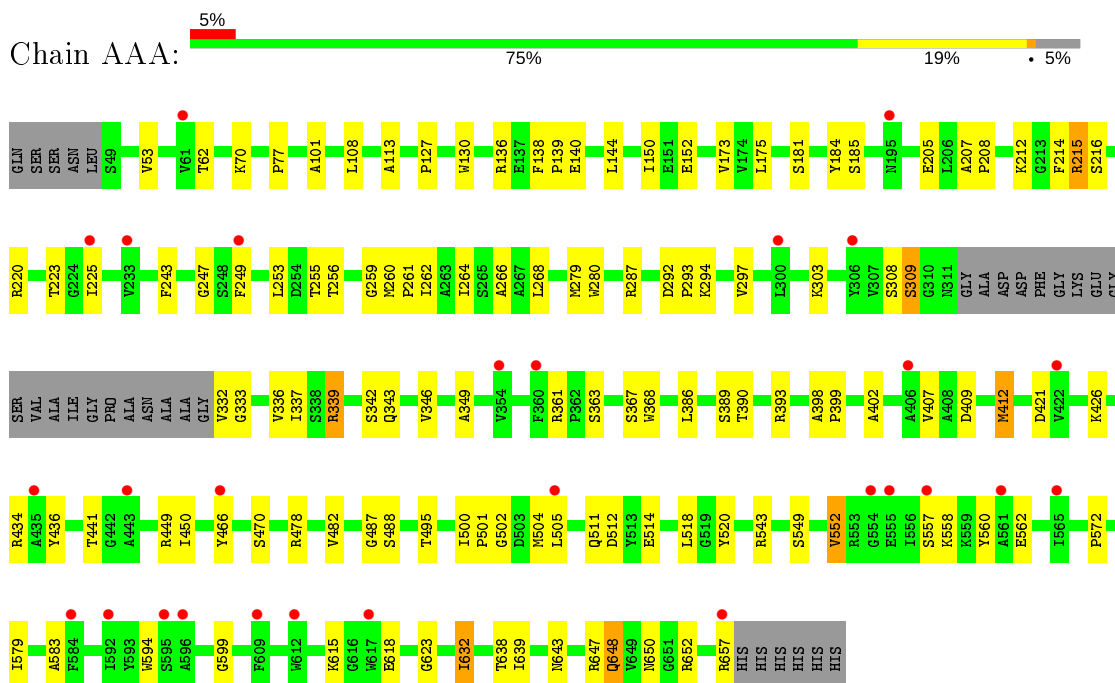
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	67	Total	O	0	0
			67	67		
3	BBB	53	Total	O	0	0
			53	53		
3	CCC	50	Total	O	0	0
			50	50		
3	DDD	39	Total	O	0	0
			39	39		

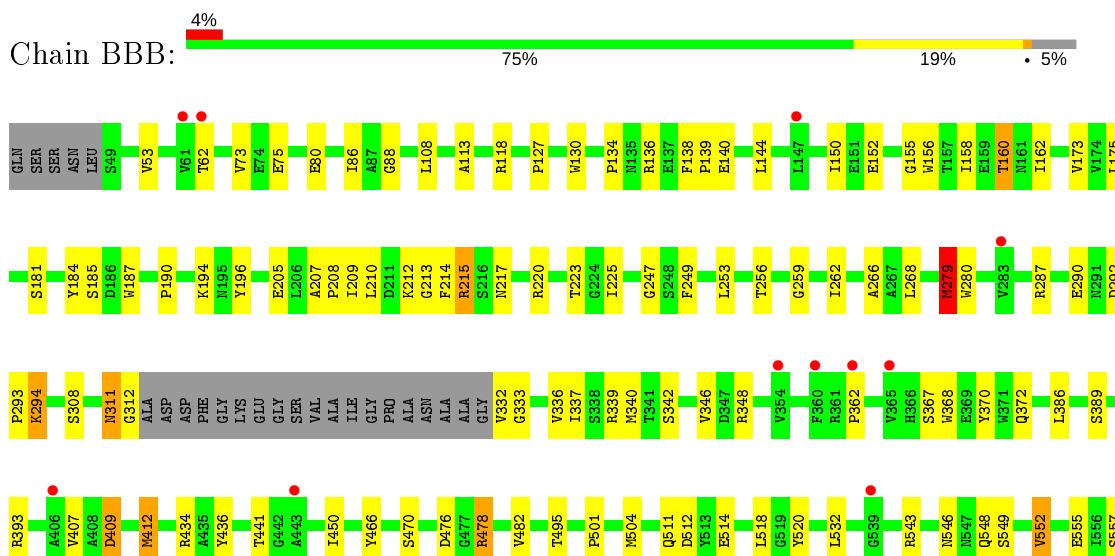
3 Residue-property plots

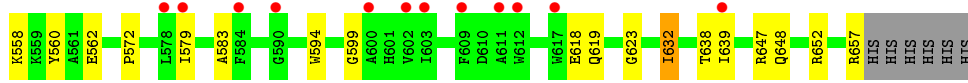
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein PS1

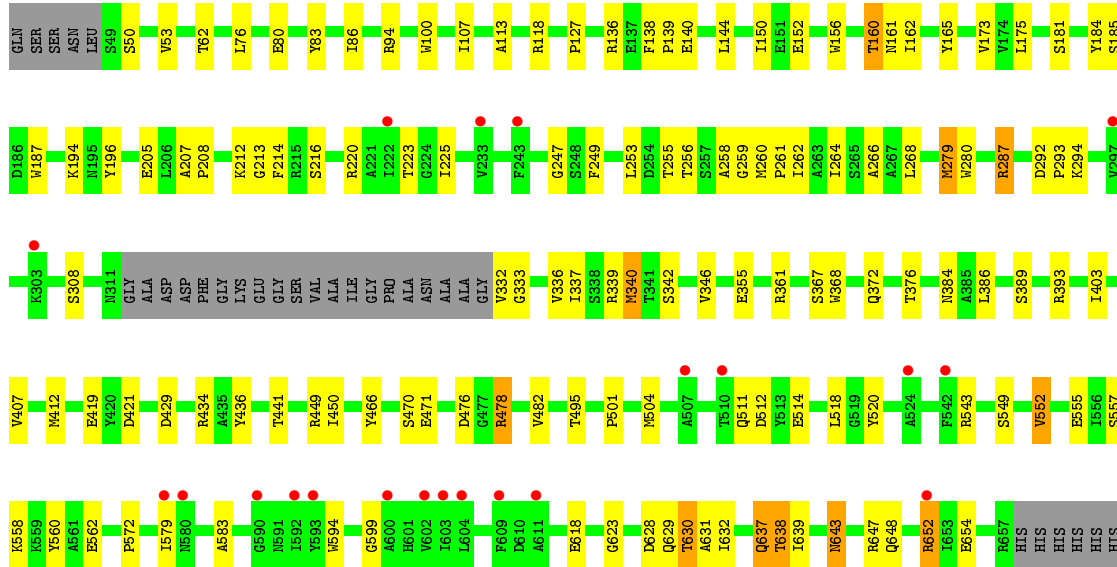
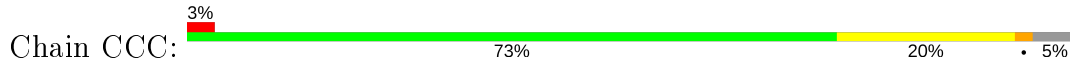


