



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 AM GMT

PDB ID : 3E76
Title : Crystal structure of Wild-type GroEL with bound Thallium ions
Authors : Kiser, P.D.; Lorimer, G.H.; Palczewski, K.
Deposited on : 2008-08-17
Resolution : 3.94 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

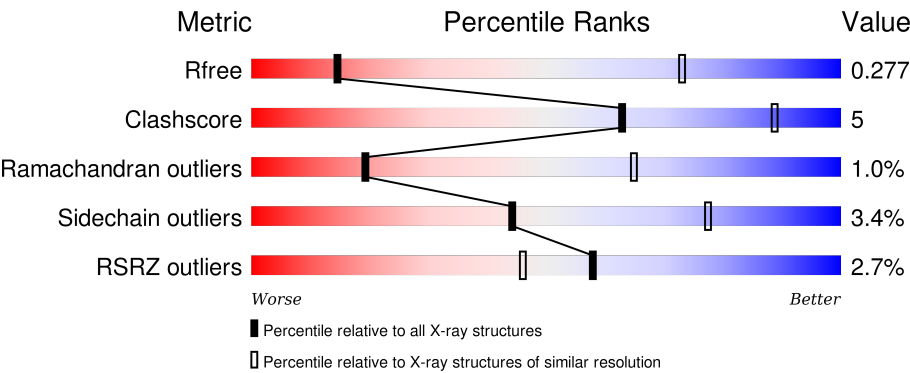
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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.



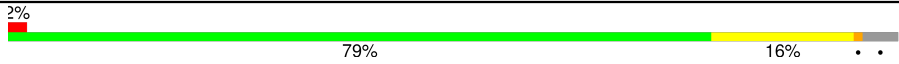

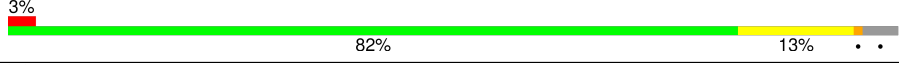



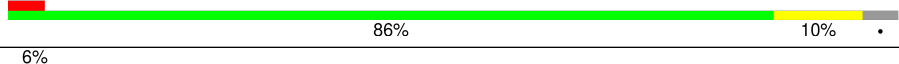

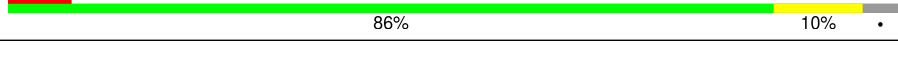
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1007 (4.34-3.54)
Clashscore	102246	1042 (4.30-3.58)
Ramachandran outliers	100387	1000 (4.30-3.58)
Sidechain outliers	100360	1021 (4.32-3.56)
RSRZ outliers	91569	1011 (4.34-3.54)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	547	<div>78%16% . .</div>
1	B	547	<div>82%14% . .</div>
1	C	547	<div>2%82%13% . .</div>
1	D	547	<div>%81%14% . .</div>
1	E	547	<div>2%82%13% . .</div>

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Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

2 Entry composition [i](#)

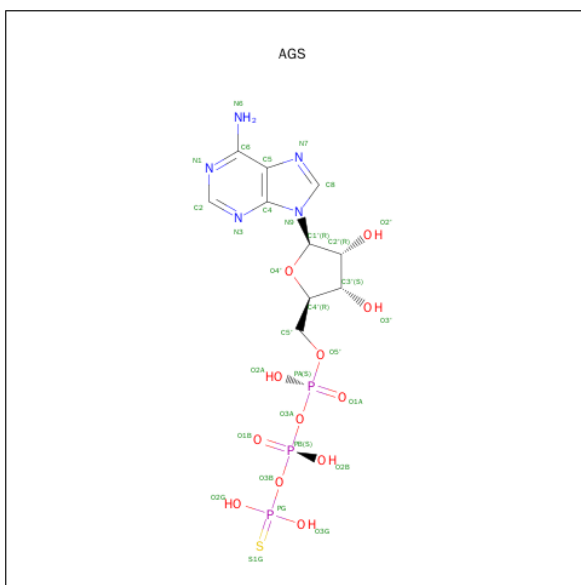
There are 4 unique types of molecules in this entry. The entry contains 54464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 3 is THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Tl 3	0	0
3	J	3	Total 3	Tl 3	0	0
3	D	4	Total 4	Tl 4	0	0
3	K	3	Total 3	Tl 3	0	0
3	E	3	Total 3	Tl 3	0	0
3	H	4	Total 4	Tl 4	0	0
3	B	4	Total 4	Tl 4	0	0
3	I	3	Total 3	Tl 3	0	0
3	C	3	Total 3	Tl 3	0	0
3	A	4	Total 4	Tl 4	0	0
3	N	2	Total 2	Tl 2	0	0
3	L	3	Total 3	Tl 3	0	0
3	F	4	Total 4	Tl 4	0	0
3	M	3	Total 3	Tl 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: Mg) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0

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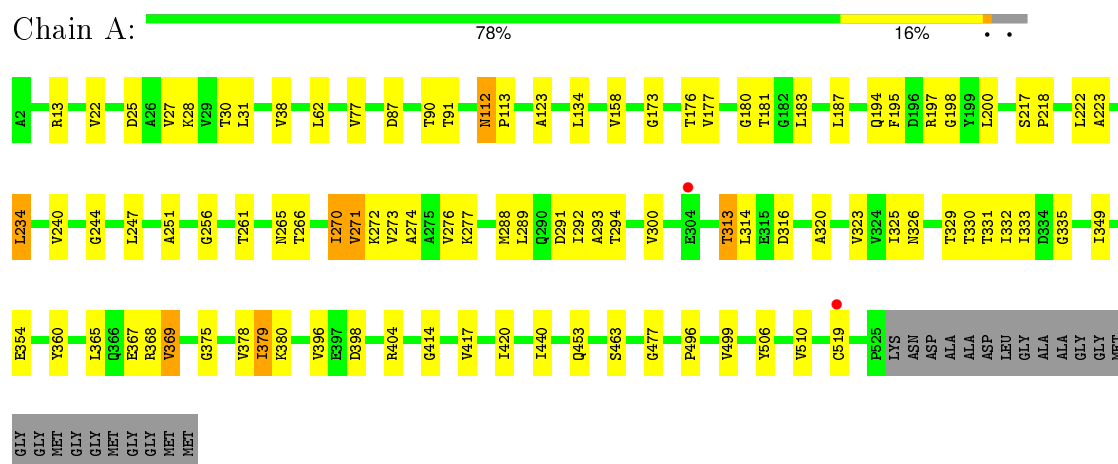
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

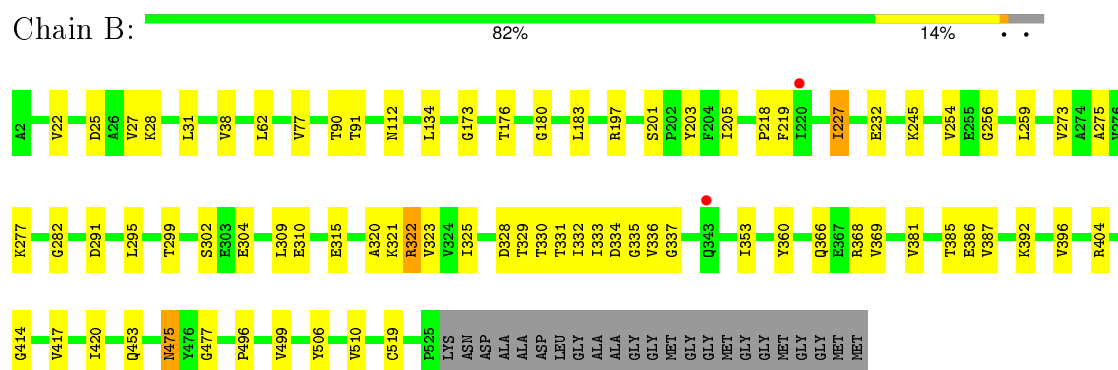
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

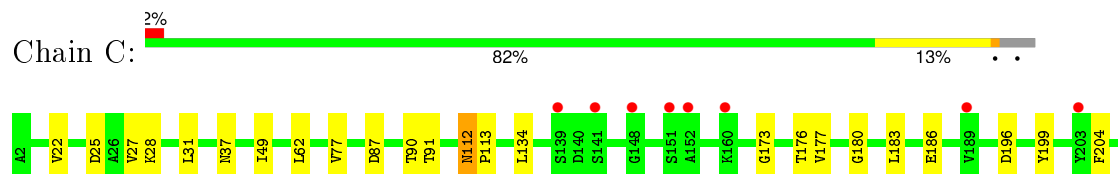
• Molecule 1: 60 kDa chaperonin

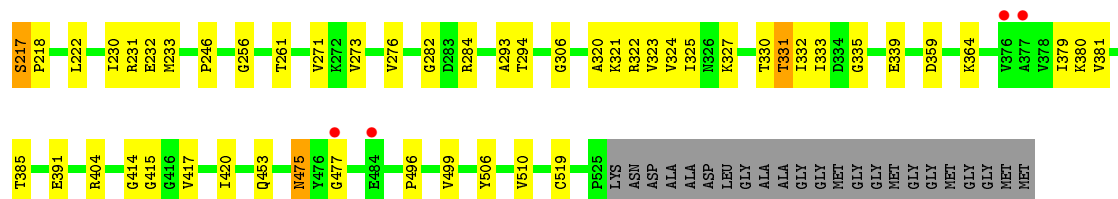


• Molecule 1: 60 kDa chaperonin

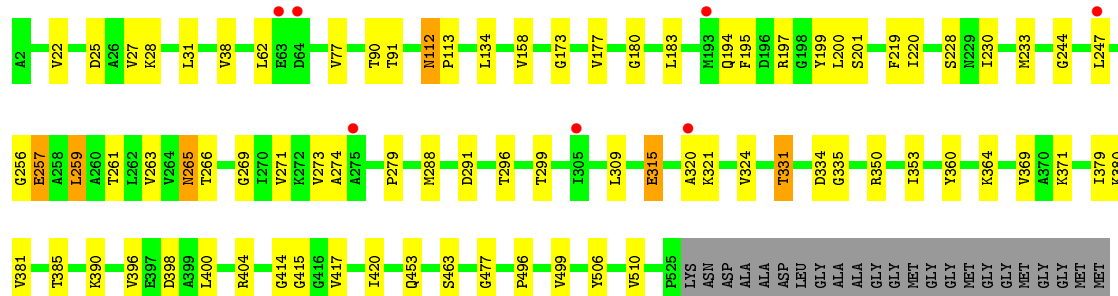
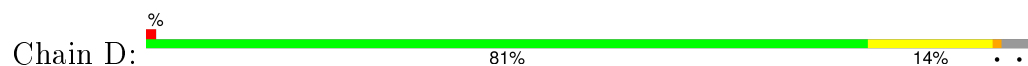


• Molecule 1: 60 kDa chaperonin

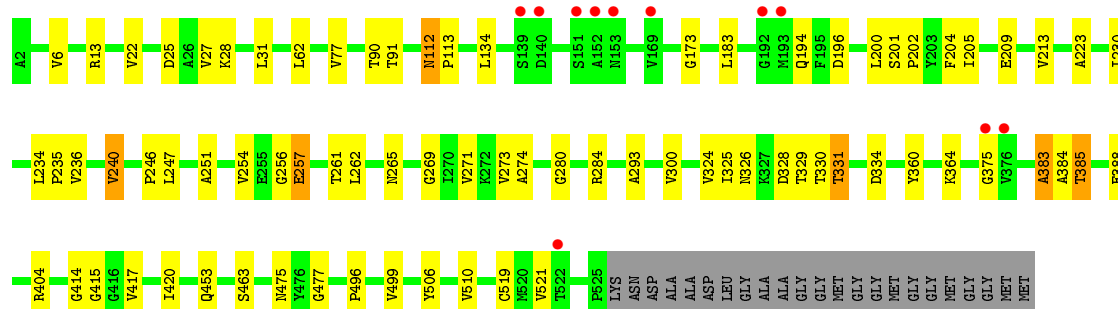
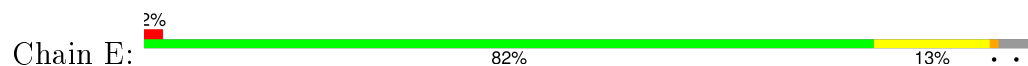




