



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2021 – 06:13 pm GMT

PDB ID : 7NZB
Title : Mutant V517L of the SH3 domain of JNK-interacting protein 1 (JIP1)
Authors : Perez, L.M.; Ielasi, F.S.; Jensen, M.R.; Palencia, A.
Deposited on : 2021-03-23
Resolution : 1.96 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.24
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

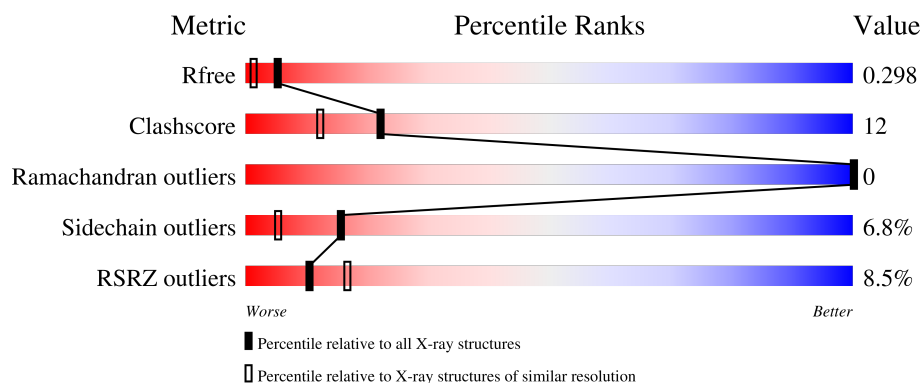
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	63	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	BBB	63	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>10%</div> <div>5%</div> </div> </div>
1	CCC	63	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>
1	DDD	63	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div> </div>
1	EEE	63	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	63	<div><div></div><div>14%</div><div>67%</div><div>27%</div><div>5%</div><div></div></div>
1	GGG	63	<div><div></div><div>8%</div><div>73%</div><div>19%</div><div>5%</div><div></div></div>
1	HHH	63	<div><div></div><div>8%</div><div>75%</div><div>17%</div><div>5%</div><div></div></div>
1	III	63	<div><div></div><div>10%</div><div>76%</div><div>19%</div><div></div><div></div></div>
1	JJJ	63	<div><div></div><div>5%</div><div>71%</div><div>17%</div><div>6%</div><div>5%</div></div>
1	KKK	63	<div><div></div><div>16%</div><div>62%</div><div>30%</div><div>6%</div><div></div></div>
1	LLL	63	<div><div></div><div>13%</div><div>73%</div><div>16%</div><div>5%</div><div>6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6835 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 SH3 domain of JNK-interacting protein 1 (JIP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	61	Total	C	N	O	S	0	0	0
			519	333	85	99	2			
1	BBB	60	Total	C	N	O	S	0	0	0
			506	325	83	97	1			
1	CCC	63	Total	C	N	O	S	0	0	0
			533	341	89	101	2			
1	DDD	60	Total	C	N	O	S	0	0	0
			511	328	84	98	1			
1	EEE	62	Total	C	N	O	S	0	0	0
			524	336	86	100	2			
1	FFF	62	Total	C	N	O	S	0	0	0
			524	336	86	100	2			
1	GGG	61	Total	C	N	O	S	0	0	0
			519	333	85	99	2			
1	HHH	61	Total	C	N	O	S	0	0	0
			514	330	84	98	2			
1	III	62	Total	C	N	O	S	0	0	0
			521	334	86	100	1			
1	JJJ	60	Total	C	N	O	S	0	0	0
			509	327	83	97	2			
1	KKK	62	Total	C	N	O	S	0	0	0
			524	336	86	100	2			
1	LLL	59	Total	C	N	O	S	0	0	0
			500	322	82	94	2			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	487	GLY	-	expression tag	UNP Q9UQF2
AAA	488	HIS	-	expression tag	UNP Q9UQF2
AAA	489	MET	-	expression tag	UNP Q9UQF2
AAA	517	LEU	VAL	engineered mutation	UNP Q9UQF2
BBB	487	GLY	-	expression tag	UNP Q9UQF2

