Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:15 AM GMT

PDB ID	:	3DUG
Title	:	Crystal structure of zn-dependent arginine carboxypeptidase complexed with zinc
Authors	:	Patskovsky, Y.; Ramagopal, U.A.; Toro, R.; Meyer, A.J.; Freeman, J.; Iizuka, M.; Bain, K.; Rodgers, L.; Raushel, F.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-07-17
Resolution	:	2.62 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

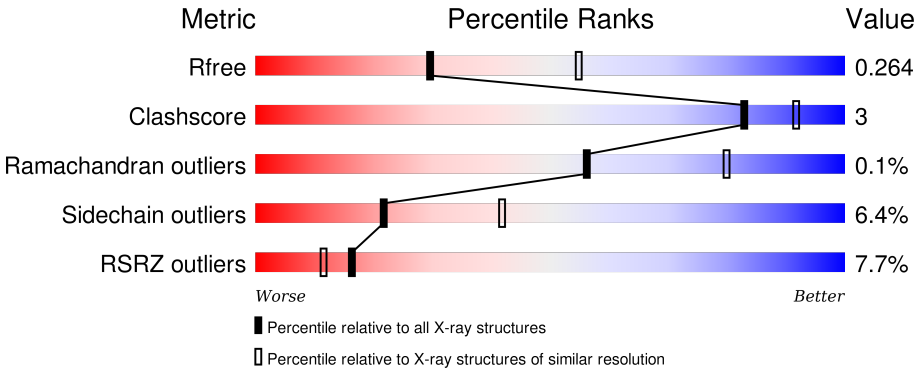
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.62 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 <=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	408	4% 84% 12%
1	B	408	4% 84% 11%
1	C	408	11% 85% 11%
1	D	408	7% 85% 11%
1	E	408	6% 84% 11%

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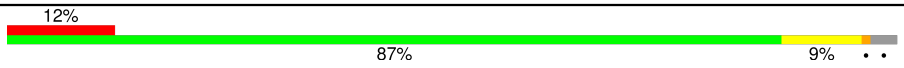
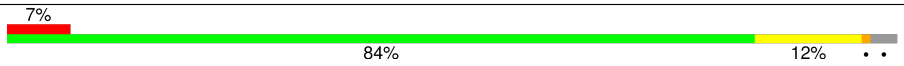
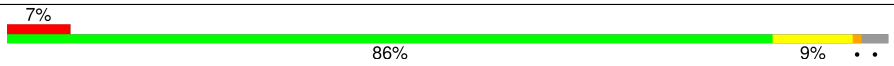
Mol	Chain	Length	Quality of chain
1	F	408	
1	G	408	
1	H	408	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	427	-	-	-	X
2	ZN	D	427	-	-	-	X
2	ZN	E	427	-	-	-	X
2	ZN	G	427	-	-	-	X
4	GOL	A	430	-	-	-	X
4	GOL	B	430	-	-	-	X
4	GOL	B	432	-	-	-	X
4	GOL	B	433	-	-	-	X
4	GOL	E	431	-	-	-	X
4	GOL	G	430	-	-	-	X
4	GOL	H	430	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24575 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 ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	2	0
			3012	1893	525	578	16			
1	B	394	Total	C	N	O	S	0	2	0
			3012	1893	525	578	16			
1	C	395	Total	C	N	O	S	0	2	0
			3026	1901	529	580	16			
1	D	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	E	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	F	395	Total	C	N	O	S	0	2	0
			3021	1898	524	583	16			
1	G	394	Total	C	N	O	S	0	0	0
			3001	1886	522	577	16			
1	H	394	Total	C	N	O	S	0	4	0
			3027	1902	529	580	16			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		
2	E	4	Total	Zn	0	0
			4	4		
2	H	4	Total	Zn	0	0
			4	4		
2	B	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		