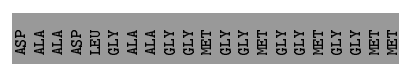
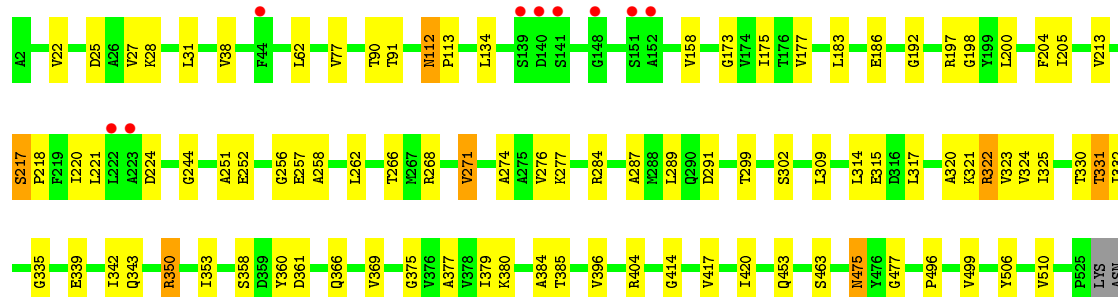
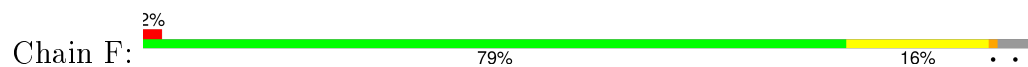
• Molecule 1: 60 kDa chaperonin



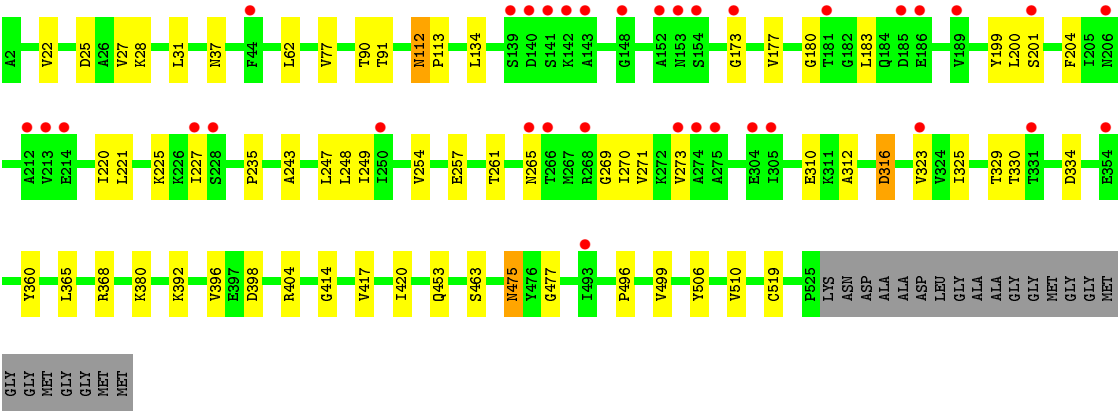
• Molecule 1: 60 kDa chaperonin



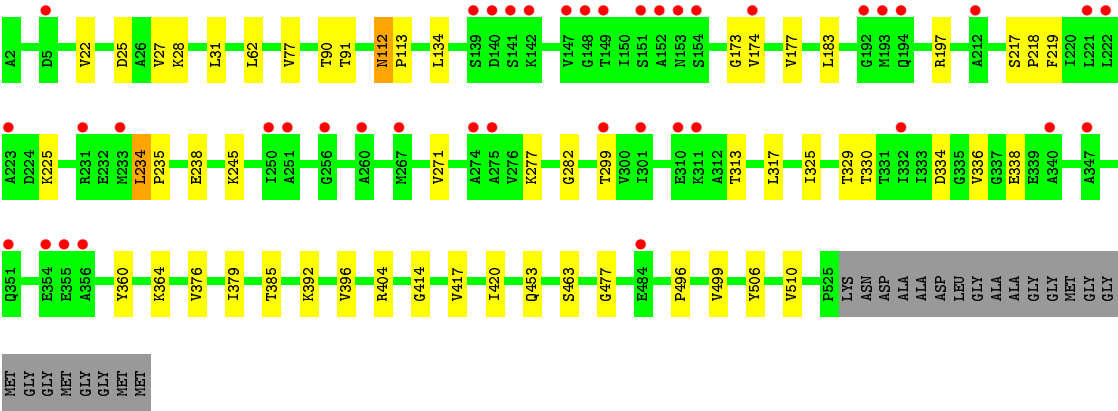
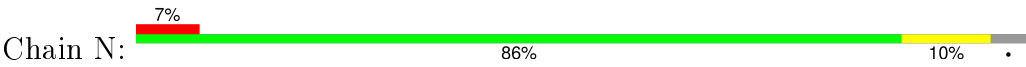
• Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 260.95Å 287.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.94 49.36 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.39-3.94) 96.5 (49.36-3.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.261 , 0.293 0.249 , 0.277	Depositor DCC
R_{free} test set	4472 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	115.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 112.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 90288 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	54464	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, AGS, TL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/3883	0.63	4/5243 (0.1%)
1	B	0.36	0/3883	0.48	0/5243
1	C	0.46	4/3883 (0.1%)	0.49	0/5243
1	D	0.43	2/3883 (0.1%)	0.50	0/5243
1	E	0.37	0/3883	0.63	4/5243 (0.1%)
1	F	0.36	0/3883	0.50	0/5243
1	G	0.37	0/3883	0.50	0/5243
1	H	0.43	2/3883 (0.1%)	0.50	0/5243
1	I	0.40	2/3883 (0.1%)	0.49	0/5243
1	J	0.36	0/3883	0.49	0/5243
1	K	0.40	2/3883 (0.1%)	0.49	0/5243
1	L	0.34	0/3883	0.47	0/5243
1	M	0.37	2/3883 (0.1%)	0.47	0/5243
1	N	0.44	3/3883 (0.1%)	0.49	1/5243 (0.0%)
All	All	0.39	17/54362 (0.0%)	0.51	9/73402 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	GLU	CD-OE2	12.24	1.39	1.25
1	N	338	GLU	CD-OE2	11.57	1.38	1.25
1	H	367	GLU	CD-OE2	10.24	1.36	1.25
1	D	315	GLU	CD-OE1	9.77	1.36	1.25
1	H	367	GLU	CD-OE1	9.42	1.36	1.25
1	C	339	GLU	CG-CD	9.28	1.65	1.51
1	D	315	GLU	CD-OE2	9.06	1.35	1.25
1	K	363	GLU	CD-OE1	8.62	1.35	1.25
1	C	232	GLU	CD-OE1	7.40	1.33	1.25
1	N	238	GLU	CD-OE2	7.30	1.33	1.25
1	M	37	ASN	CG-ND2	-6.96	1.15	1.32
1	C	339	GLU	CD-OE1	6.85	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	238	GLU	CD-OE1	6.59	1.32	1.25
1	I	209	GLU	CD-OE1	6.18	1.32	1.25
1	M	37	ASN	CG-OD1	-6.08	1.10	1.24
1	I	209	GLU	CD-OE2	5.91	1.32	1.25
1	K	363	GLU	CD-OE2	5.55	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	A	13	ARG	NE-CZ-NH2	-19.42	110.59	120.30
1	E	13	ARG	NE-CZ-NH1	18.12	129.36	120.30
1	A	13	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	13	ARG	CD-NE-CZ	8.14	135.00	123.60
1	E	13	ARG	CD-NE-CZ	7.95	134.73	123.60
1	N	338	GLU	OE1-CD-OE2	5.91	130.39	123.30
1	A	13	ARG	CB-CG-CD	-5.53	97.23	111.60
1	E	13	ARG	CB-CG-CD	-5.40	97.55	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	60	0
1	B	3855	0	3974	40	0
1	C	3855	0	3976	41	0
1	D	3855	0	3976	43	0
1	E	3855	0	3974	43	0
1	F	3855	0	3976	50	0
1	G	3855	0	3975	55	0
1	H	3855	0	3976	44	0
1	I	3855	0	3975	56	0
1	J	3855	0	3974	45	0
1	K	3855	0	3975	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3855	0	3976	30	0
1	M	3855	0	3976	36	0
1	N	3855	0	3976	34	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	2	0
2	H	31	0	12	0	0
2	I	31	0	12	1	0
2	J	31	0	12	1	0
2	K	31	0	12	1	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	G	3	0	0	0	0
3	H	4	0	0	0	0
3	I	3	0	0	1	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	54464	0	55823	586	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 5.