- Molecule 1: Protein PS1

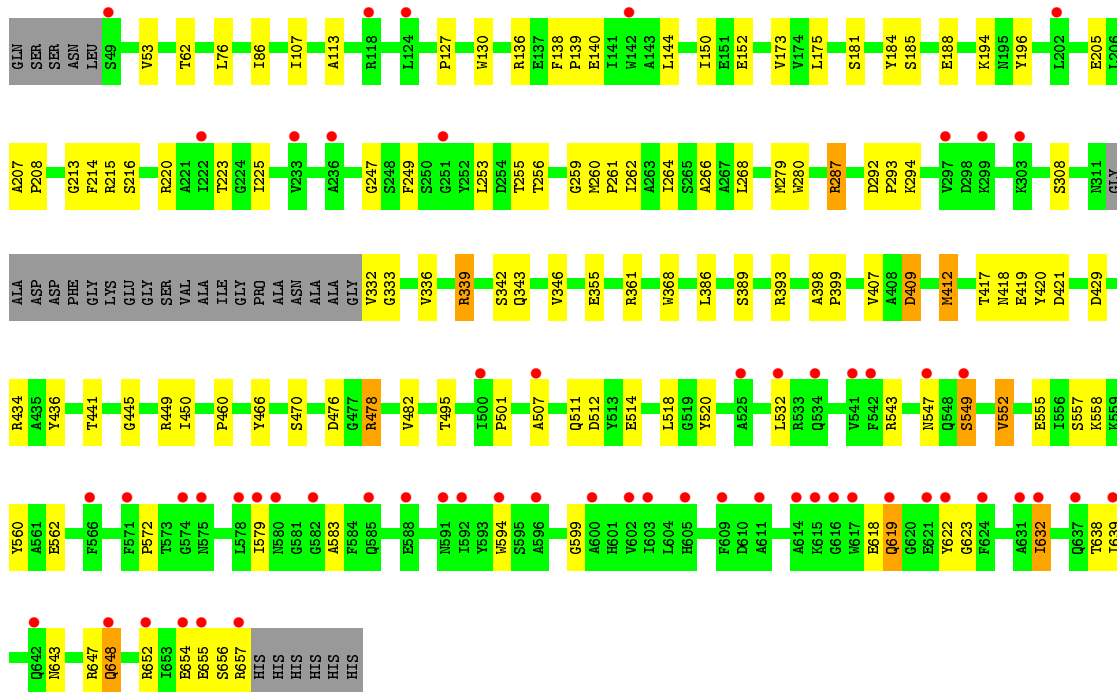
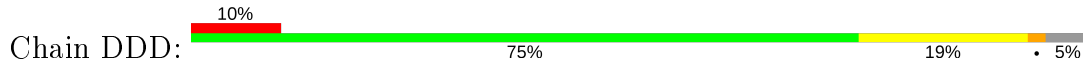




• Molecule 1: Protein PS1



• Molecule 1: Protein PS1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.15Å 170.48Å 241.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 2.80 48.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.57-2.80) 99.7 (48.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.242 , 0.262 0.246 , 0.268	Depositor DCC
R_{free} test set	3444 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtrriage
Anisotropy	0.806	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35499	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8338e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ACT

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	0.68	0/4622	0.80	1/6272 (0.0%)
1	BBB	0.67	0/4626	0.80	2/6277 (0.0%)
1	CCC	0.67	0/4622	0.80	3/6272 (0.0%)
1	DDD	0.68	0/4622	0.79	2/6272 (0.0%)
All	All	0.67	0/18492	0.80	8/25093 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	279	MSE	CG-SE-CE	6.09	112.30	98.90
1	CCC	214	PHE	CB-CA-C	5.52	121.45	110.40
1	AAA	412	MSE	CG-SE-CE	5.33	110.62	98.90
1	DDD	214	PHE	CB-CA-C	5.28	120.96	110.40
1	CCC	340	MSE	CG-SE-CE	5.24	110.42	98.90
1	DDD	412	MSE	CG-SE-CE	5.17	110.27	98.90
1	BBB	279	MSE	CG-SE-CE	5.13	110.19	98.90
1	BBB	412	MSE	CG-SE-CE	5.08	110.07	98.90

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	4513	4264	4254	95	1
1	BBB	4517	4267	4257	104	0
1	CCC	4513	4264	4254	94	1
1	DDD	4513	4264	4254	89	0
2	AAA	28	21	21	6	0
2	BBB	20	15	15	8	0
2	CCC	24	18	18	6	0
2	DDD	28	21	21	7	0
3	AAA	67	0	0	2	0
3	BBB	53	0	0	4	0
3	CCC	50	0	0	4	0
3	DDD	39	0	0	3	0
All	All	18365	17134	17094	379	1

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 11.