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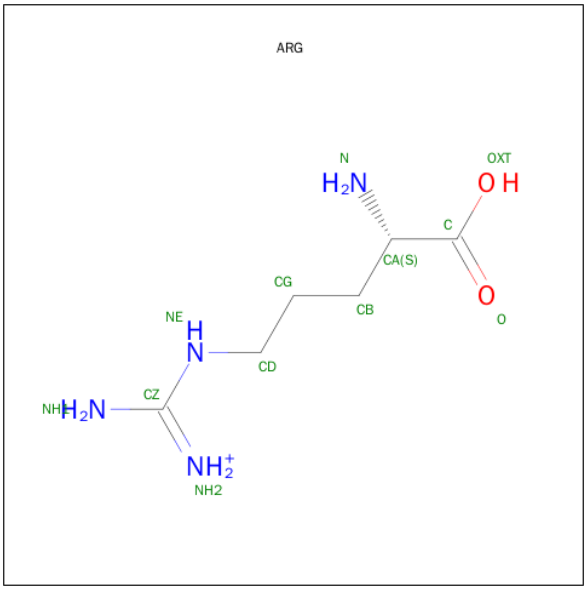
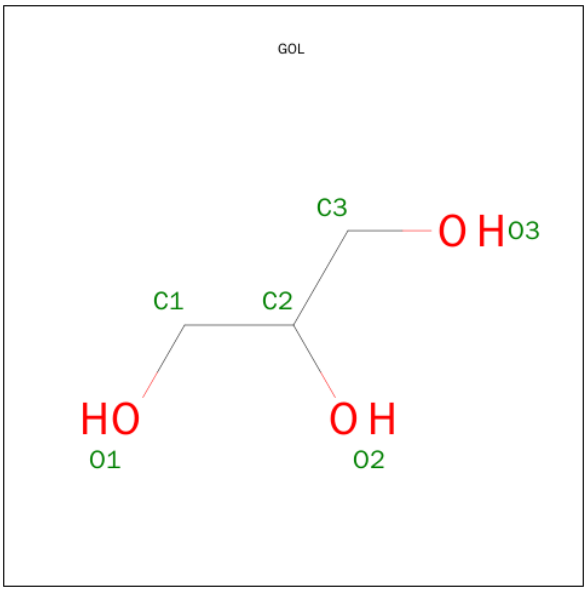
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Zn 4 4	0	0
2	F	4	Total Zn 4 4	0	0

- Molecule 3 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 6 4 2	0	0
3	B	1	Total C N O 12 6 4 2	0	0
3	C	1	Total C N O 12 6 4 2	0	0
3	D	1	Total C N O 12 6 4 2	0	0
3	E	1	Total C N O 12 6 4 2	0	0
3	F	1	Total C N O 12 6 4 2	0	0
3	G	1	Total C N O 12 6 4 2	0	0
3	H	1	Total C N O 12 6 4 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0
5	B	37	Total O 37 37	0	0

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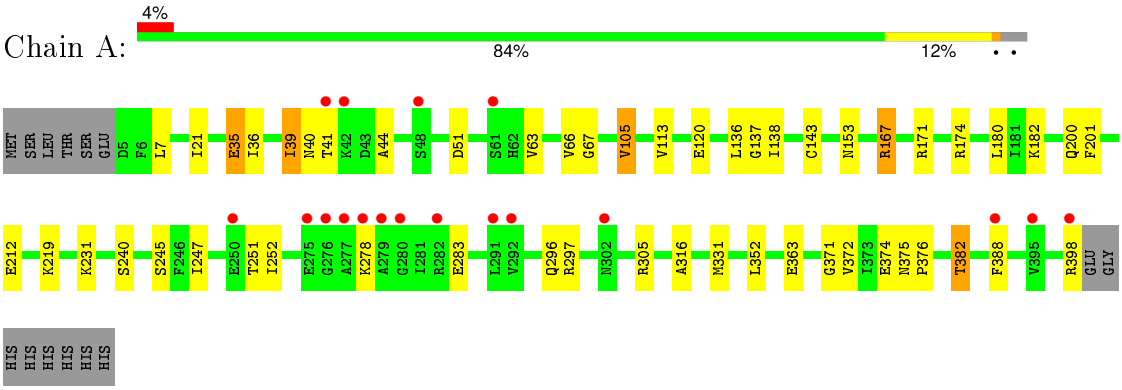
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	34	Total O 34 34	0	0
5	D	27	Total O 27 27	0	0
5	E	40	Total O 40 40	0	0
5	F	40	Total O 40 40	0	0
5	G	31	Total O 31 31	0	0
5	H	53	Total O 53 53	0	0

3 Residue-property plots (i)

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.