All (586) 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:M:183:LEU:HD22	1:N:360:TYR:CB	1.96	0.95
1:A:87:ASP:OD2	1:A:499:VAL:HG21	1.69	0.91
1:C:87:ASP:OD2	1:C:499:VAL:HG21	1.75	0.86
1:M:183:LEU:HD22	1:N:360:TYR:HB3	1.54	0.86
1:H:360:TYR:CG	1:N:183:LEU:HD22	2.13	0.84
1:D:320:ALA:HA	1:D:335:GLY:HA2	1.60	0.83
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.63	0.80
1:N:234:LEU:H	1:N:235:PRO:HD2	1.48	0.77
1:H:349:ILE:HA	1:H:352:GLN:HG2	1.68	0.76
1:E:280:GLY:HA2	1:E:284:ARG:HH21	1.51	0.75
1:N:219:PHE:HE2	1:N:245:LYS:HB2	1.52	0.75
1:G:266:THR:HG21	1:G:273:VAL:HB	1.69	0.73
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.71	0.72
1:H:219:PHE:HE2	1:H:245:LYS:HB2	1.56	0.71
1:J:219:PHE:CD2	1:J:240:VAL:HG13	2.25	0.70
1:A:187:LEU:HD13	1:A:379:ILE:HG23	1.72	0.70
1:G:415:GLY:N	2:G:549:AGS:O2'	2.20	0.70
1:H:219:PHE:CE2	1:H:245:LYS:HB2	2.27	0.70
1:I:247:LEU:HB3	1:I:273:VAL:HG13	1.74	0.69
1:J:77:VAL:HG21	1:J:510:VAL:HG11	1.74	0.69
1:H:321:LYS:O	1:H:322:ARG:HB2	1.90	0.69
1:D:38:VAL:HG22	1:E:519:CYS:HB3	1.76	0.68
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.74	0.68
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.76	0.68
1:M:365:LEU:HD22	1:M:368:ARG:HH21	1.59	0.67
1:F:339:GLU:HA	1:F:342:ILE:HB	1.76	0.66
1:H:288:MET:HA	1:H:291:ASP:HB2	1.77	0.66
1:A:197:ARG:HD2	1:A:277:LYS:HB2	1.76	0.66
1:F:198:GLY:O	1:F:276:VAL:HG13	1.95	0.65
1:M:325:ILE:HG12	1:M:330:THR:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:LEU:HD22	1:N:360:TYR:HB2	1.78	0.65
1:H:349:ILE:HA	1:H:352:GLN:CG	2.27	0.65
1:K:219:PHE:CE2	1:K:245:LYS:HB2	2.32	0.65
1:F:220:ILE:HD11	1:F:320:ALA:HB2	1.79	0.65
1:J:37:ASN:HD22	1:J:49:ILE:HG22	1.62	0.65
1:E:417:VAL:HA	1:E:420:ILE:HG22	1.79	0.64
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.78	0.64
1:I:358:SER:HB3	1:I:361:ASP:HB2	1.79	0.64
1:F:38:VAL:HG22	1:G:519:CYS:HB3	1.78	0.64
1:A:291:ASP:OD2	1:A:368:ARG:HD3	1.97	0.64
1:E:77:VAL:HG21	1:E:510:VAL:HG11	1.79	0.64
1:C:37:ASN:HD22	1:C:49:ILE:HG22	1.63	0.64
1:J:181:THR:O	1:K:282:GLY:HA3	1.99	0.63
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.80	0.63
1:N:234:LEU:N	1:N:235:PRO:HD2	2.12	0.63
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.81	0.63
1:I:77:VAL:HG21	1:I:510:VAL:HG11	1.80	0.63
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.81	0.63
1:F:77:VAL:HG21	1:F:510:VAL:HG11	1.81	0.63
1:J:202:PRO:O	1:J:205:ILE:HG13	1.99	0.63
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.81	0.63
1:C:320:ALA:HA	1:C:335:GLY:HA2	1.81	0.62
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.80	0.62
1:M:77:VAL:HG21	1:M:510:VAL:HG11	1.80	0.62
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.80	0.62
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.81	0.62
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.80	0.62
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.80	0.62
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.82	0.62
1:D:77:VAL:HG21	1:D:510:VAL:HG11	1.80	0.62
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.81	0.62
1:L:77:VAL:HG21	1:L:510:VAL:HG11	1.80	0.62
1:K:385:THR:HG22	1:L:284:ARG:HH22	1.64	0.61
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.82	0.61
1:F:321:LYS:O	1:F:322:ARG:HB2	2.01	0.61
1:A:30:THR:O	3:A:552:TL:TL	2.22	0.61
1:C:77:VAL:HG21	1:C:510:VAL:HG11	1.82	0.61
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.82	0.61
1:D:173:GLY:O	1:D:404:ARG:NH2	2.33	0.61
1:A:158:VAL:HG13	1:A:396:VAL:HG22	1.82	0.61
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.83	0.61
1:K:77:VAL:HG21	1:K:510:VAL:HG11	1.81	0.61
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.36	0.61
1:H:417:VAL:HA	1:H:420:ILE:HG22	1.82	0.61
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.83	0.61
1:G:77:VAL:HG21	1:G:510:VAL:HG11	1.83	0.61
1:B:77:VAL:HG21	1:B:510:VAL:HG11	1.82	0.60
1:I:483:GLU:OE2	3:I:551:TL:TL	2.23	0.60
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.83	0.60
1:N:417:VAL:HA	1:N:420:ILE:HG22	1.81	0.60
1:I:288:MET:HG2	1:I:368:ARG:HD3	1.83	0.60
1:H:77:VAL:HG21	1:H:510:VAL:HG11	1.83	0.60
1:E:324:VAL:HB	1:E:331:THR:HG23	1.83	0.60
1:K:417:VAL:HA	1:K:420:ILE:HG22	1.84	0.60
1:G:87:ASP:OD2	1:G:499:VAL:HG21	2.00	0.60
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.84	0.60
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.84	0.59
1:I:325:ILE:HG12	1:I:330:THR:HG23	1.84	0.59
1:N:77:VAL:HG21	1:N:510:VAL:HG11	1.84	0.59
1:F:197:ARG:NE	1:F:277:LYS:HB2	2.17	0.59
1:E:173:GLY:O	1:E:404:ARG:NH2	2.36	0.59
1:F:197:ARG:HE	1:F:277:LYS:HB2	1.67	0.59
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.83	0.59
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.85	0.59
1:A:200:LEU:HD11	1:A:277:LYS:HG3	1.84	0.59
1:K:219:PHE:HE2	1:K:245:LYS:HB2	1.67	0.59
1:E:204:PHE:CD1	1:E:274:ALA:HA	2.38	0.59
1:I:240:VAL:HG21	1:I:247:LEU:HD22	1.84	0.59
1:D:261:THR:O	1:D:265:ASN:HB2	2.03	0.59
1:A:195:PHE:HE2	1:A:197:ARG:HB2	1.66	0.59
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.85	0.59
1:G:173:GLY:O	1:G:404:ARG:NH2	2.36	0.59
1:J:266:THR:HG22	1:J:273:VAL:H	1.68	0.59
1:I:173:GLY:O	1:I:404:ARG:NH2	2.36	0.59
1:J:262:LEU:O	1:J:266:THR:HG23	2.02	0.58
1:A:261:THR:O	1:A:265:ASN:HB2	2.03	0.58
1:C:284:ARG:HB3	1:C:364:LYS:NZ	2.18	0.58
1:A:173:GLY:O	1:A:404:ARG:NH2	2.36	0.58
1:E:183:LEU:HD22	1:F:360:TYR:CG	2.38	0.58
1:F:350:ARG:HA	1:F:353:ILE:HD12	1.84	0.58
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:O	1:B:404:ARG:NH2	2.37	0.58
1:G:221:LEU:HB3	1:G:249:ILE:HG23	1.85	0.58
1:K:358:SER:HB3	1:K:361:ASP:HB2	1.84	0.58
1:M:173:GLY:O	1:M:404:ARG:NH2	2.36	0.58
1:N:392:LYS:O	1:N:396:VAL:HG23	2.02	0.58
1:D:269:GLY:HA3	1:E:257:GLU:HB2	1.86	0.58
1:K:382:GLY:HA2	1:K:389:MET:HG2	1.84	0.58
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.85	0.58
1:K:234:LEU:N	1:K:235:PRO:HD2	2.19	0.58
1:A:326:ASN:HB2	1:A:329:THR:HB	1.85	0.57
1:J:173:GLY:O	1:J:404:ARG:NH2	2.37	0.57
1:F:173:GLY:O	1:F:404:ARG:NH2	2.38	0.57
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.86	0.57
1:H:173:GLY:O	1:H:404:ARG:NH2	2.37	0.57
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.85	0.57
1:A:313:THR:HG22	1:A:314:LEU:H	1.68	0.57
1:A:176:THR:HG21	1:A:333:ILE:HD11	1.85	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.38	0.57
1:C:173:GLY:O	1:C:404:ARG:NH2	2.36	0.57
1:L:350:ARG:HG3	1:L:353:ILE:HD12	1.87	0.57
1:K:173:GLY:O	1:K:404:ARG:NH2	2.38	0.57
1:N:173:GLY:O	1:N:404:ARG:NH2	2.37	0.57
1:F:287:ALA:O	1:F:291:ASP:HB2	2.05	0.57
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.87	0.57
1:A:519:CYS:HB3	1:G:38:VAL:HG22	1.85	0.56
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.87	0.56
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.85	0.56
1:A:38:VAL:HG22	1:B:519:CYS:HB3	1.85	0.56
1:G:213:VAL:HB	1:G:325:ILE:HB	1.86	0.56
1:J:77:VAL:HG12	1:J:506:TYR:HB3	1.87	0.56
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:A:77:VAL:HG21	1:A:510:VAL:HG11	1.85	0.56
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.87	0.56
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.88	0.56
1:B:219:PHE:CE2	1:B:245:LYS:HB2	2.40	0.56
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.87	0.56
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.87	0.56
1:E:202:PRO:O	1:E:205:ILE:HG12	2.06	0.56
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.88	0.56
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.87	0.55
1:K:313:THR:HG22	1:K:314:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:PRO:HG3	1:M:310:GLU:HG3	1.88	0.55
1:G:223:ALA:O	1:G:251:ALA:HA	2.06	0.55
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.88	0.55
1:C:180:GLY:HA3	1:C:381:VAL:O	2.06	0.55
1:D:220:ILE:HD13	1:D:296:THR:HG21	1.89	0.55
1:B:325:ILE:HG13	1:B:330:THR:HG23	1.89	0.54
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.89	0.54
1:E:415:GLY:N	2:E:549:AGS:O2'	2.36	0.54
1:C:496:PRO:O	1:C:499:VAL:HG12	2.08	0.53
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.89	0.53
1:J:496:PRO:O	1:J:499:VAL:HG12	2.08	0.53
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.90	0.53
1:F:224:ASP:HB3	1:F:302:SER:HA	1.90	0.53
1:E:496:PRO:O	1:E:499:VAL:HG12	2.07	0.53
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.90	0.53
1:D:230:ILE:HA	1:D:233:MET:HB2	1.90	0.53
1:G:496:PRO:O	1:G:499:VAL:HG12	2.08	0.53
1:C:415:GLY:N	2:C:549:AGS:O2'	2.36	0.53
1:A:496:PRO:O	1:A:499:VAL:HG12	2.09	0.53
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.91	0.53
1:C:230:ILE:HD13	1:C:261:THR:HB	1.91	0.53
1:I:496:PRO:O	1:I:499:VAL:HG12	2.09	0.53
1:B:323:VAL:HG12	1:B:332:ILE:HA	1.90	0.53
1:I:223:ALA:O	1:I:251:ALA:HA	2.09	0.53
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.91	0.53
1:K:233:MET:C	1:K:235:PRO:HD2	2.29	0.52
1:J:77:VAL:CG1	1:J:506:TYR:HB3	2.38	0.52
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.91	0.52
1:B:385:THR:O	1:B:387:VAL:N	2.40	0.52
1:J:415:GLY:N	2:J:549:AGS:O2'	2.28	0.52
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.92	0.52
1:I:180:GLY:HA3	1:I:381:VAL:O	2.10	0.52
1:D:288:MET:O	1:D:291:ASP:HB2	2.09	0.52
1:L:183:LEU:HD22	1:M:360:TYR:CG	2.45	0.52
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.91	0.52
1:F:258:ALA:O	1:F:262:LEU:HG	2.10	0.52
1:L:496:PRO:O	1:L:499:VAL:HG12	2.09	0.52
1:G:323:VAL:HG12	1:G:332:ILE:HA	1.92	0.52
1:G:177:VAL:HG22	1:G:379:ILE:HB	1.91	0.52
1:N:234:LEU:H	1:N:235:PRO:CD	2.19	0.51
1:M:77:VAL:HG12	1:M:506:TYR:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PRO:HG3	1:A:323:VAL:HG22	1.92	0.51
1:J:324:VAL:HB	1:J:331:THR:HG23	1.91	0.51
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.91	0.51
1:I:26:ALA:HA	1:J:8:PHE:HE1	1.75	0.51
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.92	0.51
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.93	0.51
1:C:176:THR:HG21	1:C:333:ILE:HD11	1.93	0.51
1:D:266:THR:CG2	1:D:273:VAL:HG12	2.40	0.51
1:I:288:MET:O	1:I:292:ILE:HG13	2.10	0.51
1:D:415:GLY:N	2:D:549:AGS:O2'	2.29	0.51
1:N:496:PRO:O	1:N:499:VAL:HG12	2.10	0.51
1:I:87:ASP:OD2	1:I:499:VAL:HG21	2.11	0.51
1:G:218:PRO:HG3	1:G:323:VAL:HG22	1.92	0.51
1:H:496:PRO:O	1:H:499:VAL:HG12	2.10	0.51
1:I:366:GLN:HA	1:I:369:VAL:HG22	1.93	0.51
1:H:77:VAL:HG12	1:H:506:TYR:HB3	1.92	0.51
1:B:392:LYS:O	1:B:396:VAL:HG23	2.11	0.51
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.93	0.51
1:N:77:VAL:HG12	1:N:506:TYR:HB3	1.91	0.51
1:H:284:ARG:HH22	1:N:385:THR:HG22	1.76	0.50
1:M:261:THR:O	1:M:265:ASN:HB2	2.11	0.50
1:M:221:LEU:HD23	1:M:249:ILE:HG23	1.92	0.50
1:A:197:ARG:NH2	1:G:386:GLU:OE2	2.44	0.50
1:B:353:ILE:HD13	1:B:366:GLN:HE21	1.76	0.50
1:F:496:PRO:O	1:F:499:VAL:HG12	2.10	0.50
1:B:496:PRO:O	1:B:499:VAL:HG12	2.12	0.50
1:L:77:VAL:HG12	1:L:506:TYR:HB3	1.92	0.50
1:D:496:PRO:O	1:D:499:VAL:HG12	2.10	0.50
1:C:177:VAL:HG22	1:C:379:ILE:HB	1.93	0.50
1:M:496:PRO:O	1:M:499:VAL:HG12	2.11	0.50
1:B:219:PHE:HE2	1:B:245:LYS:HB2	1.75	0.50
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.94	0.50
1:G:234:LEU:HB2	1:G:235:PRO:HD3	1.94	0.50
1:A:320:ALA:HA	1:A:335:GLY:HA2	1.93	0.50
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.92	0.50
1:J:187:LEU:HD13	1:J:379:ILE:HG12	1.93	0.50
1:A:200:LEU:HD13	1:A:276:VAL:HA	1.93	0.50
1:B:197:ARG:HH11	1:B:277:LYS:HD3	1.77	0.50
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.94	0.50
1:D:194:GLN:HG3	1:D:331:THR:HB	1.94	0.50
1:E:383:ALA:O	1:E:384:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.93	0.50
1:K:496:PRO:O	1:K:499:VAL:HG12	2.12	0.49
1:C:222:LEU:HD13	1:C:293:ALA:HA	1.93	0.49
1:N:183:LEU:O	1:N:183:LEU:HG	2.11	0.49
1:I:225:LYS:HG2	1:I:303:GLU:HG3	1.93	0.49
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.93	0.49
1:A:183:LEU:HD22	1:B:360:TYR:CD2	2.47	0.49
1:D:360:TYR:CE1	1:D:364:LYS:HE3	2.48	0.49
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.94	0.49
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.93	0.49
1:E:194:GLN:HG3	1:E:331:THR:HB	1.92	0.49
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.94	0.49
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.94	0.49
1:D:266:THR:HG21	1:D:273:VAL:HG12	1.93	0.49
1:B:321:LYS:O	1:B:322:ARG:HB2	2.11	0.49
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.95	0.49
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.94	0.49
1:H:183:LEU:HD22	1:I:360:TYR:CD2	2.48	0.49
1:L:183:LEU:O	1:L:183:LEU:HG	2.13	0.49
1:A:349:ILE:HG21	1:A:369:VAL:HG13	1.93	0.49
1:H:194:GLN:HG3	1:H:331:THR:HB	1.95	0.49
1:F:183:LEU:HD22	1:G:360:TYR:CD2	2.48	0.49
1:K:320:ALA:HA	1:K:335:GLY:HA2	1.95	0.49
1:K:269:GLY:HA3	1:L:257:GLU:HB2	1.95	0.49
1:F:204:PHE:CD1	1:F:274:ALA:HA	2.48	0.49
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.94	0.49
1:M:77:VAL:CG1	1:M:506:TYR:HB3	2.43	0.49
1:K:414:GLY:O	1:K:417:VAL:HG22	2.13	0.49
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.94	0.49
1:B:180:GLY:HA3	1:B:381:VAL:O	2.12	0.49
1:F:324:VAL:HB	1:F:331:THR:HG23	1.95	0.48
1:I:224:ASP:HB3	1:I:302:SER:HB3	1.95	0.48
1:G:219:PHE:HE2	1:G:245:LYS:HB2	1.77	0.48
1:D:414:GLY:O	1:D:417:VAL:HG22	2.13	0.48
1:K:77:VAL:HG12	1:K:506:TYR:HB3	1.94	0.48
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.94	0.48
1:J:183:LEU:HG	1:J:183:LEU:O	2.13	0.48
1:H:31:LEU:HD23	1:H:453:GLN:HB3	1.96	0.48
1:H:392:LYS:O	1:H:396:VAL:HG23	2.13	0.48
1:I:314:LEU:HA	1:I:317:LEU:HD13	1.94	0.48
1:E:223:ALA:O	1:E:251:ALA:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:384:ALA:HB3	1:K:388:GLU:HB2	1.95	0.48
1:H:198:GLY:HA3	1:H:327:LYS:O	2.13	0.48
1:D:197:ARG:HE	1:D:279:PRO:HA	1.79	0.48
1:C:284:ARG:HB3	1:C:364:LYS:HZ1	1.79	0.48