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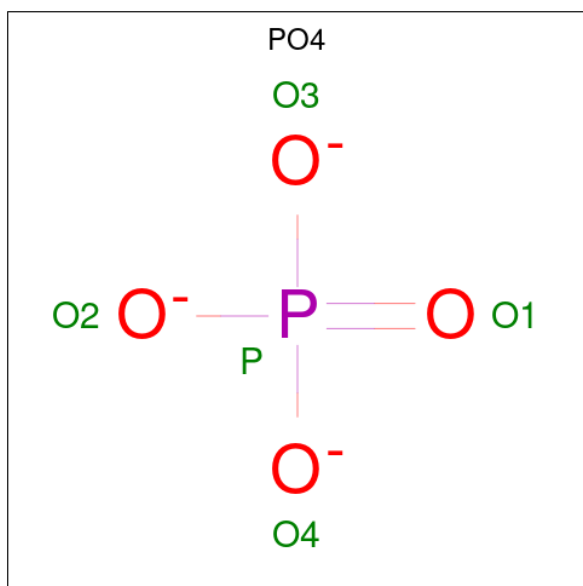
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	488	HIS	-	expression tag	UNP Q9UQF2
BBB	489	MET	-	expression tag	UNP Q9UQF2
BBB	517	LEU	VAL	engineered mutation	UNP Q9UQF2
CCC	487	GLY	-	expression tag	UNP Q9UQF2
CCC	488	HIS	-	expression tag	UNP Q9UQF2
CCC	489	MET	-	expression tag	UNP Q9UQF2
CCC	517	LEU	VAL	engineered mutation	UNP Q9UQF2
DDD	487	GLY	-	expression tag	UNP Q9UQF2
DDD	488	HIS	-	expression tag	UNP Q9UQF2
DDD	489	MET	-	expression tag	UNP Q9UQF2
DDD	517	LEU	VAL	engineered mutation	UNP Q9UQF2
EEE	487	GLY	-	expression tag	UNP Q9UQF2
EEE	488	HIS	-	expression tag	UNP Q9UQF2
EEE	489	MET	-	expression tag	UNP Q9UQF2
EEE	517	LEU	VAL	engineered mutation	UNP Q9UQF2
FFF	487	GLY	-	expression tag	UNP Q9UQF2
FFF	488	HIS	-	expression tag	UNP Q9UQF2
FFF	489	MET	-	expression tag	UNP Q9UQF2
FFF	517	LEU	VAL	engineered mutation	UNP Q9UQF2
GGG	487	GLY	-	expression tag	UNP Q9UQF2
GGG	488	HIS	-	expression tag	UNP Q9UQF2
GGG	489	MET	-	expression tag	UNP Q9UQF2
GGG	517	LEU	VAL	engineered mutation	UNP Q9UQF2
HHH	487	GLY	-	expression tag	UNP Q9UQF2
HHH	488	HIS	-	expression tag	UNP Q9UQF2
HHH	489	MET	-	expression tag	UNP Q9UQF2
HHH	517	LEU	VAL	engineered mutation	UNP Q9UQF2
III	487	GLY	-	expression tag	UNP Q9UQF2
III	488	HIS	-	expression tag	UNP Q9UQF2
III	489	MET	-	expression tag	UNP Q9UQF2
III	517	LEU	VAL	engineered mutation	UNP Q9UQF2
JJJ	487	GLY	-	expression tag	UNP Q9UQF2
JJJ	488	HIS	-	expression tag	UNP Q9UQF2
JJJ	489	MET	-	expression tag	UNP Q9UQF2
JJJ	517	LEU	VAL	engineered mutation	UNP Q9UQF2
KKK	487	GLY	-	expression tag	UNP Q9UQF2
KKK	488	HIS	-	expression tag	UNP Q9UQF2
KKK	489	MET	-	expression tag	UNP Q9UQF2
KKK	517	LEU	VAL	engineered mutation	UNP Q9UQF2
LLL	487	GLY	-	expression tag	UNP Q9UQF2
LLL	488	HIS	-	expression tag	UNP Q9UQF2
LLL	489	MET	-	expression tag	UNP Q9UQF2

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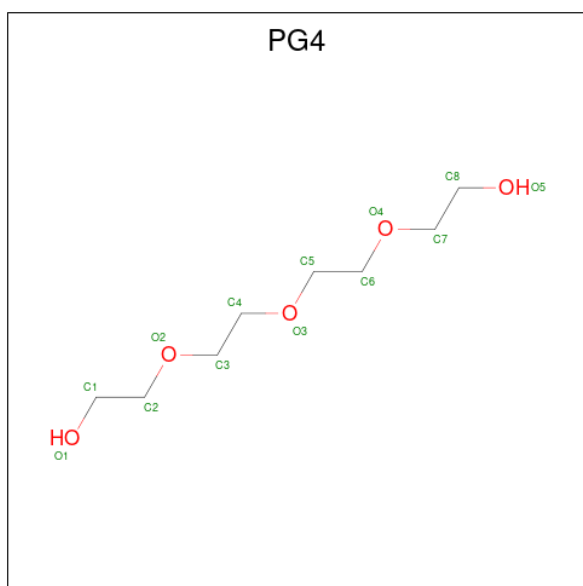
Chain	Residue	Modelled	Actual	Comment	Reference
LLL	517	LEU	VAL	engineered mutation	UNP Q9UQF2

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 13 8 5	0	0
3	DDD	1	Total C O 13 8 5	0	0
3	FFF	1	Total C O 13 8 5	0	0
3	KKK	1	Total C O 13 8 5	0	0

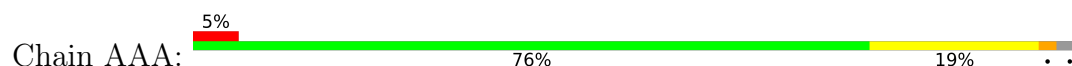
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	59	Total O 59 59	0	0
4	BBB	41	Total O 41 41	0	0
4	CCC	49	Total O 49 49	0	0
4	DDD	49	Total O 49 49	0	0
4	EEE	59	Total O 59 59	0	0
4	FFF	46	Total O 46 46	0	0
4	GGG	37	Total O 37 37	0	0
4	HHH	58	Total O 58 58	0	0
4	III	42	Total O 42 42	0	0
4	JJJ	36	Total O 36 36	0	0
4	KKK	58	Total O 58 58	0	0
4	LLL	40	Total O 40 40	0	0