All (379) 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:BBB:638:THR:HG22	1:BBB:647:ARG:HG2	1.23	1.10
1:AAA:500:ILE:HB	1:AAA:505:LEU:HD21	1.20	1.10
1:AAA:130:TRP:O	1:AAA:215:ARG:NH1	1.84	1.09
1:BBB:134:PRO:HA	1:BBB:215:ARG:HH12	1.15	1.04
1:AAA:500:ILE:HB	1:AAA:505:LEU:CD2	1.88	1.01
1:BBB:134:PRO:HA	1:BBB:215:ARG:NH1	1.86	0.91
1:BBB:312:GLY:HA2	1:BBB:367:SER:H	1.35	0.91
1:DDD:130:TRP:O	1:DDD:215:ARG:NH2	2.06	0.87
1:BBB:209:ILE:O	1:BBB:213:GLY:N	2.07	0.87
1:DDD:417:THR:HG22	1:DDD:418:ASN:O	1.75	0.86
1:DDD:339:ARG:HH12	1:DDD:343:GLN:HG2	1.42	0.83
1:BBB:187:TRP:CE2	1:BBB:279:MSE:HG3	2.15	0.81
1:BBB:407:VAL:HG22	1:BBB:412:MSE:HG3	1.62	0.81
1:BBB:638:THR:HG22	1:BBB:647:ARG:CG	2.08	0.80
1:BBB:187:TRP:CZ2	1:BBB:279:MSE:HG3	2.17	0.79
1:AAA:638:THR:HG22	1:AAA:647:ARG:HG2	1.63	0.79
1:CCC:187:TRP:CZ2	1:CCC:279:MSE:HE3	2.18	0.78
1:AAA:543:ARG:HH22	2:AAA:707:ACT:C	1.97	0.78
1:AAA:502:GLY:HA2	1:AAA:505:LEU:HD12	1.65	0.77
1:DDD:361:ARG:NH2	1:DDD:421:ASP:HB2	2.00	0.76
1:AAA:136:ARG:HD3	1:AAA:138:PHE:CE2	2.21	0.75
1:CCC:160:THR:HG22	1:CCC:162:ILE:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:136:ARG:HD3	1:DDD:138:PHE:CE2	2.22	0.74
1:CCC:136:ARG:HD3	1:CCC:138:PHE:CE2	2.23	0.74
1:BBB:136:ARG:HD3	1:BBB:138:PHE:CE2	2.22	0.74
1:BBB:130:TRP:CZ3	1:BBB:215:ARG:HD2	2.23	0.74
1:BBB:311:ASN:O	1:BBB:370:TYR:CE2	2.41	0.73
1:CCC:361:ARG:NH2	1:CCC:421:ASP:HB2	2.04	0.73
1:BBB:75:GLU:HG3	3:BBB:849:HOH:O	1.90	0.72
1:DDD:511:GLN:NE2	1:DDD:518:LEU:H	1.88	0.72
1:CCC:187:TRP:CZ2	1:CCC:279:MSE:CE	2.73	0.72
1:BBB:441:THR:HG21	1:BBB:466:TYR:HB2	1.71	0.72
1:DDD:441:THR:HG21	1:DDD:466:TYR:HB2	1.72	0.72
1:CCC:441:THR:HG21	1:CCC:466:TYR:HB2	1.71	0.72
1:AAA:441:THR:HG21	1:AAA:466:TYR:HB2	1.71	0.71
1:CCC:511:GLN:NE2	1:CCC:518:LEU:H	1.88	0.71
1:CCC:225:ILE:HG22	1:CCC:249:PHE:HB2	1.73	0.71
1:BBB:311:ASN:O	1:BBB:370:TYR:CD2	2.44	0.70
1:CCC:628:ASP:O	1:CCC:630:THR:HG22	1.91	0.70
1:BBB:501:PRO:HB3	2:BBB:705:ACT:CH3	2.21	0.70
1:BBB:511:GLN:NE2	1:BBB:518:LEU:H	1.89	0.70
1:AAA:511:GLN:NE2	1:AAA:518:LEU:H	1.89	0.70
1:AAA:500:ILE:CB	1:AAA:505:LEU:CD2	2.68	0.69
1:DDD:225:ILE:HG22	1:DDD:249:PHE:HB2	1.73	0.69
1:BBB:501:PRO:HB3	2:BBB:705:ACT:H3	1.74	0.69
1:BBB:187:TRP:CE2	1:BBB:279:MSE:CG	2.77	0.68
1:BBB:108:LEU:HD21	1:BBB:214:PHE:HZ	1.58	0.68
1:AAA:500:ILE:CG2	1:AAA:505:LEU:HD23	2.24	0.68
1:BBB:225:ILE:HG22	1:BBB:249:PHE:HB2	1.74	0.68
1:CCC:156:TRP:O	1:CCC:160:THR:HB	1.93	0.68
1:BBB:130:TRP:CH2	1:BBB:215:ARG:HD2	2.29	0.67
1:AAA:225:ILE:HG22	1:AAA:249:PHE:HB2	1.76	0.66
1:DDD:255:THR:HG22	1:DDD:264:ILE:HD11	1.77	0.66
1:BBB:108:LEU:HD21	1:BBB:214:PHE:CZ	2.32	0.65
1:BBB:210:LEU:O	1:BBB:214:PHE:O	2.15	0.65
1:BBB:130:TRP:O	1:BBB:215:ARG:NH1	2.29	0.64
1:CCC:632:ILE:HD11	1:CCC:638:THR:HG23	1.78	0.64
1:AAA:77:PRO:HG2	1:AAA:101:ALA:HB1	1.80	0.64
1:DDD:647:ARG:HG3	1:DDD:654:GLU:HB2	1.80	0.64
1:CCC:543:ARG:HH22	2:CCC:706:ACT:C	2.11	0.64
1:DDD:449:ARG:HB2	2:DDD:702:ACT:H1	1.80	0.64
1:AAA:543:ARG:NH2	2:AAA:707:ACT:OXT	2.30	0.63
1:CCC:647:ARG:HG3	1:CCC:654:GLU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:543:ARG:NH1	2:AAA:707:ACT:OXT	2.31	0.63
1:BBB:160:THR:HG22	1:BBB:162:ILE:H	1.62	0.63
1:CCC:160:THR:HG22	1:CCC:162:ILE:N	2.14	0.63
1:CCC:643:ASN:N	1:CCC:643:ASN:OD1	2.31	0.62
1:BBB:217:ASN:HB2	3:BBB:842:HOH:O	2.00	0.62
1:AAA:53:VAL:HG11	1:AAA:333:GLY:HA2	1.81	0.62
1:BBB:209:ILE:O	1:BBB:213:GLY:CA	2.47	0.62
1:CCC:86:ILE:HD13	1:CCC:213:GLY:HA3	1.81	0.62
1:BBB:543:ARG:HH12	2:BBB:705:ACT:C	2.12	0.62
1:AAA:361:ARG:CZ	1:AAA:421:ASP:HB2	2.30	0.61
1:AAA:108:LEU:HD11	1:AAA:214:PHE:CE2	2.36	0.61
1:DDD:619:GLN:HE21	1:DDD:619:GLN:CA	2.13	0.61
1:AAA:407:VAL:HG22	1:AAA:412:MSE:HG3	1.82	0.61
1:DDD:419:GLU:HG3	3:DDD:807:HOH:O	2.01	0.61
1:BBB:156:TRP:O	1:BBB:160:THR:HB	2.02	0.60
1:DDD:407:VAL:HG22	1:DDD:412:MSE:HG3	1.83	0.60
1:BBB:160:THR:HG22	1:BBB:162:ILE:HG22	1.83	0.60
1:AAA:632:ILE:HD11	1:AAA:638:THR:HG23	1.82	0.59
1:CCC:355:GLU:HB3	3:CCC:808:HOH:O	2.02	0.59
1:CCC:594:TRP:HA	1:CCC:599:GLY:O	2.03	0.59
1:DDD:594:TRP:HA	1:DDD:599:GLY:O	2.03	0.59
1:AAA:594:TRP:HA	1:AAA:599:GLY:O	2.03	0.58
1:BBB:638:THR:CG2	1:BBB:647:ARG:HG2	2.16	0.58
1:DDD:339:ARG:NH1	1:DDD:343:GLN:HG2	2.15	0.58
1:DDD:619:GLN:HA	1:DDD:619:GLN:HE21	1.68	0.58
1:BBB:140:GLU:HB2	1:BBB:220:ARG:HG2	1.86	0.58
1:BBB:86:ILE:N	1:BBB:86:ILE:HD12	2.19	0.58
1:DDD:647:ARG:CZ	1:DDD:654:GLU:HB3	2.34	0.58
1:AAA:207:ALA:HB3	1:AAA:208:PRO:HD3	1.86	0.58
1:BBB:594:TRP:HA	1:BBB:599:GLY:O	2.04	0.58
1:BBB:312:GLY:HA2	1:BBB:367:SER:N	2.15	0.57