1:B:366:GLN:HA	1:B:369:VAL:HG22	1.96	0.48
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.95	0.48
1:A:222:LEU:HD13	1:A:293:ALA:HA	1.95	0.48
1:M:183:LEU:O	1:M:183:LEU:HG	2.12	0.48
1:A:198:GLY:O	1:A:276:VAL:HG12	2.13	0.48
1:K:183:LEU:HG	1:K:183:LEU:O	2.14	0.48
1:L:77:VAL:CG1	1:L:506:TYR:HB3	2.44	0.47
1:I:220:ILE:N	1:I:318:GLY:O	2.45	0.47
1:F:183:LEU:HG	1:F:183:LEU:O	2.12	0.47
1:G:414:GLY:O	1:G:417:VAL:HG22	2.14	0.47
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.95	0.47
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.95	0.47
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.47
1:A:313:THR:H	1:A:316:ASP:HB2	1.79	0.47
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.47
1:G:183:LEU:HG	1:G:183:LEU:O	2.13	0.47
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.96	0.47
1:G:251:ALA:O	1:G:252:GLU:C	2.52	0.47
1:F:323:VAL:HG12	1:F:332:ILE:HA	1.97	0.47
1:N:77:VAL:CG1	1:N:506:TYR:HB3	2.45	0.47
1:I:236:VAL:O	1:I:240:VAL:HG23	2.15	0.47
1:I:247:LEU:HG	1:I:249:ILE:HD11	1.97	0.47
1:H:414:GLY:O	1:H:417:VAL:HG22	2.14	0.47
1:F:213:VAL:HB	1:F:325:ILE:HB	1.96	0.47
1:B:183:LEU:HG	1:B:183:LEU:O	2.15	0.47
1:A:87:ASP:OD2	1:A:499:VAL:HG11	2.15	0.47
1:A:414:GLY:O	1:A:417:VAL:HG22	2.15	0.47
1:B:335:GLY:C	1:B:337:GLY:H	2.17	0.47
1:G:194:GLN:HG3	1:G:330:THR:O	2.14	0.47
1:E:326:ASN:HB2	1:E:329:THR:HB	1.97	0.47
1:J:314:LEU:HA	1:J:317:LEU:HD13	1.97	0.47
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.96	0.47
1:F:175:ILE:HA	1:F:377:ALA:HB3	1.96	0.47
1:E:234:LEU:N	1:E:235:PRO:HD2	2.30	0.47
1:E:230:ILE:HD13	1:E:261:THR:HB	1.97	0.47
1:N:234:LEU:N	1:N:235:PRO:CD	2.75	0.46
1:F:192:GLY:H	1:F:375:GLY:HA2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.97	0.46
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.97	0.46
1:D:324:VAL:HB	1:D:331:THR:HG23	1.97	0.46
1:A:183:LEU:O	1:A:183:LEU:HG	2.15	0.46
1:K:258:ALA:O	1:K:262:LEU:HG	2.15	0.46
1:N:174:VAL:HB	1:N:376:VAL:HG22	1.97	0.46
1:K:321:LYS:O	1:K:322:ARG:HB2	2.15	0.46
1:J:269:GLY:HA3	1:K:257:GLU:HB2	1.96	0.46
1:C:77:VAL:CG1	1:C:506:TYR:HB3	2.46	0.46
1:E:183:LEU:O	1:E:183:LEU:HG	2.15	0.46
1:J:230:ILE:C	1:J:232:GLU:H	2.17	0.46
1:F:251:ALA:O	1:F:252:GLU:C	2.54	0.46
1:K:77:VAL:CG1	1:K:506:TYR:HB3	2.46	0.46
1:A:77:VAL:CG1	1:A:506:TYR:HB3	2.45	0.46
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.97	0.46
1:D:259:LEU:O	1:D:263:VAL:HG23	2.15	0.46
1:H:183:LEU:HG	1:H:183:LEU:O	2.15	0.46
1:G:336:VAL:O	1:G:337:GLY:C	2.54	0.46
1:I:194:GLN:HG3	1:I:331:THR:HB	1.97	0.46
1:K:31:LEU:HD23	1:K:453:GLN:HB3	1.98	0.46
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.98	0.46
1:E:112:ASN:HD22	1:E:113:PRO:HD2	1.81	0.46
1:K:222:LEU:HB3	1:K:289:LEU:HD22	1.98	0.46
1:C:183:LEU:O	1:C:183:LEU:HG	2.16	0.46
1:H:218:PRO:HD2	1:H:320:ALA:O	2.15	0.46
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.98	0.46
1:D:77:VAL:CG1	1:D:506:TYR:HB3	2.46	0.46
1:H:77:VAL:CG1	1:H:506:TYR:HB3	2.45	0.46
1:H:25:ASP:HA	1:H:28:LYS:HG2	1.98	0.46
1:H:112:ASN:HD22	1:H:113:PRO:HD2	1.81	0.46
1:A:87:ASP:CG	1:A:499:VAL:HG21	2.34	0.46
1:F:414:GLY:O	1:F:417:VAL:HG22	2.16	0.46
1:I:222:LEU:HD21	1:I:250:ILE:HD12	1.97	0.46
1:N:197:ARG:HD2	1:N:277:LYS:HB2	1.97	0.46
1:B:31:LEU:HD23	1:B:453:GLN:HB3	1.97	0.46
1:D:177:VAL:HG22	1:D:379:ILE:HB	1.97	0.46
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.97	0.45
1:C:112:ASN:HD22	1:C:113:PRO:HD2	1.81	0.45
1:J:222:LEU:HB3	1:J:289:LEU:HD21	1.97	0.45
1:L:217:SER:N	1:L:218:PRO:HD3	2.32	0.45
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.97	0.45
1:N:414:GLY:O	1:N:417:VAL:HG22	2.15	0.45
1:G:219:PHE:CE2	1:G:245:LYS:HB2	2.52	0.45
1:F:77:VAL:CG1	1:F:506:TYR:HB3	2.47	0.45
1:G:77:VAL:CG1	1:G:506:TYR:HB3	2.46	0.45
1:J:313:THR:HG22	1:J:314:LEU:H	1.81	0.45
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.98	0.45
1:H:338:GLU:O	1:H:342:ILE:HG13	2.15	0.45
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.98	0.45
1:C:25:ASP:HA	1:C:28:LYS:HG2	1.98	0.45
1:D:112:ASN:HD22	1:D:113:PRO:HD2	1.82	0.45
1:M:220:ILE:HG12	1:M:248:LEU:HD23	1.99	0.45
1:K:266:THR:HG22	1:K:273:VAL:H	1.80	0.45
1:I:77:VAL:CG1	1:I:506:TYR:HB3	2.47	0.45
1:B:201:SER:C	1:B:203:TYR:H	2.19	0.45
1:H:360:TYR:CD1	1:N:183:LEU:HD22	2.50	0.45
1:F:220:ILE:HD11	1:F:320:ALA:CB	2.46	0.45
1:F:217:SER:N	1:F:218:PRO:HD3	2.31	0.45
1:E:31:LEU:HD23	1:E:453:GLN:HB3	1.99	0.45
1:G:214:GLU:OE2	1:G:322:ARG:NH2	2.50	0.45
1:J:26:ALA:HA	1:K:8:PHE:HE1	1.82	0.45
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.98	0.45
1:H:321:LYS:O	1:H:322:ARG:CB	2.62	0.45
1:B:414:GLY:O	1:B:417:VAL:HG22	2.17	0.45
1:L:25:ASP:HA	1:L:28:LYS:HG2	1.99	0.45
1:M:227:ILE:HD12	1:M:254:VAL:HG22	1.98	0.45
1:I:230:ILE:HD13	1:I:261:THR:HB	1.98	0.45
1:A:417:VAL:HG11	1:A:477:GLY:HA3	1.99	0.45
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.97	0.45
1:M:112:ASN:HD22	1:M:113:PRO:HD2	1.82	0.45
1:H:360:TYR:CB	1:N:183:LEU:HD22	2.46	0.45
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.98	0.45
1:D:183:LEU:O	1:D:183:LEU:HG	2.17	0.45
1:G:302:SER:H	1:G:307:MET:HE1	1.81	0.45
1:I:158:VAL:HG13	1:I:396:VAL:HG22	2.00	0.44
1:F:218:PRO:HG3	1:F:323:VAL:HG22	1.99	0.44
1:L:31:LEU:HD23	1:L:453:GLN:HB3	1.99	0.44
1:I:39:VAL:HG23	1:J:517:THR:HG23	1.99	0.44
1:I:183:LEU:O	1:I:183:LEU:HG	2.16	0.44
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.99	0.44
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:LYS:O	1:C:322:ARG:HB2	2.17	0.44
1:L:112:ASN:HD22	1:L:113:PRO:HD2	1.83	0.44
1:J:112:ASN:HD22	1:J:113:PRO:HD2	1.81	0.44
1:I:229:ASN:HB3	1:I:231:ARG:HG3	1.99	0.44
1:D:350:ARG:HG3	1:D:353:ILE:HD11	2.00	0.44
1:B:232:GLU:HB3	1:B:309:LEU:HB2	1.98	0.44
1:C:414:GLY:O	1:C:417:VAL:HG22	2.18	0.44
1:I:112:ASN:HD22	1:I:113:PRO:HD2	1.81	0.44
1:F:221:LEU:HD21	1:F:309:LEU:HD21	1.99	0.44
1:B:417:VAL:HG11	1:B:477:GLY:HA3	1.99	0.44
1:H:417:VAL:HG11	1:H:477:GLY:HA3	2.00	0.44
1:E:360:TYR:OH	1:E:364:LYS:HE3	2.17	0.44
1:G:203:TYR:HB3	1:G:267:MET:SD	2.58	0.44
1:I:227:ILE:HB	1:I:254:VAL:HG13	1.99	0.44
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.99	0.44
1:L:38:VAL:HG22	1:M:519:CYS:HB3	2.00	0.44
1:G:180:GLY:HA3	1:G:381:VAL:O	2.18	0.44
1:C:324:VAL:HB	1:C:331:THR:HG23	2.00	0.44
1:L:392:LYS:O	1:L:396:VAL:HG23	2.18	0.44
1:I:31:LEU:HD23	1:I:453:GLN:HB3	1.99	0.44
1:C:37:ASN:HD22	1:C:49:ILE:CG2	2.28	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:D:247:LEU:HB3	1:D:273:VAL:HG23	1.99	0.44
1:J:220:ILE:HG13	1:J:248:LEU:HB3	2.00	0.44
1:A:112:ASN:HD22	1:A:113:PRO:HD2	1.82	0.44
1:D:273:VAL:HG22	1:D:274:ALA:H	1.82	0.43
1:J:305:ILE:HG21	1:J:307:MET:HE2	2.00	0.43
1:H:258:ALA:O	1:H:262:LEU:HG	2.18	0.43
1:H:353:ILE:H	1:H:353:ILE:HG13	1.66	0.43
1:K:177:VAL:HG22	1:K:379:ILE:HB	2.00	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:I:417:VAL:HG11	1:I:477:GLY:HA3	2.01	0.43
1:C:417:VAL:HG11	1:C:477:GLY:HA3	1.99	0.43
1:M:417:VAL:HG11	1:M:477:GLY:HA3	2.00	0.43
1:B:25:ASP:HA	1:B:28:LYS:HG2	1.99	0.43
1:J:417:VAL:HG11	1:J:477:GLY:HA3	2.00	0.43
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.01	0.43
1:A:273:VAL:HG12	1:A:274:ALA:N	2.33	0.43
1:E:112:ASN:HD22	1:E:113:PRO:CD	2.31	0.43
1:F:177:VAL:HG22	1:F:379:ILE:HB	1.99	0.43
1:F:25:ASP:HA	1:F:28:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:HD12	1:B:254:VAL:HG22	1.99	0.43
1:E:77:VAL:CG1	1:E:506:TYR:HB3	2.48	0.43
1:A:323:VAL:HG12	1:A:332:ILE:HA	2.00	0.43
1:B:475:ASN:N	1:B:475:ASN:HD22	2.17	0.43
1:M:25:ASP:HA	1:M:28:LYS:HG2	2.01	0.43
1:I:25:ASP:HA	1:I:28:LYS:HG2	2.01	0.43
1:B:77:VAL:CG1	1:B:506:TYR:HB3	2.48	0.43
1:J:232:GLU:HB3	1:J:309:LEU:HD12	2.01	0.43
1:G:25:ASP:HA	1:G:28:LYS:HG2	1.99	0.43
1:N:25:ASP:HA	1:N:28:LYS:HG2	2.01	0.43
1:F:112:ASN:HD22	1:F:113:PRO:HD2	1.84	0.43
1:E:25:ASP:HA	1:E:28:LYS:HG2	2.00	0.43
1:E:414:GLY:O	1:E:417:VAL:HG22	2.18	0.43
1:G:219:PHE:HB3	1:G:317:LEU:HD23	2.01	0.43
1:D:180:GLY:HA3	1:D:381:VAL:O	2.18	0.43
1:G:216:GLU:H	1:G:246:PRO:HG3	1.83	0.43
1:K:291:ASP:OD1	1:K:368:ARG:NH1	2.52	0.43
1:A:31:LEU:HD23	1:A:453:GLN:HB3	2.01	0.43
1:N:112:ASN:HD22	1:N:113:PRO:HD2	1.83	0.43
1:E:236:VAL:O	1:E:240:VAL:N	2.51	0.43
1:K:475:ASN:HD22	1:K:475:ASN:N	2.16	0.43
1:A:177:VAL:HG22	1:A:379:ILE:HG13	2.01	0.43
1:F:320:ALA:HA	1:F:335:GLY:HA2	2.01	0.43
1:J:414:GLY:O	1:J:417:VAL:HG22	2.19	0.43
1:H:224:ASP:O	1:H:225:LYS:HB3	2.19	0.43
1:F:314:LEU:HG	1:F:315:GLU:N	2.34	0.43
1:G:198:GLY:HA3	1:G:327:LYS:O	2.18	0.43
1:C:112:ASN:HD22	1:C:113:PRO:CD	2.32	0.43
1:D:112:ASN:HD22	1:D:113:PRO:CD	2.32	0.43
1:J:112:ASN:HD22	1:J:113:PRO:CD	2.31	0.43
1:C:199:TYR:HA	1:C:276:VAL:HG12	2.01	0.43
1:K:88:GLY:HA2	2:K:549:AGS:O2B	2.18	0.43
1:G:232:GLU:HA	1:G:310:GLU:HG3	2.01	0.43
1:B:302:SER:HB2	1:B:304:GLU:HG2	2.01	0.43
1:G:417:VAL:HG11	1:G:477:GLY:HA3	2.00	0.43
1:L:414:GLY:O	1:L:417:VAL:HG22	2.19	0.42
1:J:496:PRO:HB2	1:J:499:VAL:HG12	1.99	0.42
1:J:496:PRO:O	1:J:499:VAL:CG1	2.67	0.42
1:A:360:TYR:CB	1:G:183:LEU:HD22	2.49	0.42
1:A:25:ASP:HA	1:A:28:LYS:HG2	2.00	0.42
1:M:201:SER:HB3	1:M:204:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:417:VAL:HG11	1:K:477:GLY:HA3	2.01	0.42
1:H:112:ASN:HD22	1:H:113:PRO:CD	2.33	0.42
1:H:248:LEU:HD13	1:H:325:ILE:HD11	2.00	0.42
1:H:261:THR:O	1:H:265:ASN:HB2	2.18	0.42
1:E:293:ALA:HB2	1:E:300:VAL:HG23	2.01	0.42
1:C:496:PRO:O	1:C:499:VAL:CG1	2.68	0.42
1:D:228:SER:O	1:D:257:GLU:HB3	2.19	0.42
1:K:25:ASP:HA	1:K:28:LYS:HG2	2.01	0.42
1:A:112:ASN:HD22	1:A:113:PRO:CD	2.32	0.42
1:A:289:LEU:HD22	1:A:300:VAL:HG23	2.01	0.42
1:I:415:GLY:N	2:I:549:AGS:O2'	2.48	0.42
1:I:414:GLY:O	1:I:417:VAL:HG22	2.19	0.42
1:F:183:LEU:HD22	1:G:360:TYR:CG	2.55	0.42
1:G:236:VAL:HG13	1:G:317:LEU:HD11	2.01	0.42
1:N:325:ILE:HG13	1:N:330:THR:HG23	2.01	0.42
1:E:385:THR:OG1	1:E:388:GLU:HB2	2.20	0.42
1:E:200:LEU:HD13	1:E:254:VAL:HB	2.01	0.42
1:C:204:PHE:HE1	1:C:273:VAL:O	2.03	0.42
1:L:365:LEU:HD22	1:L:368:ARG:HH21	1.84	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	2.20	0.42
1:K:338:GLU:HG2	1:K:338:GLU:H	1.66	0.42
1:J:57:ALA:O	1:J:75:LYS:HD2	2.19	0.42
1:J:345:ARG:HA	1:J:348:GLN:HB2	2.01	0.42
1:J:343:GLN:O	1:J:346:VAL:HB	2.19	0.42
1:G:112:ASN:HD22	1:G:113:PRO:HD2	1.84	0.42
1:I:59:GLU:O	1:J:4:LYS:HG3	2.19	0.42
1:A:181:THR:O	1:B:282:GLY:HA3	2.20	0.42
1:I:112:ASN:HD22	1:I:113:PRO:CD	2.32	0.42
1:K:392:LYS:O	1:K:396:VAL:HG23	2.19	0.42
1:K:112:ASN:HD22	1:K:113:PRO:HD2	1.85	0.42
1:H:177:VAL:HG22	1:H:379:ILE:HB	2.01	0.42
1:I:340:ALA:O	1:I:344:GLY:N	2.49	0.42
1:D:321:LYS:HB2	1:D:334:ASP:HB3	2.02	0.42
1:M:177:VAL:HG21	1:M:396:VAL:HG12	2.00	0.42
1:I:475:ASN:HD22	1:I:475:ASN:N	2.18	0.42
1:C:475:ASN:N	1:C:475:ASN:HD22	2.18	0.42
1:A:223:ALA:O	1:A:251:ALA:HA	2.19	0.42
1:C:218:PRO:HD2	1:C:320:ALA:HB3	2.01	0.42
1:B:254:VAL:HG21	1:B:275:ALA:HB1	2.01	0.42
1:I:217:SER:N	1:I:218:PRO:HD3	2.34	0.42
1:M:312:ALA:HA	1:M:316:ASP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:PHE:HA	1:D:371:LYS:HE3	2.00	0.42
1:M:392:LYS:O	1:M:396:VAL:HG23	2.20	0.41
1:E:417:VAL:HG11	1:E:477:GLY:HA3	2.01	0.41
1:A:270:ILE:O	1:A:272:LYS:N	2.47	0.41
1:A:349:ILE:HG23	1:A:365:LEU:HD22	2.02	0.41
1:K:266:THR:CG2	1:K:273:VAL:H	2.33	0.41
1:E:240:VAL:HG21	1:E:247:LEU:HD22	2.02	0.41
1:D:25:ASP:HA	1:D:28:LYS:HG2	2.01	0.41
1:J:39:VAL:HG23	1:K:517:THR:HG23	2.01	0.41
1:M:31:LEU:HD23	1:M:453:GLN:HB3	2.01	0.41
1:N:217:SER:N	1:N:218:PRO:HD3	2.35	0.41
1:G:480:ALA:H	2:G:549:AGS:C2	2.33	0.41
1:F:417:VAL:HG11	1:F:477:GLY:HA3	2.01	0.41
1:D:417:VAL:HG11	1:D:477:GLY:HA3	2.01	0.41
1:G:197:ARG:HD2	1:G:277:LYS:HB2	2.03	0.41
1:M:112:ASN:HD22	1:M:113:PRO:CD	2.32	0.41
1:G:6:VAL:HG22	1:G:521:VAL:HG22	2.02	0.41
1:L:177:VAL:HG22	1:L:379:ILE:HB	2.02	0.41
1:H:6:VAL:HG22	1:H:521:VAL:HG22	2.03	0.41
1:G:281:PHE:HA	1:G:285:ARG:HB2	2.02	0.41
1:M:414:GLY:O	1:M:417:VAL:HG22	2.19	0.41
1:E:496:PRO:O	1:E:499:VAL:CG1	2.68	0.41
1:N:177:VAL:HG22	1:N:379:ILE:HB	2.03	0.41
1:K:87:ASP:HB3	1:K:499:VAL:HG21	2.03	0.41
1:A:360:TYR:CG	1:G:183:LEU:HD22	2.55	0.41
1:L:269:GLY:HA3	1:M:257:GLU:HB2	2.03	0.41
1:G:123:ALA:HB2	1:G:440:ILE:HG23	2.02	0.41
1:J:25:ASP:HA	1:J:28:LYS:HG2	2.02	0.41
1:G:496:PRO:O	1:G:499:VAL:CG1	2.69	0.41
1:M:248:LEU:HD22	1:M:323:VAL:HG11	2.02	0.41
1:E:204:PHE:HD1	1:E:273:VAL:O	2.03	0.41
1:A:194:GLN:HG3	1:A:330:THR:O	2.21	0.41
1:I:496:PRO:O	1:I:499:VAL:CG1	2.69	0.41
1:B:254:VAL:O	1:B:259:LEU:HD12	2.21	0.41
1:E:269:GLY:HA3	1:F:257:GLU:HB2	2.02	0.41
1:C:230:ILE:HG13	1:C:233:MET:HG3	2.03	0.41
1:A:222:LEU:CD1	1:A:293:ALA:HA	2.52	0.41
1:L:112:ASN:HD22	1:L:113:PRO:CD	2.34	0.41
1:I:254:VAL:O	1:I:259:LEU:HB2	2.20	0.41
1:H:26:ALA:HA	1:I:8:PHE:HE1	1.85	0.41
1:H:475:ASN:N	1:H:475:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PRO:O	1:A:499:VAL:CG1	2.69	0.40
1:B:218:PRO:HG3	1:B:323:VAL:HG22	2.03	0.40
1:K:240:VAL:HG11	1:K:271:VAL:HG13	2.03	0.40
1:N:112:ASN:HD22	1:N:113:PRO:CD	2.34	0.40
1:A:266:THR:HG22	1:A:271:VAL:HG13	2.04	0.40
1:G:136:VAL:HA	1:G:137:PRO:HD3	1.96	0.40
1:L:417:VAL:HG11	1:L:477:GLY:HA3	2.03	0.40
1:C:199:TYR:OH	1:C:327:LYS:HG3	2.20	0.40
1:G:242:LYS:O	1:G:243:ALA:HB3	2.21	0.40
1:L:356:ALA:HB3	1:L:362:ARG:NH2	2.37	0.40
1:I:364:LYS:HD3	1:I:364:LYS:HA	1.94	0.40
1:D:219:PHE:C	1:D:220:ILE:HG13	2.42	0.40
1:F:475:ASN:N	1:F:475:ASN:HD22	2.18	0.40
1:I:292:ILE:HG13	1:I:292:ILE:H	1.69	0.40
1:E:201:SER:O	1:E:204:PHE:HD2	2.05	0.40
1:A:123:ALA:HB2	1:A:440:ILE:HG23	2.03	0.40
1:E:6:VAL:HG22	1:E:521:VAL:HG22	2.03	0.40
1:M:475:ASN:HD22	1:M:475:ASN:N	2.19	0.40
1:L:496:PRO:O	1:L:499:VAL:CG1	2.69	0.40
1:D:177:VAL:HG23	1:D:379:ILE:HD12	2.04	0.40
1:K:254:VAL:O	1:K:259:LEU:HB2	2.21	0.40
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.21	0.40
1:N:364:LYS:HA	1:N:364:LYS:HD3	1.91	0.40