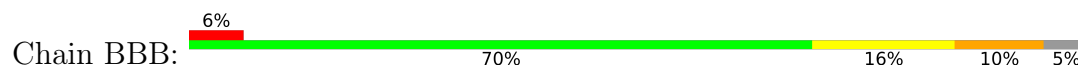
3 Residue-property plots

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: SH3 domain of JNK-interacting protein 1 (JIP1)



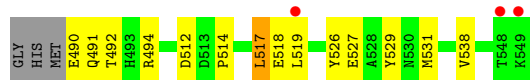
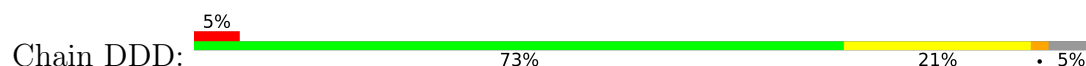
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



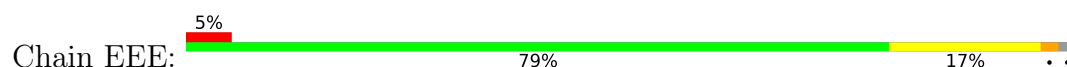
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



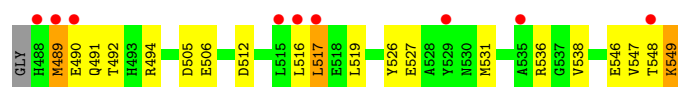
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



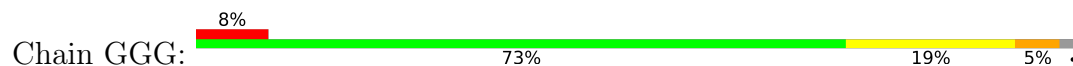
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



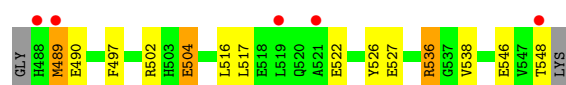
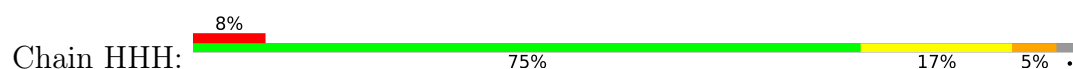
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



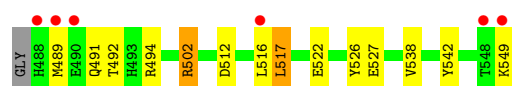
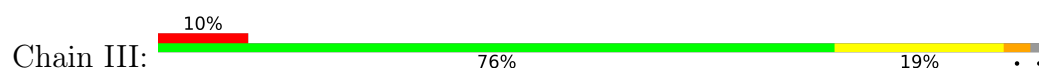
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



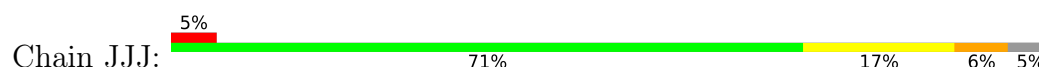
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



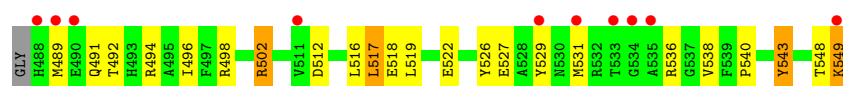
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



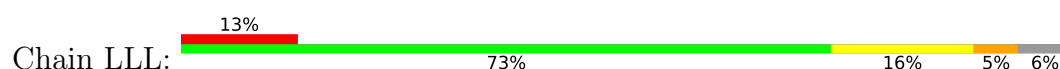
- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



- Molecule 1: SH3 domain of JNK-interacting protein 1 (JIP1)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.84Å 149.72Å 68.09Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	67.66 – 1.96 67.66 – 1.96	Depositor EDS
% Data completeness (in resolution range)	86.8 (67.66-1.96) 86.8 (67.66-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.95Å)	Xtriage
Refinement program	REFMAC 7.1.007	Depositor
R, R_{free}	0.225 , 0.281 0.242 , 0.298	Depositor DCC
R_{free} test set	2330 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.46 % 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 5.8139e-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: PG4, PO4