1:AAA:434:ARG:HD2	1:AAA:436:TYR:OH	2.04	0.57
1:CCC:207:ALA:HB3	1:CCC:208:PRO:HD3	1.87	0.57
1:DDD:543:ARG:HH12	2:DDD:707:ACT:H2	1.70	0.57
1:AAA:140:GLU:HB2	1:AAA:220:ARG:HG2	1.87	0.57
1:CCC:449:ARG:HB2	2:CCC:702:ACT:H1	1.87	0.57
1:DDD:194:LYS:HD2	1:DDD:196:TYR:OH	2.04	0.57
1:DDD:207:ALA:HB3	1:DDD:208:PRO:HD3	1.86	0.57
1:AAA:500:ILE:HG21	1:AAA:505:LEU:HD23	1.88	0.56
1:AAA:70:LYS:HE2	1:CCC:429:ASP:OD2	2.05	0.56
1:BBB:209:ILE:O	1:BBB:213:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:140:GLU:HB2	1:DDD:220:ARG:HG2	1.88	0.56
1:CCC:160:THR:HG23	1:CCC:372:GLN:HG2	1.88	0.56
1:CCC:140:GLU:HB2	1:CCC:220:ARG:HG2	1.87	0.56
1:CCC:53:VAL:HG11	1:CCC:333:GLY:HA2	1.87	0.56
1:CCC:511:GLN:HE22	1:CCC:518:LEU:H	1.53	0.56
1:BBB:511:GLN:HE22	1:BBB:518:LEU:H	1.54	0.56
1:CCC:181:SER:O	1:CCC:279:MSE:HE1	2.06	0.56
1:CCC:407:VAL:HG22	1:CCC:412:MSE:HG3	1.88	0.56
1:BBB:207:ALA:HB3	1:BBB:208:PRO:HD3	1.87	0.55
1:BBB:618:GLU:HA	1:BBB:623:GLY:O	2.06	0.55
1:CCC:618:GLU:HA	1:CCC:623:GLY:O	2.06	0.55
1:DDD:511:GLN:HE22	1:DDD:518:LEU:H	1.54	0.55
1:DDD:507:ALA:HB2	1:DDD:549:SER:HB3	1.87	0.55
1:AAA:511:GLN:HE22	1:AAA:518:LEU:H	1.53	0.55
1:AAA:500:ILE:CG2	1:AAA:505:LEU:CD2	2.84	0.55
1:DDD:618:GLU:HA	1:DDD:623:GLY:O	2.07	0.55
1:DDD:225:ILE:HA	1:DDD:249:PHE:O	2.07	0.55
1:BBB:73:VAL:HG21	1:DDD:429:ASP:OD2	2.07	0.55
1:AAA:618:GLU:HA	1:AAA:623:GLY:O	2.06	0.54
1:CCC:543:ARG:NH2	2:CCC:706:ACT:OXT	2.31	0.54
1:BBB:53:VAL:HG11	1:BBB:333:GLY:HA2	1.89	0.54
1:DDD:638:THR:HG22	1:DDD:647:ARG:HB3	1.88	0.54
1:CCC:552:VAL:HG13	1:CCC:557:SER:CB	2.38	0.54
1:BBB:434:ARG:HD2	1:BBB:436:TYR:OH	2.07	0.54
1:DDD:552:VAL:HG13	1:DDD:557:SER:CB	2.38	0.54
1:AAA:402:ALA:H	2:AAA:705:ACT:H1	1.72	0.53
1:BBB:632:ILE:HD11	1:BBB:638:THR:HG23	1.89	0.53
1:CCC:434:ARG:HD2	1:CCC:436:TYR:OH	2.08	0.53
1:BBB:280:TRP:O	1:BBB:287:ARG:HB2	2.09	0.53
1:AAA:225:ILE:HA	1:AAA:249:PHE:O	2.08	0.53
1:AAA:262:ILE:HG23	3:AAA:836:HOH:O	2.07	0.53
1:CCC:255:THR:HG22	1:CCC:264:ILE:HD11	1.90	0.53
1:CCC:83:TYR:C	3:CCC:813:HOH:O	2.47	0.53
1:CCC:225:ILE:HA	1:CCC:249:PHE:O	2.08	0.53
1:CCC:555:GLU:H	2:CCC:703:ACT:H2	1.73	0.53
1:DDD:434:ARG:HD2	1:DDD:436:TYR:OH	2.07	0.53
1:CCC:260:MSE:HE3	1:CCC:260:MSE:HA	1.91	0.53
1:DDD:501:PRO:HB3	2:DDD:707:ACT:H1	1.91	0.53
1:AAA:487:GLY:HA2	1:AAA:505:LEU:CD1	2.38	0.53
1:BBB:108:LEU:HD11	1:BBB:214:PHE:CE1	2.44	0.53
1:CCC:501:PRO:HB3	2:CCC:706:ACT:OXT	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:225:ILE:HA	1:BBB:249:PHE:O	2.09	0.52
1:BBB:62:THR:HG22	1:BBB:266:ALA:HB1	1.90	0.52
1:CCC:187:TRP:CZ2	1:CCC:279:MSE:HE2	2.44	0.52
1:BBB:552:VAL:HG13	1:BBB:557:SER:CB	2.40	0.52
1:AAA:389:SER:O	1:AAA:393:ARG:HG3	2.10	0.52
1:AAA:361:ARG:NH2	1:AAA:421:ASP:HB2	2.23	0.52
1:DDD:361:ARG:HH21	1:DDD:421:ASP:HB2	1.73	0.52
1:AAA:255:THR:HG22	1:AAA:264:ILE:HD11	1.92	0.51
1:DDD:86:ILE:HD13	1:DDD:213:GLY:HA3	1.92	0.51
1:DDD:139:PRO:HB2	1:DDD:386:LEU:HD13	1.93	0.51
1:DDD:389:SER:O	1:DDD:393:ARG:HG3	2.11	0.51
1:DDD:409:ASP:OD1	1:DDD:409:ASP:N	2.42	0.51
1:BBB:150:ILE:HD12	1:BBB:152:GLU:HB2	1.93	0.51
1:CCC:637:GLN:N	1:CCC:637:GLN:HE21	2.09	0.51
1:DDD:259:GLY:O	1:DDD:262:ILE:HG12	2.10	0.51
1:AAA:615:LYS:CE	1:AAA:657:ARG:NH1	2.74	0.51
1:BBB:389:SER:O	1:BBB:393:ARG:HG3	2.11	0.51
1:AAA:259:GLY:O	1:AAA:262:ILE:HG12	2.12	0.50
1:CCC:259:GLY:O	1:CCC:262:ILE:HG12	2.10	0.50
1:AAA:478:ARG:HG2	1:AAA:478:ARG:O	2.10	0.50
1:CCC:389:SER:O	1:CCC:393:ARG:HG3	2.11	0.50
1:AAA:139:PRO:HB2	1:AAA:386:LEU:HD13	1.92	0.50
1:AAA:552:VAL:HG13	1:AAA:557:SER:CB	2.41	0.50
1:BBB:311:ASN:N	1:BBB:311:ASN:OD1	2.43	0.50
1:AAA:62:THR:HG22	1:AAA:266:ALA:HB1	1.94	0.50
1:BBB:194:LYS:HD2	1:BBB:196:TYR:OH	2.12	0.50
1:AAA:108:LEU:HD21	1:AAA:214:PHE:CZ	2.47	0.50
1:CCC:495:THR:HG21	1:CCC:520:TYR:HB2	1.93	0.49
1:BBB:294:LYS:HD2	1:BBB:348:ARG:HD2	1.93	0.49
1:DDD:255:THR:HG22	1:DDD:264:ILE:CD1	2.42	0.49
1:CCC:150:ILE:HD12	1:CCC:152:GLU:HB2	1.93	0.49
1:BBB:259:GLY:O	1:BBB:262:ILE:HG12	2.12	0.49
1:AAA:615:LYS:HE2	1:AAA:657:ARG:NH1	2.27	0.49
1:BBB:139:PRO:HB2	1:BBB:386:LEU:HD13	1.94	0.49
1:BBB:495:THR:HG21	1:BBB:520:TYR:HB2	1.95	0.49
1:AAA:449:ARG:HB2	2:AAA:702:ACT:H1	1.95	0.49
1:DDD:150:ILE:HD12	1:DDD:152:GLU:HB2	1.95	0.49
1:AAA:543:ARG:CZ	2:AAA:707:ACT:OXT	2.62	0.48
1:BBB:476:ASP:OD1	1:BBB:478:ARG:HG2	2.13	0.48
1:CCC:139:PRO:HB2	1:CCC:386:LEU:HD13	1.94	0.48
1:AAA:280:TRP:O	1:AAA:287:ARG:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:134:PRO:HA	1:BBB:215:ARG:CZ	2.42	0.48
1:DDD:417:THR:HG22	1:DDD:418:ASN:N	2.28	0.48