There are no symmetry-related clashes.

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	A	522/547 (95%)	494 (95%)	23 (4%)	5 (1%)	19 65
1	B	522/547 (95%)	490 (94%)	25 (5%)	7 (1%)	15 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	522/547 (95%)	490 (94%)	27 (5%)	5 (1%)	19	65
1	D	522/547 (95%)	487 (93%)	30 (6%)	5 (1%)	19	65
1	E	522/547 (95%)	493 (94%)	22 (4%)	7 (1%)	15	60
1	F	522/547 (95%)	496 (95%)	19 (4%)	7 (1%)	15	60
1	G	522/547 (95%)	490 (94%)	28 (5%)	4 (1%)	24	69
1	H	522/547 (95%)	496 (95%)	18 (3%)	8 (2%)	13	58
1	I	522/547 (95%)	495 (95%)	25 (5%)	2 (0%)	39	79
1	J	522/547 (95%)	496 (95%)	21 (4%)	5 (1%)	19	65
1	K	522/547 (95%)	485 (93%)	33 (6%)	4 (1%)	24	69
1	L	522/547 (95%)	501 (96%)	20 (4%)	1 (0%)	52	86
1	M	522/547 (95%)	495 (95%)	22 (4%)	5 (1%)	19	65
1	N	522/547 (95%)	483 (92%)	32 (6%)	7 (1%)	15	60
All	All	7308/7658 (95%)	6891 (94%)	345 (5%)	72 (1%)	19	65