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	0.94	2/533 (0.4%)	1.08	1/722 (0.1%)
1	BBB	1.05	3/520 (0.6%)	1.01	1/708 (0.1%)
1	CCC	0.87	1/548 (0.2%)	1.01	0/742
1	DDD	0.94	0/525	0.96	0/712
1	EEE	1.04	2/538 (0.4%)	1.02	0/729
1	FFF	0.77	1/538 (0.2%)	0.91	0/729
1	GGG	0.82	0/533	0.92	0/722
1	HHH	0.94	2/528 (0.4%)	1.05	1/718 (0.1%)
1	III	0.89	0/535	1.01	1/726 (0.1%)
1	JJJ	0.89	2/523 (0.4%)	1.01	0/711
1	KKK	0.82	1/538 (0.2%)	1.01	1/729 (0.1%)
1	LLL	0.92	1/513 (0.2%)	1.04	0/696
All	All	0.91	15/6372 (0.2%)	1.00	5/8644 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	518	GLU	CD-OE1	9.07	1.35	1.25
1	HHH	504	GLU	CD-OE1	7.84	1.34	1.25
1	BBB	527	GLU	CD-OE2	6.54	1.32	1.25
1	LLL	506	GLU	CD-OE1	6.35	1.32	1.25
1	BBB	518	GLU	CD-OE2	6.27	1.32	1.25
1	CCC	527	GLU	CD-OE2	5.85	1.32	1.25
1	JJJ	504	GLU	CD-OE1	5.83	1.32	1.25
1	EEE	546	GLU	CD-OE1	5.58	1.31	1.25
1	BBB	504	GLU	CD-OE1	5.56	1.31	1.25
1	AAA	510	GLU	CD-OE1	5.51	1.31	1.25
1	KKK	522	GLU	CD-OE2	5.49	1.31	1.25
1	HHH	546	GLU	CD-OE2	-5.47	1.19	1.25
1	AAA	504	GLU	CD-OE2	5.46	1.31	1.25
1	FFF	506	GLU	CD-OE2	-5.29	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	JJJ	504	GLU	CD-OE2	5.18	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	536	ARG	CB-CG-CD	5.70	126.41	111.60
1	AAA	524	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	BBB	502	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	III	502	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	KKK	543	TYR	CB-CG-CD2	5.07	124.04	121.00

There are no chirality outliers.

There are no planarity outliers.

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	519	0	485	11	0
1	BBB	506	0	465	9	0
1	CCC	533	0	495	6	0
1	DDD	511	0	476	17	0
1	EEE	524	0	487	11	0
1	FFF	524	0	487	25	0
1	GGG	519	0	485	12	0
1	HHH	514	0	474	8	1
1	III	521	0	480	10	0
1	JJJ	509	0	472	13	1
1	KKK	524	0	487	30	0
1	LLL	500	0	465	10	0
2	AAA	5	0	0	0	0
3	BBB	13	0	18	1	0
3	DDD	13	0	18	0	0
3	FFF	13	0	18	3	0
3	KKK	13	0	18	2	0
4	AAA	59	0	0	5	0
4	BBB	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CCC	49	0	0	0	0
4	DDD	49	0	0	1	0
4	EEE	59	0	0	3	0
4	FFF	46	0	0	5	0
4	GGG	37	0	0	2	0
4	HHH	58	0	0	2	1
4	III	42	0	0	1	0
4	JJJ	36	0	0	5	0
4	KKK	58	0	0	7	0
4	LLL	40	0	0	0	0
All	All	6835	0	5830	142	3

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 12.