1:AAA:243:PHE:O	1:AAA:303:LYS:HE3	2.13	0.48
1:AAA:495:THR:HG21	1:AAA:520:TYR:HB2	1.95	0.48
1:CCC:223:THR:HA	1:CCC:247:GLY:O	2.14	0.48
1:DDD:495:THR:HG21	1:DDD:520:TYR:HB2	1.95	0.48
1:BBB:223:THR:HA	1:BBB:247:GLY:O	2.14	0.47
1:BBB:160:THR:OG1	1:BBB:372:GLN:HB2	2.13	0.47
1:CCC:187:TRP:HZ2	1:CCC:279:MSE:CE	2.22	0.47
1:CCC:62:THR:HG22	1:CCC:266:ALA:HB1	1.96	0.47
1:AAA:223:THR:HA	1:AAA:247:GLY:O	2.15	0.47
1:AAA:150:ILE:HB	3:AAA:806:HOH:O	2.14	0.47
1:BBB:543:ARG:HH12	2:BBB:705:ACT:CH3	2.28	0.47
1:DDD:262:ILE:HG23	3:DDD:821:HOH:O	2.14	0.47
1:BBB:409:ASP:N	1:BBB:409:ASP:OD1	2.43	0.47
1:DDD:223:THR:HA	1:DDD:247:GLY:O	2.14	0.47
1:DDD:62:THR:HG22	1:DDD:266:ALA:HB1	1.96	0.47
1:CCC:361:ARG:HH21	1:CCC:421:ASP:HB2	1.78	0.47
1:BBB:501:PRO:CB	2:BBB:705:ACT:CH3	2.93	0.47
1:BBB:80:GLU:HG2	3:BBB:836:HOH:O	2.15	0.47
1:CCC:94:ARG:HD2	3:CCC:848:HOH:O	2.14	0.47
1:CCC:279:MSE:HG2	1:CCC:280:TRP:CD1	2.50	0.46
1:DDD:279:MSE:HE3	1:DDD:280:TRP:CE3	2.49	0.46
1:AAA:500:ILE:O	1:AAA:505:LEU:HD11	2.14	0.46
1:DDD:136:ARG:O	1:DDD:215:ARG:HD2	2.15	0.46
1:DDD:342:SER:O	1:DDD:346:VAL:HG23	2.15	0.46
1:DDD:476:ASP:OD1	1:DDD:478:ARG:HG2	2.15	0.46
1:DDD:445:GLY:H	2:DDD:706:ACT:H2	1.79	0.46
1:AAA:150:ILE:HD12	1:AAA:152:GLU:HB2	1.97	0.46
1:AAA:363:SER:HA	1:AAA:426:LYS:HE3	1.96	0.46
1:AAA:487:GLY:HA2	1:AAA:505:LEU:HD12	1.98	0.46
1:AAA:500:ILE:CB	1:AAA:505:LEU:HD23	2.44	0.46
1:CCC:118:ARG:HH12	1:CCC:194:LYS:HE2	1.79	0.46
1:DDD:260:MSE:HE3	1:DDD:260:MSE:HA	1.98	0.46
1:AAA:279:MSE:HG2	1:AAA:280:TRP:CD1	2.50	0.46
1:DDD:181:SER:HB3	1:DDD:268:LEU:HD22	1.98	0.46
1:AAA:361:ARG:NH2	1:AAA:421:ASP:H	2.14	0.46
1:BBB:134:PRO:CA	1:BBB:215:ARG:HH12	2.05	0.46
1:BBB:579:ILE:HG12	1:BBB:583:ALA:HA	1.98	0.46
1:AAA:504:MSE:HA	1:AAA:549:SER:OG	2.16	0.45
1:BBB:342:SER:O	1:BBB:346:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:631:ALA:HA	1:CCC:637:GLN:HA	1.97	0.45
1:AAA:279:MSE:HE3	1:AAA:280:TRP:CE3	2.50	0.45
1:AAA:579:ILE:HG12	1:AAA:583:ALA:HA	1.98	0.45
1:BBB:311:ASN:HD21	1:BBB:362:PRO:HA	1.82	0.45
1:CCC:173:VAL:HG12	1:CCC:175:LEU:HD11	1.98	0.45
1:CCC:342:SER:O	1:CCC:346:VAL:HG23	2.16	0.45
1:AAA:342:SER:O	1:AAA:346:VAL:HG23	2.15	0.45
1:CCC:255:THR:HG22	1:CCC:264:ILE:CD1	2.46	0.45
1:CCC:579:ILE:HG12	1:CCC:583:ALA:HA	1.98	0.45
1:CCC:181:SER:HB3	1:CCC:268:LEU:HD22	1.99	0.45
1:CCC:476:ASP:OD1	1:CCC:478:ARG:HG2	2.15	0.45
1:AAA:127:PRO:HG3	1:AAA:138:PHE:CG	2.52	0.45
1:BBB:504:MSE:HA	1:BBB:549:SER:OG	2.17	0.45
1:AAA:450:ILE:HG21	1:AAA:482:VAL:CG2	2.47	0.45
1:BBB:127:PRO:HG3	1:BBB:138:PHE:CG	2.52	0.45
1:BBB:187:TRP:CE2	1:BBB:279:MSE:HG2	2.51	0.45
1:AAA:253:LEU:HA	1:AAA:293:PRO:HG2	1.99	0.45
1:BBB:648:GLN:HA	1:BBB:652:ARG:O	2.17	0.45
1:BBB:543:ARG:NH1	2:BBB:705:ACT:H2	2.32	0.45
1:CCC:558:LYS:O	1:CCC:562:GLU:HG3	2.17	0.45
1:AAA:309:SER:HB3	1:AAA:339:ARG:HD3	1.97	0.44
1:DDD:253:LEU:HA	1:DDD:293:PRO:HG2	1.99	0.44
1:CCC:140:GLU:OE1	1:CCC:216:SER:OG	2.21	0.44
1:AAA:500:ILE:CB	1:AAA:505:LEU:HD21	2.14	0.44
1:DDD:647:ARG:HH22	1:DDD:656:SER:CB	2.31	0.44
1:AAA:639:ILE:O	1:AAA:639:ILE:HG23	2.18	0.44
1:AAA:260:MSE:HB2	1:AAA:261:PRO:HD3	2.00	0.44
1:AAA:648:GLN:HA	1:AAA:652:ARG:O	2.17	0.44
1:BBB:253:LEU:HA	1:BBB:293:PRO:HG2	1.98	0.44
1:AAA:398:ALA:HA	1:AAA:399:PRO:HD3	1.89	0.44
1:BBB:558:LYS:O	1:BBB:562:GLU:HG3	2.17	0.44
1:CCC:253:LEU:HA	1:CCC:293:PRO:HG2	1.99	0.44
1:CCC:504:MSE:HA	1:CCC:549:SER:OG	2.18	0.44
1:CCC:638:THR:CG2	1:CCC:647:ARG:HB3	2.48	0.44
1:DDD:76:LEU:HD13	1:DDD:107:ILE:HG12	1.99	0.44
1:DDD:113:ALA:HB3	1:DDD:205:GLU:OE2	2.18	0.44
1:CCC:384:ASN:ND2	3:CCC:802:HOH:O	2.46	0.44
1:DDD:558:LYS:O	1:DDD:562:GLU:HG3	2.17	0.44
1:AAA:173:VAL:HG12	1:AAA:175:LEU:HD11	2.00	0.43
1:AAA:558:LYS:O	1:AAA:562:GLU:HG3	2.17	0.43
1:BBB:173:VAL:HG12	1:BBB:175:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:127:PRO:HG3	1:DDD:138:PHE:CG	2.53	0.43
1:DDD:560:TYR:OH	1:DDD:572:PRO:HD3	2.18	0.43
1:DDD:579:ILE:HG12	1:DDD:583:ALA:HA	2.00	0.43
1:AAA:140:GLU:OE1	1:AAA:216:SER:OG	2.21	0.43
1:BBB:212:LYS:NZ	3:BBB:804:HOH:O	2.50	0.43
1:BBB:546:ASN:OD1	1:BBB:548:GLN:NE2	2.51	0.43
1:CCC:260:MSE:HB2	1:CCC:261:PRO:HD3	2.00	0.43
1:DDD:53:VAL:HG21	1:DDD:333:GLY:HA2	2.00	0.43
1:DDD:648:GLN:HA	1:DDD:652:ARG:O	2.18	0.43
1:CCC:560:TYR:OH	1:CCC:572:PRO:HD3	2.18	0.43
1:DDD:279:MSE:HG2	1:DDD:280:TRP:CD1	2.53	0.43
1:AAA:332:VAL:O	1:AAA:336:VAL:HG23	2.19	0.43
1:AAA:560:TYR:OH	1:AAA:572:PRO:HD3	2.18	0.43
1:BBB:532:LEU:HD12	1:BBB:543:ARG:HD2	2.00	0.43
1:BBB:560:TYR:OH	1:BBB:572:PRO:HD3	2.18	0.43
1:CCC:332:VAL:O	1:CCC:336:VAL:HG23	2.19	0.43