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLY
1	A	375	GLY
1	B	205	ILE
1	H	322	ARG
1	H	336	VAL
1	I	244	GLY
1	K	208	PRO
1	A	256	GLY
1	B	256	GLY
1	B	334	ASP
1	B	336	VAL
1	D	256	GLY
1	E	256	GLY
1	G	271	VAL
1	G	293	ALA
1	G	337	GLY
1	J	270	ILE
1	J	271	VAL
1	K	356	ALA
1	B	310	GLU
1	C	282	GLY

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Mol	Chain	Res	Type
1	E	375	GLY
1	E	385	THR
1	F	322	ARG
1	F	384	ALA
1	F	385	THR
1	H	271	VAL
1	H	334	ASP
1	I	271	VAL
1	J	334	ASP
1	M	334	ASP
1	N	313	THR
1	N	317	LEU
1	B	322	ARG
1	B	386	GLU
1	D	244	GLY
1	D	385	THR
1	E	246	PRO
1	E	334	ASP
1	F	271	VAL
1	H	356	ALA
1	J	231	ARG
1	M	271	VAL
1	N	271	VAL
1	N	334	ASP
1	A	271	VAL
1	D	271	VAL
1	E	271	VAL
1	H	244	GLY
1	K	322	ARG
1	L	271	VAL
1	M	243	ALA
1	A	234	LEU
1	C	246	PRO
1	C	256	GLY
1	C	271	VAL
1	D	259	LEU
1	E	383	ALA
1	G	270	ILE
1	H	205	ILE
1	M	270	ILE
1	N	336	VAL
1	F	205	ILE

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Mol	Chain	Res	Type
1	F	244	GLY
1	F	256	GLY
1	N	282	GLY
1	C	306	GLY
1	H	256	GLY
1	K	202	PRO
1	J	244	GLY
1	M	269	GLY
1	N	234	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/414 (98%)	386 (96%)	18 (4%)	34	71
1	B	404/414 (98%)	392 (97%)	12 (3%)	48	79
1	C	404/414 (98%)	392 (97%)	12 (3%)	48	79
1	D	404/414 (98%)	387 (96%)	17 (4%)	36	72
1	E	404/414 (98%)	392 (97%)	12 (3%)	48	79
1	F	404/414 (98%)	389 (96%)	15 (4%)	41	75
1	G	404/414 (98%)	385 (95%)	19 (5%)	32	70
1	H	404/414 (98%)	393 (97%)	11 (3%)	52	80
1	I	404/414 (98%)	389 (96%)	15 (4%)	41	75
1	J	404/414 (98%)	388 (96%)	16 (4%)	38	73
1	K	404/414 (98%)	385 (95%)	19 (5%)	32	70
1	L	404/414 (98%)	393 (97%)	11 (3%)	52	80
1	M	404/414 (98%)	393 (97%)	11 (3%)	52	80
1	N	404/414 (98%)	397 (98%)	7 (2%)	68	88
All	All	5656/5796 (98%)	5461 (97%)	195 (3%)	44	77

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	112	ASN
1	A	134	LEU
1	A	217	SER
1	A	234	LEU
1	A	270	ILE
1	A	288	MET
1	A	292	ILE
1	A	294	THR
1	A	313	THR
1	A	331	THR
1	A	354	GLU
1	A	367	GLU
1	A	369	VAL
1	A	378	VAL
1	A	379	ILE
1	A	398	ASP
1	A	463	SER
1	B	91	THR
1	B	112	ASN
1	B	134	LEU
1	B	227	ILE
1	B	273	VAL
1	B	295	LEU
1	B	299	THR
1	B	315	GLU
1	B	328	ASP
1	B	329	THR
1	B	331	THR
1	B	475	ASN
1	C	91	THR
1	C	112	ASN
1	C	134	LEU
1	C	196	ASP
1	C	217	SER
1	C	231	ARG
1	C	294	THR
1	C	331	THR
1	C	359	ASP
1	C	385	THR
1	C	391	GLU
1	C	475	ASN
1	D	91	THR

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Mol	Chain	Res	Type
1	D	112	ASN
1	D	134	LEU
1	D	199	TYR
1	D	200	LEU
1	D	201	SER
1	D	257	GLU
1	D	265	ASN
1	D	299	THR
1	D	309	LEU
1	D	315	GLU
1	D	331	THR
1	D	369	VAL
1	D	390	LYS
1	D	398	ASP
1	D	400	LEU
1	D	463	SER
1	E	91	THR
1	E	112	ASN
1	E	134	LEU
1	E	196	ASP
1	E	209	GLU
1	E	240	VAL
1	E	257	GLU
1	E	265	ASN
1	E	328	ASP
1	E	331	THR
1	E	463	SER
1	E	475	ASN
1	F	91	THR
1	F	112	ASN
1	F	134	LEU
1	F	200	LEU
1	F	217	SER
1	F	268	ARG
1	F	284	ARG
1	F	289	LEU
1	F	299	THR
1	F	317	LEU
1	F	331	THR
1	F	343	GLN
1	F	350	ARG
1	F	463	SER

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Mol	Chain	Res	Type
1	F	475	ASN
1	G	91	THR
1	G	112	ASN
1	G	134	LEU
1	G	206	ASN
1	G	217	SER
1	G	242	LYS
1	G	249	ILE
1	G	288	MET
1	G	295	LEU
1	G	310	GLU
1	G	315	GLU
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	351	GLN
1	G	360	TYR
1	G	369	VAL
1	G	463	SER
1	G	475	ASN
1	H	91	THR
1	H	112	ASN
1	H	134	LEU
1	H	200	LEU
1	H	217	SER
1	H	225	LYS
1	H	314	LEU
1	H	317	LEU
1	H	331	THR
1	H	386	GLU
1	H	475	ASN
1	I	91	THR
1	I	112	ASN
1	I	134	LEU
1	I	196	ASP
1	I	199	TYR
1	I	200	LEU
1	I	209	GLU
1	I	210	THR
1	I	225	LYS
1	I	257	GLU
1	I	289	LEU

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Mol	Chain	Res	Type
1	I	294	THR
1	I	299	THR
1	I	329	THR
1	I	475	ASN
1	J	77	VAL
1	J	91	THR
1	J	112	ASN
1	J	134	LEU
1	J	200	LEU
1	J	225	LYS
1	J	228	SER
1	J	294	THR
1	J	299	THR
1	J	313	THR
1	J	327	LYS
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	390	LYS
1	J	463	SER
1	K	91	THR
1	K	112	ASN
1	K	134	LEU
1	K	200	LEU
1	K	206	ASN
1	K	210	THR
1	K	225	LYS
1	K	253	ASP
1	K	255	GLU
1	K	273	VAL
1	K	294	THR
1	K	310	GLU
1	K	316	ASP
1	K	328	ASP
1	K	329	THR
1	K	338	GLU
1	K	361	ASP
1	K	368	ARG
1	K	463	SER
1	L	91	THR
1	L	112	ASN
1	L	134	LEU

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Mol	Chain	Res	Type
1	L	200	LEU
1	L	209	GLU
1	L	225	LYS
1	L	283	ASP
1	L	295	LEU
1	L	398	ASP
1	L	463	SER
1	L	475	ASN
1	M	91	THR
1	M	112	ASN
1	M	134	LEU
1	M	199	TYR
1	M	200	LEU
1	M	225	LYS
1	M	316	ASP
1	M	329	THR
1	M	398	ASP
1	M	463	SER
1	M	475	ASN
1	N	91	THR
1	N	112	ASN
1	N	134	LEU
1	N	225	LYS
1	N	299	THR
1	N	329	THR
1	N	463	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	352	GLN
1	B	112	ASN
1	B	366	GLN
1	C	37	ASN
1	C	112	ASN
1	D	112	ASN
1	E	112	ASN
1	E	351	GLN
1	F	112	ASN
1	G	112	ASN
1	H	112	ASN