All (142) 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:FFF:516:LEU:CD1	1:KKK:489:MET:HG3	1.79	1.13
1:FFF:516:LEU:HD13	1:KKK:489:MET:HG3	1.09	1.04
1:JJJ:520:GLN:HB3	4:JJJ:609:HOH:O	1.57	1.02
1:DDD:491:GLN:HB2	1:DDD:531:MET:HE3	1.55	0.85
1:AAA:545:ILE:HD11	1:KKK:512:ASP:OD1	1.77	0.84
1:KKK:543:TYR:CG	4:KKK:740:HOH:O	2.32	0.82
1:HHH:489:MET:O	1:HHH:489:MET:HG2	1.80	0.81
1:AAA:548:THR:N	4:AAA:701:HOH:O	2.15	0.79
3:BBB:601:PG4:O1	3:KKK:601:PG4:O1	2.02	0.78
1:DDD:491:GLN:HB2	1:DDD:531:MET:CE	2.17	0.74
1:JJJ:520:GLN:NE2	4:JJJ:601:HOH:O	2.17	0.73
1:KKK:543:TYR:CD1	4:KKK:740:HOH:O	2.42	0.72
1:EEE:494:ARG:NH1	4:EEE:601:HOH:O	2.23	0.71
1:KKK:543:TYR:CE1	4:KKK:734:HOH:O	2.46	0.68
3:FFF:601:PG4:H62	4:FFF:726:HOH:O	1.94	0.68
1:KKK:518:GLU:OE2	1:KKK:536:ARG:CZ	2.44	0.66
1:FFF:516:LEU:CD1	1:KKK:489:MET:CG	2.68	0.66
1:FFF:489:MET:HG3	1:KKK:516:LEU:HD13	1.80	0.63
1:FFF:494:ARG:HD2	1:FFF:512:ASP:OD1	1.99	0.63
1:AAA:545:ILE:CD1	1:KKK:512:ASP:OD1	2.45	0.63
1:KKK:543:TYR:CD2	4:KKK:740:HOH:O	2.52	0.62
1:FFF:516:LEU:HD13	1:KKK:489:MET:CG	2.05	0.62
1:CCC:534:GLY:O	1:FFF:505:ASP:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:493:HIS:HE1	4:JJJ:616:HOH:O	1.82	0.61
1:FFF:549:LYS:NZ	4:FFF:701:HOH:O	2.32	0.60
1:GGG:496:ILE:O	4:GGG:601:HOH:O	2.17	0.60
1:KKK:498:ARG:HB2	4:KKK:702:HOH:O	2.02	0.60
1:FFF:549:LYS:HE3	1:JJJ:512:ASP:OD2	2.02	0.59
1:DDD:491:GLN:CB	1:DDD:531:MET:CE	2.80	0.59
1:DDD:494:ARG:HD2	1:DDD:512:ASP:OD1	2.03	0.58
1:FFF:489:MET:HE1	1:FFF:531:MET:HG2	1.87	0.57
1:HHH:489:MET:HG3	1:HHH:516:LEU:HD12	1.84	0.57
1:EEE:522:GLU:OE2	1:HHH:502:ARG:NH2	2.33	0.57
1:KKK:494:ARG:HD3	1:KKK:512:ASP:OD1	2.06	0.55
1:III:489:MET:HA	1:III:516:LEU:HD11	1.88	0.55
1:KKK:540:PRO:HD2	4:KKK:740:HOH:O	2.06	0.55
1:III:549:LYS:HB3	4:III:627:HOH:O	2.06	0.55
1:LLL:494:ARG:HD3	1:LLL:512:ASP:OD1	2.06	0.55
1:HHH:489:MET:O	1:HHH:489:MET:CG	2.54	0.55
1:III:494:ARG:HD3	1:III:512:ASP:OD1	2.07	0.54
1:DDD:491:GLN:HA	1:DDD:531:MET:HE1	1.90	0.53
1:AAA:547:VAL:CA	4:AAA:701:HOH:O	2.57	0.53
1:LLL:517:LEU:HD22	1:LLL:528:ALA:HB2	1.90	0.53
3:FFF:601:PG4:H12	4:FFF:726:HOH:O	2.08	0.53
1:FFF:512:ASP:OD2	1:JJJ:547:VAL:HG13	2.09	0.52
1:BBB:494:ARG:HD3	1:BBB:512:ASP:OD1	2.09	0.52
1:EEE:522:GLU:HG2	1:GGG:519:LEU:CD2	2.40	0.52
1:KKK:498:ARG:N	4:KKK:702:HOH:O	2.41	0.51
1:LLL:526:TYR:O	1:LLL:538:VAL:HA	2.11	0.51
1:HHH:527:GLU:HG2	4:HHH:623:HOH:O	2.10	0.51
1:FFF:526:TYR:O	1:FFF:538:VAL:HA	2.11	0.51
1:JJJ:526:TYR:O	1:JJJ:538:VAL:HA	2.11	0.51
1:III:526:TYR:O	1:III:538:VAL:HA	2.11	0.51
1:FFF:536:ARG:HH22	1:KKK:489:MET:C	2.14	0.51
1:GGG:494:ARG:HD3	1:GGG:512:ASP:OD1	2.10	0.50
1:AAA:517:LEU:HD22	1:AAA:528:ALA:HB2	1.91	0.50
1:AAA:526:TYR:O	1:AAA:538:VAL:HA	2.11	0.50
3:FFF:601:PG4:H82	4:FFF:726:HOH:O	2.12	0.50
1:DDD:514:PRO:HB2	1:DDD:531:MET:CE	2.42	0.50
1:DDD:491:GLN:CB	1:DDD:531:MET:HE1	2.41	0.49
1:HHH:526:TYR:O	1:HHH:538:VAL:HA	2.12	0.49
1:KKK:526:TYR:O	1:KKK:538:VAL:HA	2.13	0.49
1:DDD:526:TYR:O	1:DDD:538:VAL:HA	2.12	0.49
1:LLL:520:GLN:HB3	1:LLL:526:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:503:HIS:CE1	4:AAA:702:HOH:O	2.65	0.49
1:CCC:519:LEU:HB3	1:CCC:527:GLU:HG3	1.95	0.49
1:GGG:526:TYR:O	1:GGG:538:VAL:HA	2.12	0.49
1:DDD:519:LEU:HB3	1:DDD:527:GLU:HG3	1.95	0.48
1:III:542:TYR:CD2	1:JJJ:497:PHE:HB3	2.48	0.48
1:DDD:491:GLN:HG3	1:DDD:531:MET:HE1	1.94	0.48
1:BBB:526:TYR:O	1:BBB:538:VAL:HA	2.12	0.48