1:DDD:188:GLU:OE1	1:DDD:287:ARG:HD3	2.18	0.43
1:BBB:639:ILE:O	1:BBB:639:ILE:HG23	2.19	0.43
1:BBB:543:ARG:HH12	2:BBB:705:ACT:H2	1.83	0.43
1:CCC:76:LEU:HD13	1:CCC:107:ILE:HG12	2.00	0.43
1:AAA:500:ILE:HB	1:AAA:505:LEU:HD23	1.91	0.43
1:DDD:552:VAL:HG13	1:DDD:557:SER:HA	2.01	0.43
1:DDD:632:ILE:HD11	1:DDD:638:THR:HG23	2.01	0.43
1:DDD:555:GLU:H	2:DDD:703:ACT:H2	1.84	0.43
1:AAA:256:THR:HG23	1:AAA:292:ASP:HB2	2.01	0.43
1:AAA:500:ILE:HG22	1:AAA:505:LEU:HG	2.01	0.43
1:BBB:450:ILE:HG21	1:BBB:482:VAL:CG2	2.48	0.43
1:CCC:127:PRO:HG3	1:CCC:138:PHE:CG	2.53	0.43
1:CCC:450:ILE:HG21	1:CCC:482:VAL:CG2	2.48	0.43
1:DDD:543:ARG:HH12	2:DDD:707:ACT:CH3	2.30	0.43
1:AAA:255:THR:HG22	1:AAA:264:ILE:CD1	2.49	0.43
1:CCC:194:LYS:HD2	1:CCC:196:TYR:CE1	2.54	0.43
1:CCC:260:MSE:CE	1:CCC:260:MSE:HA	2.49	0.43
1:AAA:638:THR:CG2	1:AAA:647:ARG:HG2	2.42	0.43
1:CCC:449:ARG:HD3	1:CCC:449:ARG:HA	1.87	0.42
1:DDD:450:ILE:HG21	1:DDD:482:VAL:CG2	2.48	0.42
1:BBB:113:ALA:HB3	1:BBB:205:GLU:OE2	2.18	0.42
1:CCC:280:TRP:O	1:CCC:287:ARG:HB3	2.18	0.42
1:BBB:205:GLU:C	1:BBB:208:PRO:HD2	2.40	0.42
1:CCC:628:ASP:O	1:CCC:630:THR:CG2	2.64	0.42
1:AAA:181:SER:HB3	1:AAA:268:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:113:ALA:HB3	1:AAA:205:GLU:OE2	2.20	0.42
1:AAA:488:SER:N	1:AAA:505:LEU:HD11	2.35	0.42
1:BBB:367:SER:OG	1:BBB:368:TRP:N	2.52	0.42
1:BBB:225:ILE:HD11	1:BBB:368:TRP:CZ3	2.55	0.42
1:DDD:417:THR:CG2	1:DDD:418:ASN:N	2.82	0.42
1:DDD:632:ILE:HD11	1:DDD:638:THR:CG2	2.49	0.42
1:DDD:639:ILE:O	1:DDD:639:ILE:HG23	2.19	0.42
1:AAA:260:MSE:HE1	1:AAA:337:ILE:HG23	2.02	0.42
1:AAA:260:MSE:HA	1:AAA:260:MSE:HE3	2.00	0.42
1:AAA:552:VAL:HG13	1:AAA:557:SER:HA	2.01	0.42
1:BBB:332:VAL:O	1:BBB:336:VAL:HG23	2.19	0.42
1:CCC:639:ILE:HG23	1:CCC:639:ILE:O	2.20	0.42
1:DDD:407:VAL:CG1	1:DDD:407:VAL:O	2.67	0.42
1:BBB:108:LEU:HD11	1:BBB:214:PHE:CZ	2.55	0.42
1:BBB:256:THR:HG23	1:BBB:292:ASP:HB2	2.02	0.42
1:CCC:256:THR:HG23	1:CCC:292:ASP:HB2	2.02	0.42
1:CCC:260:MSE:HE1	1:CCC:337:ILE:HG23	2.01	0.42
1:AAA:407:VAL:O	1:AAA:407:VAL:CG1	2.68	0.42
1:CCC:648:GLN:HA	1:CCC:652:ARG:O	2.19	0.42
1:BBB:181:SER:HB3	1:BBB:268:LEU:HD22	2.01	0.42
1:BBB:214:PHE:N	1:BBB:214:PHE:CD1	2.87	0.42
1:CCC:144:LEU:HB3	1:CCC:184:TYR:CE2	2.55	0.42
1:CCC:165:TYR:CE1	1:CCC:376:THR:HG22	2.55	0.42
1:DDD:173:VAL:HG12	1:DDD:175:LEU:HD11	2.01	0.42
1:DDD:260:MSE:HB2	1:DDD:261:PRO:HD3	2.02	0.42
1:DDD:280:TRP:O	1:DDD:287:ARG:HB3	2.20	0.42
1:AAA:205:GLU:C	1:AAA:208:PRO:HD2	2.40	0.41
1:CCC:403:ILE:HD12	1:CCC:419:GLU:HG2	2.01	0.41
1:BBB:190:PRO:O	1:DDD:355:GLU:HG3	2.20	0.41
1:CCC:205:GLU:C	1:CCC:208:PRO:HD2	2.41	0.41
1:BBB:287:ARG:HH21	1:BBB:290:GLU:CD	2.23	0.41
1:CCC:113:ALA:HB3	1:CCC:205:GLU:OE2	2.20	0.41
1:DDD:205:GLU:C	1:DDD:208:PRO:HD2	2.40	0.41
1:DDD:225:ILE:HD11	1:DDD:368:TRP:CZ3	2.55	0.41
1:BBB:552:VAL:HG13	1:BBB:557:SER:HA	2.02	0.41
1:CCC:181:SER:O	1:CCC:279:MSE:CE	2.67	0.41
1:CCC:260:MSE:HE1	1:CCC:337:ILE:CG2	2.50	0.41
1:DDD:398:ALA:HA	1:DDD:399:PRO:HD3	1.89	0.41
1:BBB:144:LEU:HB3	1:BBB:184:TYR:CE2	2.55	0.41
1:BBB:555:GLU:H	2:BBB:703:ACT:H2	1.84	0.41
1:CCC:367:SER:OG	1:CCC:368:TRP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:140:GLU:OE1	1:DDD:216:SER:OG	2.22	0.41
1:AAA:502:GLY:O	1:AAA:505:LEU:HB2	2.21	0.41
1:BBB:118:ARG:HB2	3:DDD:832:HOH:O	2.20	0.41
1:CCC:50:SER:OG	1:CCC:340:MSE:SE	2.89	0.41
1:DDD:256:THR:HG23	1:DDD:292:ASP:HB2	2.01	0.41
1:BBB:88:GLY:HA3	1:BBB:212:LYS:HZ2	1.84	0.41
1:DDD:460:PRO:HB3	1:DDD:466:TYR:CE1	2.56	0.41
1:AAA:144:LEU:HB3	1:AAA:184:TYR:CE2	2.55	0.41
1:BBB:108:LEU:CD2	1:BBB:214:PHE:HZ	2.28	0.41
1:BBB:638:THR:CG2	1:BBB:647:ARG:CG	2.90	0.41
1:DDD:332:VAL:O	1:DDD:336:VAL:HG23	2.20	0.41
1:AAA:501:PRO:O	1:AAA:505:LEU:HG	2.21	0.41
1:DDD:532:LEU:HD12	1:DDD:543:ARG:HD2	2.02	0.41
1:BBB:407:VAL:O	1:BBB:407:VAL:CG1	2.69	0.41
1:CCC:407:VAL:CG1	1:CCC:407:VAL:O	2.68	0.41
1:DDD:144:LEU:HB3	1:DDD:184:TYR:CE2	2.55	0.41
1:AAA:367:SER:OG	1:AAA:368:TRP:N	2.53	0.40
1:AAA:441:THR:HG21	1:AAA:466:TYR:CB	2.48	0.40
1:CCC:471:GLU:OE2	2:CCC:702:ACT:OXT	2.40	0.40
1:BBB:155:GLY:HA2	1:BBB:158:ILE:HD12	2.03	0.40
1:CCC:225:ILE:HD11	1:CCC:368:TRP:CZ3	2.56	0.40
1:DDD:417:THR:HG21	1:DDD:420:TYR:HD2	1.86	0.40
1:DDD:622:TYR:OH	1:DDD:655:GLU:HB3	2.21	0.40
1:AAA:297:VAL:HG21	1:AAA:349:ALA:HB2	2.03	0.40
1:CCC:160:THR:CG2	1:CCC:161:ASN:N	2.84	0.40
1:DDD:417:THR:HG21	1:DDD:420:TYR:CD2	2.56	0.40
1:CCC:80:GLU:O	1:CCC:100:TRP:HD1	2.05	0.40
1:DDD:543:ARG:HH22	2:DDD:707:ACT:C	2.34	0.40
1:CCC:552:VAL:HG13	1:CCC:557:SER:HA	2.03	0.40