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Mol	Chain	Res	Type
1	H	229	ASN
1	I	112	ASN
1	J	37	ASN
1	J	112	ASN
1	J	265	ASN
1	J	366	GLN
1	L	206	ASN
1	M	351	GLN
1	N	112	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 60 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AGS	A	549	4	24,33,33	1.39	1 (4%)	28,52,52	2.34	5 (17%)
2	AGS	B	549	4	24,33,33	1.20	2 (8%)	28,52,52	2.39	6 (21%)
2	AGS	C	549	4	24,33,33	1.64	1 (4%)	28,52,52	2.43	6 (21%)
2	AGS	D	549	4	24,33,33	1.25	1 (4%)	28,52,52	2.36	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	E	549	4	24,33,33	1.32	1 (4%)	28,52,52	2.42	6 (21%)
2	AGS	F	549	4	24,33,33	1.49	1 (4%)	28,52,52	2.45	5 (17%)
2	AGS	G	549	4	24,33,33	1.58	1 (4%)	28,52,52	2.41	6 (21%)
2	AGS	H	549	4	24,33,33	1.19	1 (4%)	28,52,52	2.38	6 (21%)
2	AGS	I	549	4	24,33,33	1.34	1 (4%)	28,52,52	2.38	6 (21%)
2	AGS	J	549	4	24,33,33	1.84	1 (4%)	28,52,52	2.43	5 (17%)
2	AGS	K	549	4	24,33,33	1.67	1 (4%)	28,52,52	2.46	6 (21%)
2	AGS	L	549	4	24,33,33	1.62	2 (8%)	28,52,52	2.35	6 (21%)
2	AGS	M	549	4	24,33,33	1.06	1 (4%)	28,52,52	2.51	6 (21%)
2	AGS	N	549	4	24,33,33	1.96	1 (4%)	28,52,52	2.36	6 (21%)

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	AGS	A	549	4	-	0/15/38/38	0/3/3/3
2	AGS	B	549	4	-	0/15/38/38	0/3/3/3
2	AGS	C	549	4	-	0/15/38/38	0/3/3/3
2	AGS	D	549	4	-	0/15/38/38	0/3/3/3
2	AGS	E	549	4	-	0/15/38/38	0/3/3/3
2	AGS	F	549	4	-	0/15/38/38	0/3/3/3
2	AGS	G	549	4	-	0/15/38/38	0/3/3/3
2	AGS	H	549	4	-	0/15/38/38	0/3/3/3
2	AGS	I	549	4	-	0/15/38/38	0/3/3/3
2	AGS	J	549	4	-	0/15/38/38	0/3/3/3
2	AGS	K	549	4	-	0/15/38/38	0/3/3/3
2	AGS	L	549	4	-	0/15/38/38	0/3/3/3
2	AGS	M	549	4	-	0/15/38/38	0/3/3/3
2	AGS	N	549	4	-	0/15/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	549	AGS	PG-O2G	-2.03	1.48	1.55
2	M	549	AGS	O4'-C1'	2.17	1.44	1.41
2	L	549	AGS	O4'-C1'	2.53	1.44	1.41
2	B	549	AGS	PG-S1G	3.19	1.96	1.90
2	H	549	AGS	PG-S1G	3.28	1.97	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	549	AGS	PG-S1G	3.59	1.97	1.90
2	E	549	AGS	PG-S1G	4.14	1.98	1.90
2	I	549	AGS	PG-S1G	4.16	1.98	1.90
2	A	549	AGS	PG-S1G	4.79	1.99	1.90
2	F	549	AGS	PG-S1G	5.34	2.01	1.90
2	L	549	AGS	PG-S1G	6.16	2.02	1.90
2	G	549	AGS	PG-S1G	6.20	2.02	1.90
2	C	549	AGS	PG-S1G	6.44	2.03	1.90
2	K	549	AGS	PG-S1G	6.68	2.03	1.90
2	J	549	AGS	PG-S1G	7.76	2.05	1.90
2	N	549	AGS	PG-S1G	8.28	2.06	1.90