1:EEE:526:TYR:O	1:EEE:538:VAL:HA	2.13	0.48
1:JJJ:517:LEU:HD11	1:JJJ:526:TYR:HB3	1.95	0.48
1:DDD:514:PRO:HB2	1:DDD:531:MET:HE2	1.95	0.48
1:EEE:545:ILE:HD11	1:III:512:ASP:OD1	2.14	0.48
1:KKK:491:GLN:HE22	1:KKK:494:ARG:CZ	2.27	0.48
1:CCC:526:TYR:O	1:CCC:538:VAL:HA	2.13	0.48
1:BBB:517:LEU:HD11	1:BBB:526:TYR:HB3	1.95	0.47
1:DDD:491:GLN:CB	1:DDD:531:MET:HE3	2.37	0.47
1:KKK:492:THR:OG1	1:KKK:517:LEU:HB2	2.14	0.47
1:DDD:491:GLN:HE22	1:DDD:494:ARG:CZ	2.28	0.47
1:FFF:491:GLN:HE22	1:FFF:494:ARG:CZ	2.28	0.47
1:DDD:517:LEU:HD11	1:DDD:526:TYR:HB3	1.98	0.46
1:EEE:517:LEU:HD22	1:EEE:528:ALA:HB2	1.97	0.46
1:KKK:517:LEU:HD11	1:KKK:526:TYR:HB3	1.96	0.46
1:GGG:491:GLN:HE22	1:GGG:494:ARG:CZ	2.29	0.46
1:DDD:492:THR:OG1	1:DDD:517:LEU:HB2	2.15	0.46
1:FFF:489:MET:SD	1:KKK:529:TYR:CE2	3.08	0.45
1:FFF:489:MET:CE	1:FFF:531:MET:HG2	2.46	0.45
1:FFF:492:THR:OG1	1:FFF:517:LEU:HB2	2.16	0.45
4:FFF:718:HOH:O	1:KKK:531:MET:HB3	2.16	0.45
1:EEE:517:LEU:HD11	1:EEE:526:TYR:HB3	1.99	0.45
1:AAA:547:VAL:HA	4:AAA:701:HOH:O	2.14	0.45
1:GGG:510:GLU:HG3	1:GGG:532:ARG:HH22	1.81	0.44
1:KKK:502:ARG:NH1	1:LLL:538:VAL:HG11	2.32	0.44
1:EEE:488:HIS:N	4:EEE:606:HOH:O	2.50	0.44
1:FFF:547:VAL:HG12	1:FFF:549:LYS:CG	2.47	0.44
1:FFF:547:VAL:CG1	1:FFF:549:LYS:HG2	2.47	0.44
1:III:492:THR:OG1	1:III:517:LEU:HB2	2.18	0.44
1:EEE:488:HIS:N	4:EEE:605:HOH:O	2.49	0.44
1:JJJ:490:GLU:HA	1:JJJ:490:GLU:OE2	2.18	0.44
1:DDD:527:GLU:HB3	4:DDD:712:HOH:O	2.17	0.44
1:III:502:ARG:NH1	4:JJJ:602:HOH:O	2.26	0.44
1:III:491:GLN:HE22	1:III:494:ARG:CZ	2.31	0.43
1:LLL:517:LEU:HD21	1:LLL:526:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:492:THR:OG1	1:BBB:517:LEU:HB2	2.18	0.43
1:GGG:492:THR:OG1	1:GGG:517:LEU:HB2	2.18	0.43
1:CCC:517:LEU:HD11	1:CCC:526:TYR:HB3	2.01	0.43
1:FFF:516:LEU:HD11	1:KKK:489:MET:SD	2.58	0.43
1:AAA:545:ILE:CD1	1:KKK:512:ASP:CG	2.87	0.43
1:III:517:LEU:HD11	1:III:526:TYR:HB3	1.99	0.43
1:JJJ:492:THR:OG1	1:JJJ:517:LEU:HB2	2.18	0.43
1:CCC:492:THR:OG1	1:CCC:517:LEU:HB2	2.18	0.43
1:AAA:503:HIS:CE1	1:BBB:505:ASP:OD1	2.72	0.43
1:CCC:489:MET:HE3	1:CCC:529:TYR:CE2	2.54	0.42
1:LLL:489:MET:HG3	1:LLL:516:LEU:HD12	2.01	0.42
1:JJJ:505:ASP:OD2	4:JJJ:602:HOH:O	2.21	0.42
1:KKK:519:LEU:HB3	1:KKK:527:GLU:HG3	2.01	0.42
1:BBB:519:LEU:HB3	1:BBB:527:GLU:HG3	2.01	0.42
1:FFF:519:LEU:HB3	1:FFF:527:GLU:HG3	2.01	0.42
4:AAA:728:HOH:O	1:KKK:549:LYS:HB3	2.19	0.42
1:BBB:512:ASP:OD2	1:LLL:547:VAL:HA	2.19	0.42
1:FFF:517:LEU:HD11	1:FFF:526:TYR:HB3	2.01	0.42
1:HHH:489:MET:HE1	4:HHH:648:HOH:O	2.20	0.42
1:GGG:549:LYS:HB2	4:GGG:625:HOH:O	2.19	0.41
1:LLL:489:MET:HG3	1:LLL:516:LEU:CD1	2.50	0.41
1:FFF:546:GLU:H	1:FFF:546:GLU:HG3	1.62	0.41
1:EEE:522:GLU:HG2	1:GGG:519:LEU:HD23	2.02	0.41
1:JJJ:522:GLU:HG3	1:JJJ:523:ASP:N	2.36	0.41
1:DDD:518:GLU:OE2	1:DDD:529:TYR:CE2	2.74	0.41
1:GGG:517:LEU:HD11	1:GGG:526:TYR:HB3	2.01	0.41
1:AAA:492:THR:OG1	1:AAA:517:LEU:HB2	2.19	0.41
1:GGG:532:ARG:HE	1:GGG:533:THR:HG23	1.86	0.41
1:JJJ:520:GLN:H	1:JJJ:520:GLN:HG2	1.78	0.41
1:FFF:516:LEU:HD11	1:KKK:489:MET:HG3	1.86	0.41
1:GGG:542:TYR:CD2	1:HHH:497:PHE:HB3	2.56	0.41
1:BBB:497:PHE:HB2	1:BBB:543:TYR:CD2	2.55	0.40
1:LLL:491:GLN:HG2	1:LLL:547:VAL:HG21	2.03	0.40
1:FFF:547:VAL:HG12	1:FFF:549:LYS:HG3	2.01	0.40
1:BBB:490:GLU:OE2	1:BBB:491:GLN:HG3	2.22	0.40
1:EEE:494:ARG:HD3	1:EEE:512:ASP:OD1	2.21	0.40
1:KKK:496:ILE:HD11	3:KKK:601:PG4:H21	2.04	0.40