All (1) 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:650:ASN:HD21	1:CCC:258:ALA:H[2_555]	1.31	0.29

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	585/620 (94%)	546 (93%)	37 (6%)	2 (0%)	41	72
1	BBB	586/620 (94%)	546 (93%)	38 (6%)	2 (0%)	41	72
1	CCC	585/620 (94%)	543 (93%)	40 (7%)	2 (0%)	41	72
1	DDD	585/620 (94%)	543 (93%)	40 (7%)	2 (0%)	41	72
All	All	2341/2480 (94%)	2178 (93%)	155 (7%)	8 (0%)	41	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	512	ASP
1	BBB	512	ASP
1	CCC	512	ASP
1	CCC	629	GLN
1	DDD	512	ASP
1	BBB	632	ILE
1	DDD	632	ILE
1	AAA	632	ILE

5.3.2 Protein sidechains [i](#)

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	459/470 (98%)	444 (97%)	15 (3%)	38	72
1	BBB	459/470 (98%)	442 (96%)	17 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CCC	459/470 (98%)	443 (96%)	16 (4%)	36	70
1	DDD	459/470 (98%)	443 (96%)	16 (4%)	36	70
All	All	1836/1880 (98%)	1772 (96%)	64 (4%)	36	70

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	185	SER
1	AAA	212	LYS
1	AAA	215	ARG
1	AAA	294	LYS
1	AAA	308	SER
1	AAA	309	SER
1	AAA	339	ARG
1	AAA	343	GLN
1	AAA	390	THR
1	AAA	409	ASP
1	AAA	470	SER
1	AAA	514	GLU
1	AAA	552	VAL
1	AAA	643	ASN
1	AAA	648	GLN
1	BBB	160	THR
1	BBB	185	SER
1	BBB	215	ARG
1	BBB	279	MSE
1	BBB	294	LYS
1	BBB	308	SER
1	BBB	311	ASN
1	BBB	337	ILE
1	BBB	339	ARG
1	BBB	340	MSE
1	BBB	409	ASP
1	BBB	470	SER
1	BBB	478	ARG
1	BBB	514	GLU
1	BBB	552	VAL
1	BBB	619	GLN
1	BBB	657	ARG
1	CCC	160	THR
1	CCC	185	SER

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Mol	Chain	Res	Type
1	CCC	212	LYS
1	CCC	287	ARG
1	CCC	294	LYS
1	CCC	308	SER
1	CCC	339	ARG
1	CCC	470	SER
1	CCC	478	ARG
1	CCC	514	GLU
1	CCC	552	VAL
1	CCC	630	THR
1	CCC	637	GLN
1	CCC	638	THR
1	CCC	643	ASN
1	CCC	652	ARG
1	DDD	185	SER
1	DDD	287	ARG
1	DDD	294	LYS
1	DDD	308	SER
1	DDD	339	ARG
1	DDD	409	ASP
1	DDD	470	SER
1	DDD	478	ARG
1	DDD	514	GLU
1	DDD	547	ASN
1	DDD	549	SER
1	DDD	552	VAL
1	DDD	619	GLN
1	DDD	643	ASN
1	DDD	648	GLN
1	DDD	657	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	ACT	BBB	704	-	1,3,3	4.21	1 (100%)	0,3,3	0.00	-
2	ACT	CCC	705	-	1,3,3	5.53	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	703	-	1,3,3	4.23	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	701	-	1,3,3	4.41	1 (100%)	0,3,3	0.00	-
2	ACT	CCC	702	-	1,3,3	5.34	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	704	-	1,3,3	4.66	1 (100%)	0,3,3	0.00	-
2	ACT	CCC	706	-	1,3,3	3.04	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	705	-	1,3,3	2.49	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	702	-	1,3,3	5.56	1 (100%)	0,3,3	0.00	-
2	ACT	CCC	704	-	1,3,3	4.48	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	706	-	1,3,3	5.53	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	705	-	1,3,3	3.91	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	707	-	1,3,3	4.37	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	707	-	1,3,3	5.14	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	703	-	1,3,3	4.54	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	705	-	1,3,3	4.63	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	702	-	1,3,3	5.85	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	701	-	1,3,3	3.56	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	706	-	1,3,3	4.95	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	701	-	1,3,3	4.24	1 (100%)	0,3,3	0.00	-
2	ACT	AAA	704	-	1,3,3	4.55	1 (100%)	0,3,3	0.00	-
2	ACT	CCC	701	-	1,3,3	4.37	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	CCC	703	-	1,3,3	4.44	1 (100%)	0,3,3	0.00	-
2	ACT	DDD	703	-	1,3,3	4.55	1 (100%)	0,3,3	0.00	-
2	ACT	BBB	702	-	1,3,3	5.19	1 (100%)	0,3,3	0.00	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	702	ACT	CH3-C	5.85	1.56	1.48
2	DDD	702	ACT	CH3-C	5.56	1.55	1.48
2	CCC	705	ACT	CH3-C	5.53	1.55	1.48
2	DDD	706	ACT	CH3-C	5.53	1.55	1.48
2	CCC	702	ACT	CH3-C	5.34	1.55	1.48
2	BBB	702	ACT	CH3-C	5.19	1.55	1.48
2	AAA	707	ACT	CH3-C	5.14	1.55	1.48
2	AAA	706	ACT	CH3-C	4.95	1.55	1.48
2	DDD	704	ACT	CH3-C	4.66	1.54	1.48
2	AAA	705	ACT	CH3-C	4.63	1.54	1.48
2	AAA	704	ACT	CH3-C	4.55	1.54	1.48
2	DDD	703	ACT	CH3-C	4.55	1.54	1.48
2	BBB	703	ACT	CH3-C	4.54	1.54	1.48
2	CCC	704	ACT	CH3-C	4.48	1.54	1.48
2	CCC	703	ACT	CH3-C	4.44	1.54	1.48
2	AAA	701	ACT	CH3-C	4.41	1.54	1.48
2	CCC	701	ACT	CH3-C	4.37	1.54	1.48
2	DDD	707	ACT	CH3-C	4.37	1.54	1.48
2	DDD	701	ACT	CH3-C	4.24	1.54	1.48
2	AAA	703	ACT	CH3-C	4.23	1.54	1.48
2	BBB	704	ACT	CH3-C	4.21	1.54	1.48
2	DDD	705	ACT	CH3-C	3.91	1.53	1.48
2	BBB	701	ACT	CH3-C	3.56	1.53	1.48
2	CCC	706	ACT	CH3-C	3.04	1.52	1.48
2	BBB	705	ACT	CH3-C	2.49	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	702	ACT	2	0
2	CCC	706	ACT	3	0
2	BBB	705	ACT	7	0
2	DDD	702	ACT	1	0
2	DDD	706	ACT	1	0
2	DDD	707	ACT	4	0
2	AAA	707	ACT	4	0
2	BBB	703	ACT	1	0
2	AAA	705	ACT	1	0
2	AAA	702	ACT	1	0
2	CCC	703	ACT	1	0
2	DDD	703	ACT	1	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