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	549	AGS	N3-C2-N1	-10.03	121.21	128.89
2	K	549	AGS	N3-C2-N1	-9.96	121.27	128.89
2	C	549	AGS	N3-C2-N1	-9.93	121.29	128.89
2	J	549	AGS	N3-C2-N1	-9.92	121.30	128.89
2	E	549	AGS	N3-C2-N1	-9.81	121.38	128.89
2	B	549	AGS	N3-C2-N1	-9.76	121.42	128.89
2	H	549	AGS	N3-C2-N1	-9.71	121.46	128.89
2	G	549	AGS	N3-C2-N1	-9.67	121.49	128.89
2	D	549	AGS	N3-C2-N1	-9.59	121.55	128.89
2	A	549	AGS	N3-C2-N1	-9.56	121.57	128.89
2	I	549	AGS	N3-C2-N1	-9.49	121.63	128.89
2	L	549	AGS	N3-C2-N1	-9.41	121.69	128.89
2	N	549	AGS	N3-C2-N1	-9.35	121.73	128.89
2	M	549	AGS	N3-C2-N1	-9.35	121.74	128.89
2	N	549	AGS	C4'-O4'-C1'	-5.16	104.05	109.72
2	K	549	AGS	C4'-O4'-C1'	-5.13	104.08	109.72
2	M	549	AGS	C4'-O4'-C1'	-5.12	104.09	109.72
2	G	549	AGS	C4'-O4'-C1'	-5.05	104.17	109.72
2	F	549	AGS	C4'-O4'-C1'	-5.04	104.18	109.72
2	I	549	AGS	C4'-O4'-C1'	-5.04	104.18	109.72
2	L	549	AGS	C4'-O4'-C1'	-4.97	104.26	109.72
2	J	549	AGS	C4'-O4'-C1'	-4.91	104.32	109.72
2	E	549	AGS	C4'-O4'-C1'	-4.85	104.39	109.72
2	H	549	AGS	C4'-O4'-C1'	-4.78	104.47	109.72
2	B	549	AGS	C4'-O4'-C1'	-4.76	104.49	109.72
2	C	549	AGS	C4'-O4'-C1'	-4.74	104.51	109.72
2	D	549	AGS	C4'-O4'-C1'	-4.65	104.61	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	549	AGS	PA-O3A-PB	-4.54	119.99	132.73
2	A	549	AGS	C4'-O4'-C1'	-4.45	104.83	109.72
2	M	549	AGS	PB-O3B-PG	-3.77	120.02	132.67
2	I	549	AGS	PB-O3B-PG	-3.34	121.48	132.67
2	K	549	AGS	PB-O3B-PG	-3.30	121.60	132.67
2	J	549	AGS	PB-O3B-PG	-3.26	121.72	132.67
2	G	549	AGS	PB-O3B-PG	-3.18	121.99	132.67
2	C	549	AGS	PB-O3B-PG	-3.18	122.00	132.67
2	F	549	AGS	PB-O3B-PG	-3.16	122.08	132.67
2	E	549	AGS	PB-O3B-PG	-3.15	122.10	132.67
2	M	549	AGS	C2'-C1'-N9	-3.14	109.49	114.29
2	L	549	AGS	PB-O3B-PG	-3.11	122.23	132.67
2	N	549	AGS	PB-O3B-PG	-3.10	122.27	132.67
2	B	549	AGS	PB-O3B-PG	-3.10	122.27	132.67
2	A	549	AGS	PB-O3B-PG	-3.10	122.28	132.67
2	H	549	AGS	PB-O3B-PG	-3.08	122.34	132.67
2	D	549	AGS	PB-O3B-PG	-3.01	122.56	132.67
2	A	549	AGS	PA-O3A-PB	-2.97	124.38	132.73
2	I	549	AGS	PA-O3A-PB	-2.85	124.73	132.73
2	D	549	AGS	PA-O3A-PB	-2.85	124.74	132.73
2	E	549	AGS	PA-O3A-PB	-2.82	124.81	132.73
2	C	549	AGS	PA-O3A-PB	-2.80	124.87	132.73
2	N	549	AGS	PA-O3A-PB	-2.79	124.91	132.73
2	E	549	AGS	C5'-C4'-C3'	-2.65	104.70	115.21
2	L	549	AGS	PA-O3A-PB	-2.63	125.33	132.73
2	J	549	AGS	PA-O3A-PB	-2.62	125.36	132.73
2	D	549	AGS	C5'-C4'-C3'	-2.62	104.81	115.21
2	F	549	AGS	PA-O3A-PB	-2.62	125.38	132.73
2	K	549	AGS	PA-O3A-PB	-2.61	125.39	132.73
2	G	549	AGS	PA-O3A-PB	-2.61	125.40	132.73
2	J	549	AGS	C5'-C4'-C3'	-2.61	104.86	115.21
2	H	549	AGS	PA-O3A-PB	-2.59	125.45	132.73
2	B	549	AGS	PA-O3A-PB	-2.58	125.50	132.73
2	F	549	AGS	C5'-C4'-C3'	-2.57	105.00	115.21
2	B	549	AGS	C5'-C4'-C3'	-2.56	105.05	115.21
2	N	549	AGS	C5'-C4'-C3'	-2.55	105.08	115.21
2	G	549	AGS	C5'-C4'-C3'	-2.55	105.10	115.21
2	K	549	AGS	C5'-C4'-C3'	-2.52	105.20	115.21
2	H	549	AGS	C5'-C4'-C3'	-2.49	105.32	115.21
2	C	549	AGS	C5'-C4'-C3'	-2.48	105.38	115.21
2	I	549	AGS	C5'-C4'-C3'	-2.45	105.47	115.21
2	A	549	AGS	C5'-C4'-C3'	-2.42	105.60	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	549	AGS	C5'-C4'-C3'	-2.40	105.67	115.21
2	I	549	AGS	C4-C5-N7	-2.24	107.41	109.48
2	N	549	AGS	C4-C5-N7	-2.24	107.42	109.48
2	G	549	AGS	C4-C5-N7	-2.21	107.44	109.48
2	E	549	AGS	C4-C5-N7	-2.18	107.47	109.48
2	M	549	AGS	C4-C5-N7	-2.15	107.50	109.48
2	D	549	AGS	C4-C5-N7	-2.14	107.51	109.48
2	L	549	AGS	C4-C5-N7	-2.10	107.55	109.48
2	H	549	AGS	C4-C5-N7	-2.07	107.57	109.48
2	K	549	AGS	C4-C5-N7	-2.06	107.58	109.48
2	B	549	AGS	C4-C5-N7	-2.03	107.61	109.48
2	C	549	AGS	C4-C5-N7	-2.01	107.63	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	549	AGS	1	0
2	D	549	AGS	1	0
2	E	549	AGS	1	0
2	G	549	AGS	2	0
2	I	549	AGS	1	0
2	J	549	AGS	1	0
2	K	549	AGS	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	A	524/547 (95%)	-0.16	2 (0%) 93 90	125, 125, 125, 125	0
1	B	524/547 (95%)	-0.15	2 (0%) 93 90	125, 125, 125, 125	0
1	C	524/547 (95%)	-0.06	12 (2%) 64 52	125, 125, 125, 125	0
1	D	524/547 (95%)	-0.10	7 (1%) 79 70	125, 125, 125, 125	0
1	E	524/547 (95%)	0.00	11 (2%) 67 55	125, 125, 125, 125	0
1	F	524/547 (95%)	-0.09	9 (1%) 73 62	125, 125, 125, 125	0
1	G	524/547 (95%)	-0.11	7 (1%) 79 70	125, 125, 125, 125	0
1	H	524/547 (95%)	0.02	15 (2%) 55 42	125, 125, 125, 125	0
1	I	524/547 (95%)	-0.10	13 (2%) 61 48	125, 125, 125, 125	0
1	J	524/547 (95%)	0.01	12 (2%) 64 52	125, 125, 125, 125	0
1	K	524/547 (95%)	-0.01	13 (2%) 61 48	125, 125, 125, 125	0
1	L	524/547 (95%)	0.07	22 (4%) 40 29	125, 125, 125, 125	0
1	M	524/547 (95%)	0.25	35 (6%) 21 14	125, 125, 125, 125	0
1	N	524/547 (95%)	0.41	41 (7%) 16 11	125, 125, 125, 125	0
All	All	7336/7658 (95%)	-0.00	201 (2%) 58 46	125, 125, 125, 125	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	223	ALA	12.2
1	I	141	SER	7.4
1	M	153	ASN	7.1
1	E	152	ALA	6.9
1	N	148	GLY	6.8
1	N	355	GLU	6.5
1	N	251	ALA	6.3
1	M	331	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	M	152	ALA	5.6
1	M	140	ASP	5.4
1	J	152	ALA	5.4
1	M	139	SER	5.3
1	N	139	SER	5.2
1	N	141	SER	5.1
1	N	152	ALA	5.1
1	N	275	ALA	5.1
1	L	141	SER	5.0
1	N	151	SER	4.9
1	E	153	ASN	4.9
1	I	140	ASP	4.9
1	H	141	SER	4.8
1	N	193	MET	4.6
1	E	151	SER	4.6
1	F	223	ALA	4.5
1	N	310	GLU	4.5
1	M	141	SER	4.4
1	K	153	ASN	4.4
1	H	139	SER	4.4
1	N	153	ASN	4.3
1	N	301	ILE	4.3
1	N	149	THR	4.3
1	D	63	GLU	4.2
1	G	147	VAL	4.2
1	N	221	LEU	4.2
1	N	222	LEU	4.1
1	L	357	THR	3.9
1	K	271	VAL	3.9
1	N	484	GLU	3.9
1	J	151	SER	3.8
1	N	154	SER	3.8
1	L	169	VAL	3.8
1	M	304	GLU	3.8
1	M	275	ALA	3.8
1	M	268	ARG	3.8
1	N	354	GLU	3.8
1	N	174	VAL	3.6
1	I	274	ALA	3.6
1	J	139	SER	3.6
1	K	151	SER	3.5
1	G	148	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	141	SER	3.5
1	C	152	ALA	3.4
1	M	274	ALA	3.4
1	N	231	ARG	3.4
1	M	265	ASN	3.4
1	G	140	ASP	3.3
1	M	273	VAL	3.3
1	M	212	ALA	3.3
1	L	214	GLU	3.2
1	L	374	GLY	3.2
1	C	151	SER	3.2
1	L	191	GLU	3.2
1	M	201	SER	3.2
1	J	247	LEU	3.2
1	N	194	GLN	3.2
1	E	139	SER	3.1
1	G	139	SER	3.1
1	A	519	CYS	3.1
1	N	140	ASP	3.1
1	L	186	GLU	3.1
1	E	140	ASP	3.0
1	L	340	ALA	3.0
1	M	154	SER	3.0
1	N	192	GLY	3.0
1	M	206	ASN	3.0
1	F	140	ASP	3.0
1	N	142	LYS	3.0
1	N	147	VAL	3.0
1	I	153	ASN	3.0
1	C	139	SER	3.0
1	J	153	ASN	3.0
1	M	186	GLU	2.9
1	H	305	ILE	2.9
1	M	266	THR	2.9
1	N	267	MET	2.9
1	N	256	GLY	2.8
1	H	140	ASP	2.8
1	F	151	SER	2.8
1	F	152	ALA	2.8
1	M	142	LYS	2.8
1	C	376	VAL	2.8
1	G	151	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	144	ILE	2.8
1	H	275	ALA	2.7
1	J	141	SER	2.7
1	M	189	VAL	2.7
1	H	233	MET	2.7
1	N	212	ALA	2.7
1	H	151	SER	2.7
1	M	493	ILE	2.7
1	M	214	GLU	2.7
1	C	484	GLU	2.7
1	D	320	ALA	2.7
1	N	250	ILE	2.6
1	L	311	LYS	2.6
1	I	139	SER	2.6
1	H	222	LEU	2.6
1	J	150	ILE	2.6
1	M	228	SER	2.6
1	F	148	GLY	2.6
1	I	204	PHE	2.6
1	C	141	SER	2.6
1	N	347	ALA	2.6
1	I	142	LYS	2.6
1	N	356	ALA	2.6
1	N	340	ALA	2.6
1	H	300	VAL	2.5
1	L	283	ASP	2.5
1	M	181	THR	2.5
1	J	140	ASP	2.5
1	L	187	LEU	2.5
1	L	154	SER	2.5
1	M	227	ILE	2.5
1	F	141	SER	2.5
1	L	145	ALA	2.5
1	M	354	GLU	2.4
1	I	275	ALA	2.4
1	C	203	TYR	2.4
1	E	169	VAL	2.4
1	L	113	PRO	2.4
1	L	140	ASP	2.4
1	C	148	GLY	2.4
1	K	381	VAL	2.4
1	A	304	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	343	GLN	2.4
1	E	376	VAL	2.4
1	E	193	MET	2.4
1	F	222	LEU	2.4
1	C	189	VAL	2.3
1	N	299	THR	2.3
1	N	351	GLN	2.3
1	L	354	GLU	2.3
1	J	484	GLU	2.3
1	N	311	LYS	2.3
1	J	142	LYS	2.3
1	K	191	GLU	2.3
1	K	376	VAL	2.3
1	I	183	LEU	2.3
1	I	519	CYS	2.3
1	H	143	ALA	2.3
1	D	193	MET	2.3
1	J	149	THR	2.2
1	J	191	GLU	2.2
1	F	44	PHE	2.2
1	D	305	ILE	2.2
1	K	333	ILE	2.2
1	N	332	ILE	2.2
1	H	144	ILE	2.2
1	M	250	ILE	2.2
1	M	305	ILE	2.2
1	C	160	LYS	2.2
1	E	192	GLY	2.2
1	M	173	GLY	2.2
1	M	323	VAL	2.2
1	K	357	THR	2.2
1	D	64	ASP	2.2
1	L	243	ALA	2.2
1	H	517	THR	2.1
1	I	203	TYR	2.1
1	N	233	MET	2.1
1	D	247	LEU	2.1
1	E	375	GLY	2.1
1	L	493	ILE	2.1
1	F	139	SER	2.1
1	N	274	ALA	2.1
1	C	377	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	274	ALA	2.1
1	L	159	GLY	2.1
1	K	139	SER	2.1
1	H	323	VAL	2.1
1	M	44	PHE	2.1
1	L	188	ASP	2.1
1	N	5	ASP	2.1
1	K	273	VAL	2.1
1	K	174	VAL	2.1
1	M	148	GLY	2.1
1	L	147	VAL	2.1
1	H	331	THR	2.0
1	K	152	ALA	2.0
1	M	143	ALA	2.0
1	M	185	ASP	2.0
1	C	477	GLY	2.0
1	E	522	THR	2.0
1	H	234	LEU	2.0
1	I	194	GLN	2.0
1	N	260	ALA	2.0
1	I	172	GLU	2.0
1	D	275	ALA	2.0
1	L	167	ASP	2.0
1	M	213	VAL	2.0
1	B	220	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	AGS	C	549	31/31	0.80	0.23	-0.07	125,125,125,125	0
2	AGS	F	549	31/31	0.84	0.24	-0.15	125,125,125,125	0
2	AGS	E	549	31/31	0.76	0.27	-0.17	125,125,125,125	0
2	AGS	N	549	31/31	0.80	0.23	-0.22	125,125,125,125	0
2	AGS	L	549	31/31	0.79	0.25	-0.29	125,125,125,125	0
2	AGS	G	549	31/31	0.87	0.22	-0.34	125,125,125,125	0
3	TL	C	552	1/1	0.96	0.25	-0.40	125,125,125,125	1
2	AGS	J	549	31/31	0.82	0.27	-0.41	125,125,125,125	0
3	TL	F	550	1/1	0.99	0.21	-0.46	125,125,125,125	1
2	AGS	K	549	31/31	0.88	0.21	-0.52	125,125,125,125	0
2	AGS	H	549	31/31	0.83	0.23	-0.53	125,125,125,125	0
2	AGS	B	549	31/31	0.86	0.19	-0.72	125,125,125,125	0
3	TL	L	550	1/1	0.89	0.15	-0.77	125,125,125,125	1
2	AGS	I	549	31/31	0.90	0.17	-0.79	125,125,125,125	0
2	AGS	A	549	31/31	0.86	0.21	-0.81	125,125,125,125	0
2	AGS	M	549	31/31	0.83	0.21	-0.83	125,125,125,125	0
3	TL	J	551	1/1	0.74	0.18	-0.84	125,125,125,125	1
3	TL	M	552	1/1	0.95	0.20	-0.86	125,125,125,125	1
3	TL	A	554	1/1	0.99	0.19	-0.86	125,125,125,125	1
3	TL	N	551	1/1	0.93	0.20	-0.90	125,125,125,125	1
3	TL	H	552	1/1	0.93	0.16	-0.92	125,125,125,125	1
2	AGS	D	549	31/31	0.88	0.19	-0.95	125,125,125,125	0
3	TL	K	552	1/1	0.86	0.18	-0.96	125,125,125,125	1
3	TL	B	552	1/1	0.87	0.19	-1.04	125,125,125,125	1
3	TL	D	1	1/1	0.99	0.19	-1.11	125,125,125,125	1
3	TL	G	551	1/1	0.73	0.13	-1.12	125,125,125,125	1
3	TL	B	554	1/1	1.00	0.19	-1.14	125,125,125,125	1
3	TL	G	550	1/1	0.95	0.11	-1.22	125,125,125,125	1
3	TL	J	550	1/1	0.94	0.14	-1.25	125,125,125,125	1
3	TL	L	551	1/1	0.85	0.16	-1.26	125,125,125,125	1
3	TL	B	551	1/1	0.96	0.14	-1.29	125,125,125,125	1
3	TL	K	551	1/1	0.98	0.11	-1.50	125,125,125,125	1
3	TL	H	554	1/1	0.76	0.15	-1.66	125,125,125,125	1
3	TL	I	550	1/1	0.98	0.08	-1.67	125,125,125,125	1
3	TL	G	552	1/1	0.94	0.12	-1.68	125,125,125,125	1
3	TL	F	554	1/1	0.98	0.17	-1.71	125,125,125,125	1
3	TL	I	551	1/1	0.95	0.13	-1.75	125,125,125,125	1
3	TL	D	551	1/1	0.93	0.12	-1.85	125,125,125,125	1
3	TL	C	550	1/1	0.94	0.09	-1.94	125,125,125,125	1
3	TL	A	552	1/1	0.94	0.11	-2.15	125,125,125,125	1
3	TL	F	551	1/1	0.73	0.11	-2.21	125,125,125,125	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TL	I	552	1/1	0.98	0.06	-2.22	125,125,125,125	1
3	TL	A	550	1/1	0.96	0.08	-2.23	125,125,125,125	1
3	TL	J	552	1/1	0.98	0.04	-2.41	125,125,125,125	1
3	TL	E	550	1/1	0.85	0.13	-2.44	125,125,125,125	1
3	TL	A	551	1/1	0.88	0.17	-2.57	125,125,125,125	1
3	TL	H	550	1/1	0.94	0.07	-2.58	125,125,125,125	1
3	TL	K	550	1/1	0.88	0.10	-2.86	125,125,125,125	1
3	TL	H	551	1/1	0.93	0.07	-2.92	125,125,125,125	1
3	TL	N	550	1/1	0.94	0.07	-3.00	125,125,125,125	1
3	TL	F	552	1/1	0.97	0.08	-3.01	125,125,125,125	1
3	TL	M	551	1/1	0.96	0.09	-3.02	125,125,125,125	1
3	TL	C	551	1/1	0.89	0.08	-3.22	125,125,125,125	1
3	TL	D	552	1/1	0.91	0.05	-3.36	125,125,125,125	1
3	TL	M	550	1/1	0.96	0.10	-3.37	125,125,125,125	1
3	TL	L	552	1/1	0.96	0.04	-3.42	125,125,125,125	1
3	TL	B	550	1/1	0.95	0.11	-3.51	125,125,125,125	1
3	TL	E	552	1/1	0.99	0.25	-3.64	125,125,125,125	1
3	TL	E	551	1/1	0.94	0.06	-3.99	125,125,125,125	1
4	MG	K	553	1/1	0.95	0.12	-	125,125,125,125	0
4	MG	B	553	1/1	0.95	0.16	-	125,125,125,125	0
4	MG	F	553	1/1	0.87	0.25	-	125,125,125,125	0
4	MG	M	553	1/1	0.94	0.14	-	125,125,125,125	0
4	MG	D	553	1/1	0.89	0.21	-	125,125,125,125	0
4	MG	C	553	1/1	0.80	0.41	-	125,125,125,125	0
4	MG	I	553	1/1	0.84	0.23	-	125,125,125,125	0
4	MG	E	553	1/1	0.95	0.34	-	125,125,125,125	0
4	MG	L	553	1/1	0.92	0.22	-	125,125,125,125	0
4	MG	J	553	1/1	0.94	0.12	-	125,125,125,125	0
4	MG	A	553	1/1	0.79	0.25	-	125,125,125,125	0
4	MG	N	552	1/1	0.86	0.32	-	125,125,125,125	0
3	TL	D	550	1/1	0.96	0.11	-	125,125,125,125	1
4	MG	G	553	1/1	0.84	0.22	-	125,125,125,125	0
4	MG	H	553	1/1	0.86	0.24	-	125,125,125,125	0

6.5 Other polymers ⓘ

There are no such residues in this entry.