All (3) 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:JJJ:522:GLU:O	1:JJJ:522:GLU:O[2_656]	1.63	0.57
1:HHH:522:GLU:O	1:HHH:522:GLU:O[2_556]	1.97	0.23
4:HHH:635:HOH:O	4:HHH:635:HOH:O[2_556]	2.11	0.09

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	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
1	BBB	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
1	CCC	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
1	DDD	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
1	EEE	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
1	FFF	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
1	GGG	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
1	HHH	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
1	III	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
1	JJJ	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
1	KKK	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
1	LLL	55/63 (87%)	54 (98%)	1 (2%)	0	100	100
All	All	707/756 (94%)	688 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	53/54 (98%)	51 (96%)	2 (4%)	33	21
1	BBB	51/54 (94%)	46 (90%)	5 (10%)	8	2
1	CCC	54/54 (100%)	53 (98%)	1 (2%)	57	50
1	DDD	52/54 (96%)	50 (96%)	2 (4%)	33	21
1	EEE	53/54 (98%)	51 (96%)	2 (4%)	33	21
1	FFF	53/54 (98%)	48 (91%)	5 (9%)	8	2
1	GGG	53/54 (98%)	49 (92%)	4 (8%)	13	4
1	HHH	52/54 (96%)	46 (88%)	6 (12%)	5	1
1	III	52/54 (96%)	49 (94%)	3 (6%)	20	8
1	JJJ	52/54 (96%)	47 (90%)	5 (10%)	8	2
1	KKK	53/54 (98%)	49 (92%)	4 (8%)	13	4
1	LLL	51/54 (94%)	47 (92%)	4 (8%)	12	3
All	All	629/648 (97%)	586 (93%)	43 (7%)	16	5

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	490	GLU
1	AAA	517	LEU
1	BBB	490	GLU
1	BBB	491	GLN
1	BBB	494	ARG
1	BBB	502	ARG
1	BBB	517	LEU
1	CCC	517	LEU
1	DDD	490	GLU
1	DDD	517	LEU
1	EEE	517	LEU
1	EEE	549	LYS
1	FFF	489	MET
1	FFF	490	GLU
1	FFF	517	LEU
1	FFF	548	THR
1	FFF	549	LYS
1	GGG	517	LEU
1	GGG	532	ARG

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Mol	Chain	Res	Type
1	GGG	536	ARG
1	GGG	549	LYS
1	HHH	489	MET
1	HHH	490	GLU
1	HHH	504	GLU
1	HHH	517	LEU
1	HHH	536	ARG
1	HHH	548	THR
1	III	517	LEU
1	III	522	GLU
1	III	527	GLU
1	JJJ	490	GLU
1	JJJ	504	GLU
1	JJJ	517	LEU
1	JJJ	520	GLN
1	JJJ	527	GLU
1	KKK	502	ARG
1	KKK	517	LEU
1	KKK	548	THR
1	KKK	549	LYS
1	LLL	489	MET
1	LLL	517	LEU
1	LLL	518	GLU
1	LLL	520	GLN