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	579/620 (93%)	0.54	28 (4%) 30 21	32, 52, 74, 109	0
1	BBB	580/620 (93%)	0.56	23 (3%) 38 28	32, 55, 78, 95	0
1	CCC	579/620 (93%)	0.55	21 (3%) 42 32	33, 52, 79, 117	0
1	DDD	579/620 (93%)	0.70	59 (10%) 6 3	34, 55, 102, 133	0
All	All	2317/2480 (93%)	0.59	131 (5%) 23 15	32, 54, 83, 133	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	616	GLY	6.1
1	DDD	603	ILE	6.0
1	DDD	639	ILE	6.0
1	AAA	505	LEU	5.2
1	DDD	614	ALA	5.2
1	DDD	615	LYS	5.0
1	AAA	233	VAL	4.9
1	DDD	609	PHE	4.3
1	DDD	605	HIS	4.3
1	DDD	632	ILE	4.0
1	DDD	580	ASN	3.8
1	AAA	406	ALA	3.6
1	DDD	617	TRP	3.6
1	DDD	579	ILE	3.5
1	DDD	541	VAL	3.5
1	BBB	360	PHE	3.3
1	DDD	624	PHE	3.2
1	AAA	657	ARG	3.2
1	DDD	297	VAL	3.2
1	CCC	603	ILE	3.1
1	DDD	571	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	202	LEU	3.0
1	BBB	354	VAL	3.0
1	BBB	590	GLY	3.0
1	DDD	525	ALA	3.0
1	DDD	534	GLN	3.0
1	CCC	580	ASN	3.0
1	DDD	547	ASN	2.9
1	BBB	612	TRP	2.9
1	CCC	652	ARG	2.8
1	AAA	565	ILE	2.8
1	DDD	631	ALA	2.8
1	DDD	49	SER	2.8
1	DDD	596	ALA	2.8
1	DDD	588	GLU	2.8
1	DDD	592	ILE	2.8
1	BBB	61	VAL	2.7
1	AAA	617	TRP	2.7
1	DDD	542	PHE	2.7
1	DDD	602	VAL	2.7
1	BBB	602	VAL	2.7
1	DDD	574	GLY	2.7
1	BBB	406	ALA	2.6
1	BBB	579	ILE	2.6
1	CCC	507	ALA	2.6
1	CCC	303	LYS	2.6
1	DDD	532	LEU	2.6
1	DDD	578	LEU	2.6
1	DDD	549	SER	2.6
1	BBB	443	ALA	2.5
1	DDD	642	GLN	2.5
1	DDD	591	ASN	2.5
1	AAA	360	PHE	2.5
1	BBB	609	PHE	2.5
1	CCC	579	ILE	2.5
1	DDD	600	ALA	2.5
1	BBB	362	PRO	2.5
1	DDD	124	LEU	2.5
1	CCC	611	ALA	2.4
1	CCC	604	LEU	2.4
1	CCC	602	VAL	2.4
1	AAA	443	ALA	2.4
1	AAA	300	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	354	VAL	2.4
1	DDD	585	GLN	2.4
1	DDD	648	GLN	2.4
1	BBB	600	ALA	2.4
1	BBB	611	ALA	2.4
1	CCC	233	VAL	2.4
1	DDD	251	GLY	2.4
1	DDD	594	TRP	2.4
1	DDD	637	GLN	2.3
1	AAA	435	ALA	2.3
1	AAA	225	ILE	2.3
1	AAA	561	ALA	2.3
1	DDD	507	ALA	2.3
1	CCC	524	ALA	2.3
1	DDD	118	ARG	2.3
1	DDD	657	ARG	2.3
1	AAA	249	PHE	2.3
1	BBB	283	VAL	2.3
1	CCC	542	PHE	2.3
1	DDD	566	PHE	2.3
1	BBB	578	LEU	2.3
1	CCC	510	THR	2.3
1	DDD	303	LYS	2.3
1	DDD	655	GLU	2.3
1	AAA	306	TYR	2.3
1	CCC	593	TYR	2.2
1	AAA	592	ILE	2.2
1	BBB	365	VAL	2.2
1	AAA	609	PHE	2.2
1	CCC	590	GLY	2.2
1	BBB	639	ILE	2.2
1	DDD	621	GLU	2.2
1	AAA	596	ALA	2.2
1	DDD	236	ALA	2.2
1	CCC	609	PHE	2.2
1	AAA	61	VAL	2.2
1	BBB	617	TRP	2.2
1	AAA	584	PHE	2.2
1	DDD	622	TYR	2.2
1	DDD	222	ILE	2.2
1	AAA	612	TRP	2.2
1	DDD	582	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	555	GLU	2.1
1	DDD	575	ASN	2.1
1	BBB	62	THR	2.1
1	DDD	619	GLN	2.1
1	DDD	299	LYS	2.1
1	CCC	222	ILE	2.1
1	DDD	500	ILE	2.1
1	AAA	595	SER	2.1
1	DDD	652	ARG	2.1
1	AAA	195	ASN	2.1
1	DDD	142	TRP	2.1
1	AAA	554	GLY	2.1
1	BBB	539	GLY	2.1
1	DDD	654	GLU	2.0
1	DDD	233	VAL	2.0
1	AAA	466	TYR	2.0
1	CCC	600	ALA	2.0
1	AAA	557	SER	2.0
1	BBB	147	LEU	2.0
1	CCC	297	VAL	2.0
1	BBB	603	ILE	2.0
1	CCC	592	ILE	2.0
1	DDD	611	ALA	2.0
1	BBB	584	PHE	2.0
1	CCC	243	PHE	2.0
1	AAA	422	VAL	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no 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
2	ACT	AAA	707	4/4	0.64	0.27	52,54,60,75	0
2	ACT	CCC	706	4/4	0.73	0.39	46,49,51,57	0
2	ACT	BBB	705	4/4	0.77	0.36	45,49,53,53	0
2	ACT	DDD	706	4/4	0.79	0.22	60,60,60,63	0
2	ACT	AAA	706	4/4	0.83	0.21	44,45,45,47	0
2	ACT	CCC	701	4/4	0.83	0.18	54,54,58,60	0
2	ACT	BBB	703	4/4	0.84	0.23	31,34,36,36	0
2	ACT	DDD	702	4/4	0.85	0.20	41,46,46,46	0
2	ACT	DDD	707	4/4	0.86	0.30	38,38,39,40	0
2	ACT	CCC	702	4/4	0.89	0.23	23,26,26,26	0
2	ACT	BBB	701	4/4	0.89	0.19	35,35,36,37	0
2	ACT	AAA	702	4/4	0.90	0.20	30,32,32,32	0
2	ACT	AAA	703	4/4	0.90	0.20	29,30,30,31	0
2	ACT	BBB	702	4/4	0.90	0.18	36,37,37,38	0
2	ACT	BBB	704	4/4	0.91	0.21	51,53,55,57	0
2	ACT	AAA	701	4/4	0.91	0.26	38,38,39,40	0
2	ACT	CCC	705	4/4	0.91	0.25	40,44,44,44	0
2	ACT	CCC	703	4/4	0.92	0.17	38,38,40,43	0
2	ACT	DDD	701	4/4	0.92	0.14	41,42,44,45	0
2	ACT	AAA	705	4/4	0.93	0.16	41,42,44,44	0
2	ACT	DDD	703	4/4	0.93	0.12	40,40,43,46	0
2	ACT	DDD	705	4/4	0.93	0.22	44,48,48,48	0
2	ACT	DDD	704	4/4	0.94	0.15	48,51,52,53	0
2	ACT	CCC	704	4/4	0.94	0.14	44,44,47,50	0
2	ACT	AAA	704	4/4	0.95	0.12	45,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.