Sometimes 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

5 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	$\# Z > 2$
3	PG4	KKK	601	-	12,12,12	0.28	0	11,11,11	0.25	0
2	PO4	AAA	601	-	4,4,4	0.91	0	6,6,6	0.47	0
3	PG4	DDD	601	-	12,12,12	0.31	0	11,11,11	0.27	0
3	PG4	BBB	601	-	12,12,12	0.29	0	11,11,11	0.26	0
3	PG4	FFF	601	-	12,12,12	0.33	0	11,11,11	0.27	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
3	PG4	KKK	601	-	-	5/10/10/10	-
3	PG4	DDD	601	-	-	6/10/10/10	-
3	PG4	BBB	601	-	-	5/10/10/10	-
3	PG4	FFF	601	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DDD	601	PG4	O3-C5-C6-O4
3	BBB	601	PG4	O3-C5-C6-O4
3	FFF	601	PG4	O2-C3-C4-O3
3	BBB	601	PG4	O1-C1-C2-O2
3	KKK	601	PG4	O1-C1-C2-O2
3	KKK	601	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
3	DDD	601	PG4	O1-C1-C2-O2
3	FFF	601	PG4	O1-C1-C2-O2
3	FFF	601	PG4	O3-C5-C6-O4
3	BBB	601	PG4	O4-C7-C8-O5
3	DDD	601	PG4	O4-C7-C8-O5
3	DDD	601	PG4	O2-C3-C4-O3
3	KKK	601	PG4	C3-C4-O3-C5
3	DDD	601	PG4	C1-C2-O2-C3
3	FFF	601	PG4	C3-C4-O3-C5
3	KKK	601	PG4	C8-C7-O4-C6
3	BBB	601	PG4	C5-C6-O4-C7
3	DDD	601	PG4	C4-C3-O2-C2
3	FFF	601	PG4	C6-C5-O3-C4
3	KKK	601	PG4	C1-C2-O2-C3
3	FFF	601	PG4	C1-C2-O2-C3
3	BBB	601	PG4	C8-C7-O4-C6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	KKK	601	PG4	2	0
3	BBB	601	PG4	1	0
3	FFF	601	PG4	3	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	61/63 (96%)	0.06	3 (4%) 29 39	18, 30, 73, 101	0
1	BBB	60/63 (95%)	0.52	4 (6%) 17 26	19, 42, 73, 119	0
1	CCC	63/63 (100%)	0.21	3 (4%) 30 40	25, 36, 67, 93	0
1	DDD	60/63 (95%)	0.42	3 (5%) 28 39	27, 42, 69, 131	0
1	EEE	62/63 (98%)	0.04	3 (4%) 30 40	20, 31, 62, 89	0
1	FFF	62/63 (98%)	1.13	9 (14%) 2 4	47, 68, 115, 150	0
1	GGG	61/63 (96%)	0.70	5 (8%) 11 18	48, 57, 83, 122	0
1	HHH	61/63 (96%)	0.53	5 (8%) 11 18	35, 43, 71, 99	0
1	III	62/63 (98%)	0.53	6 (9%) 7 12	20, 38, 93, 118	0
1	JJJ	60/63 (95%)	0.41	3 (5%) 28 39	29, 43, 69, 104	0
1	KKK	62/63 (98%)	1.12	10 (16%) 1 2	27, 53, 96, 178	0
1	LLL	59/63 (93%)	0.62	8 (13%) 3 4	19, 39, 98, 115	0
All	All	733/756 (96%)	0.52	62 (8%) 10 17	18, 44, 93, 178	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	KKK	488	HIS	14.3
1	LLL	519	LEU	11.7
1	III	548	THR	10.5
1	BBB	489	MET	9.4
1	FFF	548	THR	7.7
1	FFF	488	HIS	7.2
1	BBB	548	THR	7.0
1	DDD	549	LYS	6.8
1	HHH	488	HIS	6.0
1	KKK	489	MET	6.0
1	III	488	HIS	5.7

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Mol	Chain	Res	Type	RSRZ
1	GGG	548	THR	5.7
1	III	549	LYS	5.4
1	LLL	489	MET	4.9
1	DDD	548	THR	4.7
1	JJJ	489	MET	4.7
1	GGG	549	LYS	4.6
1	KKK	529	TYR	4.6
1	LLL	548	THR	4.5
1	CCC	487	GLY	4.2
1	GGG	489	MET	3.9
1	CCC	548	THR	3.9
1	LLL	518	GLU	3.7
1	LLL	523	ASP	3.7
1	BBB	531	MET	3.6
1	EEE	548	THR	3.5
1	KKK	490	GLU	3.4
1	EEE	549	LYS	3.4
1	KKK	533	THR	3.4
1	III	489	MET	3.3
1	JJJ	548	THR	3.3
1	KKK	535	ALA	3.2
1	CCC	549	LYS	3.2
1	KKK	549	LYS	3.0
1	JJJ	547	VAL	3.0
1	AAA	549	LYS	3.0
1	GGG	490	GLU	2.9
1	EEE	488	HIS	2.9
1	AAA	548	THR	2.9
1	FFF	490	GLU	2.8
1	FFF	516	LEU	2.8
1	AAA	489	MET	2.7
1	DDD	519	LEU	2.7
1	HHH	519	LEU	2.6
1	KKK	511	VAL	2.5
1	HHH	548	THR	2.5
1	HHH	489	MET	2.4
1	FFF	517	LEU	2.4
1	FFF	529	TYR	2.4
1	LLL	492	THR	2.4
1	FFF	535	ALA	2.3
1	III	490	GLU	2.3
1	LLL	524	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	FFF	515	LEU	2.3
1	LLL	547	VAL	2.2
1	III	516	LEU	2.2
1	HHH	521	ALA	2.1
1	FFF	489	MET	2.1
1	BBB	529	TYR	2.1
1	GGG	522	GLU	2.0
1	KKK	534	GLY	2.0
1	KKK	531	MET	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
3	PG4	BBB	601	13/13	0.88	0.20	30,59,81,81	0
3	PG4	DDD	601	13/13	0.90	0.16	35,38,51,52	0
3	PG4	FFF	601	13/13	0.90	0.11	34,36,44,47	0
3	PG4	KKK	601	13/13	0.90	0.15	29,46,69,72	0
2	PO4	AAA	601	5/5	0.94	0.14	59,59,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.