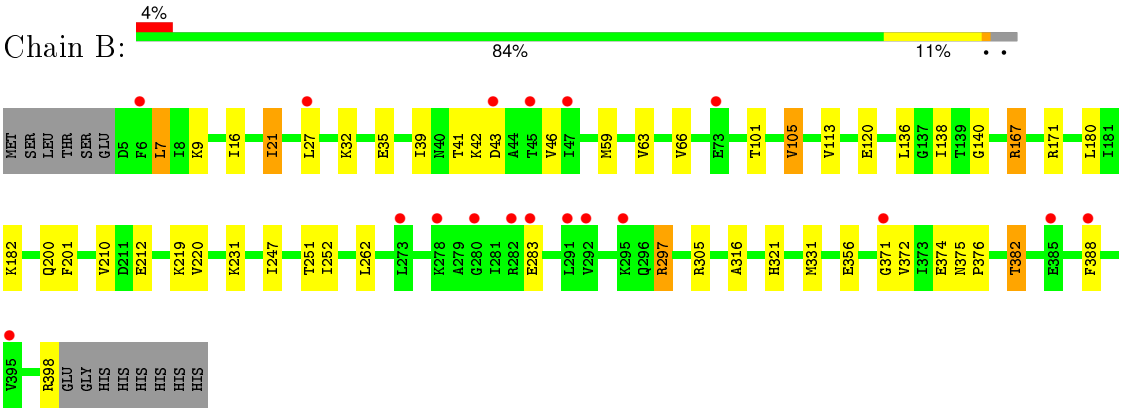
- Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

Chain A:



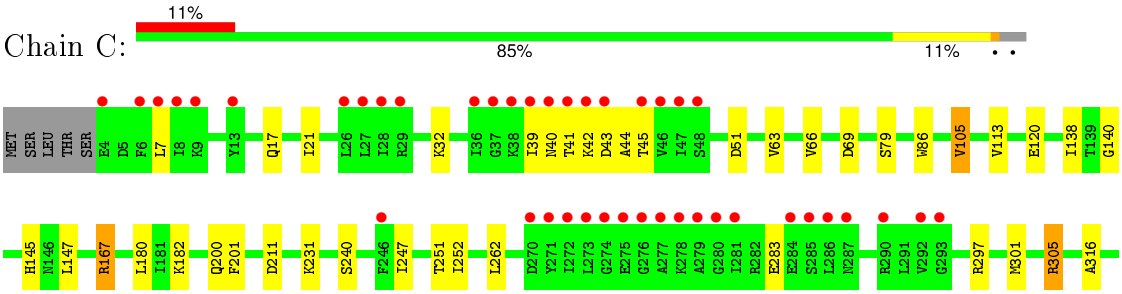
- Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

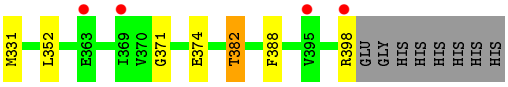
Chain B:



- Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

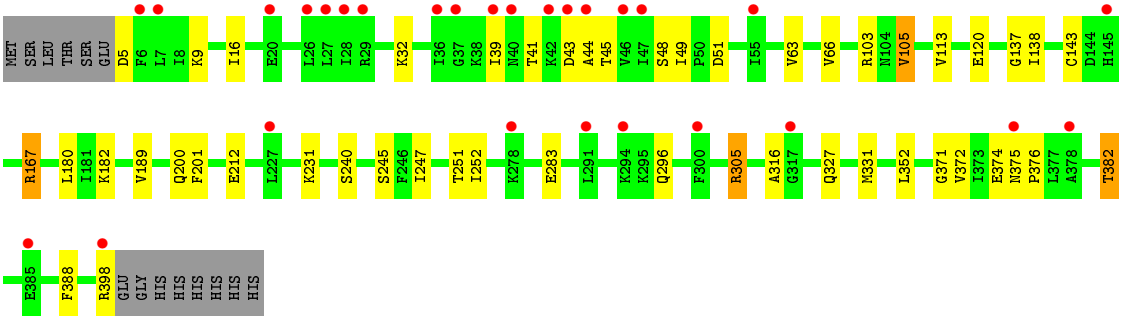
Chain C:





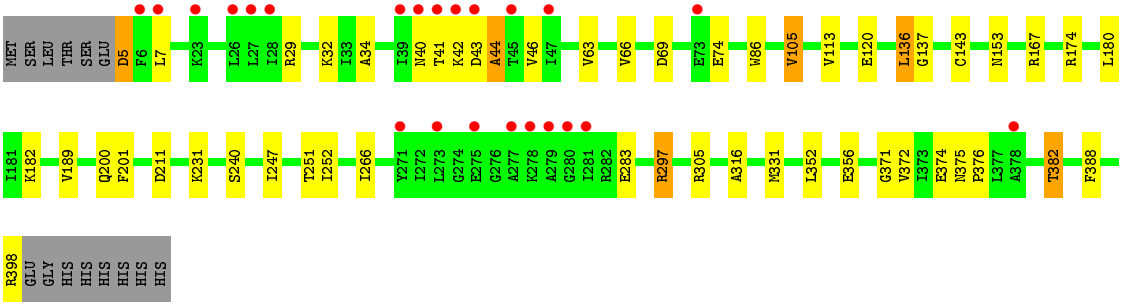
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

Chain D:



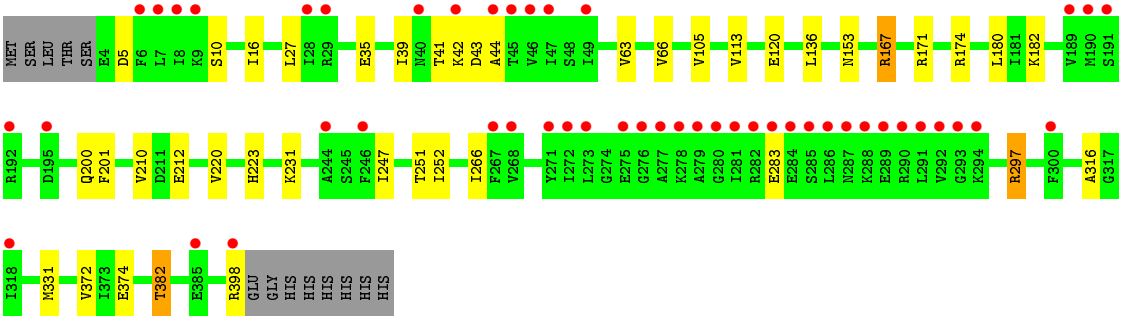
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

Chain E:



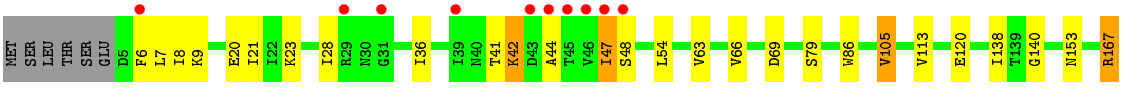
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

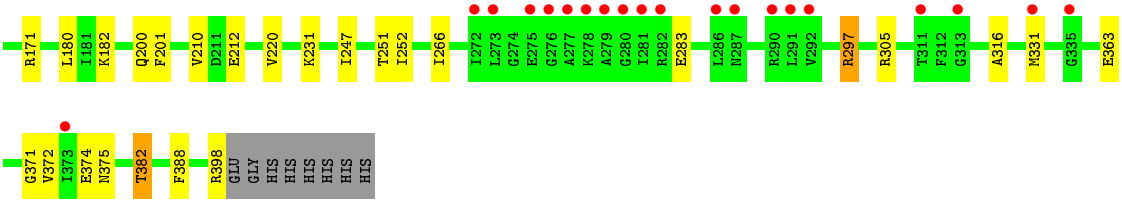
Chain F:



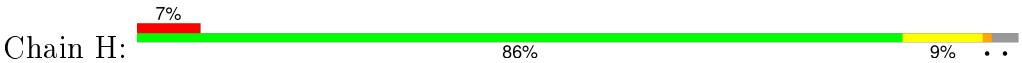
• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE

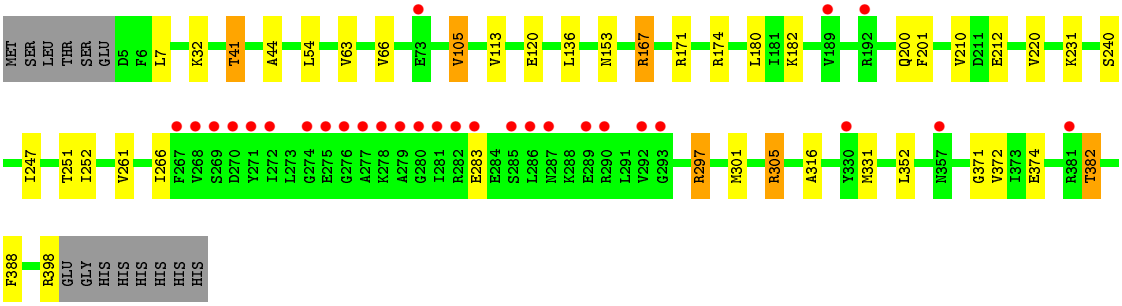
Chain G:





• Molecule 1: ZN-DEPENDENT ARGININE CARBOXYPEPTIDASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.33Å 146.04Å 255.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 37.37 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.62) 99.1 (37.37-2.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.264 0.232 , 0.264	Depositor DCC
R_{free} test set	3808 reflections (3.11%)	DCC
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 126664 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24575	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, ZN, KCX

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	0.37	0/3052	0.58	1/4115 (0.0%)
1	B	0.38	0/3052	0.59	2/4115 (0.0%)
1	C	0.39	0/3066	0.57	0/4133
1	D	0.38	0/3035	0.57	0/4093
1	E	0.38	0/3035	0.58	1/4093 (0.0%)
1	F	0.40	0/3061	0.59	0/4128
1	G	0.38	0/3035	0.58	0/4093
1	H	0.39	0/3071	0.59	1/4141 (0.0%)
All	All	0.38	0/24407	0.58	5/32911 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	2
1	F	0	1
1	G	0	2
1	H	0	2
All	All	0	12

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	ARG	CG-CD-NE	5.72	123.82	111.80
1	A	136	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	297	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	E	136	LEU	CA-CB-CG	5.23	127.34	115.30
1	H	136	LEU	CA-CB-CG	5.16	127.18	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ALA	Peptide
1	B	42	LYS	Peptide
1	C	42	LYS	Peptide
1	C	44	ALA	Peptide
1	D	43	ASP	Peptide
1	E	42	LYS	Peptide
1	E	44	ALA	Peptide
1	F	42	LYS	Peptide
1	G	42	LYS	Peptide
1	G	44	ALA	Peptide
1	H	41	THR	Peptide
1	H	44	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3012	0	3020	20	0
1	B	3012	0	3019	20	0
1	C	3026	0	3034	18	0
1	D	3001	0	3002	23	0
1	E	3001	0	3002	22	0
1	F	3021	0	3019	16	0
1	G	3001	0	3002	20	0
1	H	3027	0	3032	18	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	1	0
3	E	12	0	12	1	0
3	F	12	0	12	1	0
3	G	12	0	12	0	0
3	H	12	0	12	0	0
4	A	6	0	8	1	0
4	B	24	0	32	2	0
4	D	6	0	8	0	0
4	E	12	0	16	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	A	24	0	0	0	0
5	B	37	0	0	0	0
5	C	34	0	0	0	0
5	D	27	0	0	1	0
5	E	40	0	0	0	0
5	F	40	0	0	0	0
5	G	31	0	0	0	0
5	H	53	0	0	0	0
All	All	24575	0	24306	149	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 3.

All (149) 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:E:305:ARG:HG2	1:E:305:ARG:HH21	1.16	1.07
1:D:305:ARG:HH21	1:D:305:ARG:HG2	1.19	1.06
1:D:305:ARG:NH2	1:D:305:ARG:HG2	1.78	0.93
1:E:305:ARG:CG	1:E:305:ARG:HH21	1.83	0.91
1:D:305:ARG:CG	1:D:305:ARG:HH21	1.85	0.88
1:B:105:VAL:HG22	1:B:182:KCX:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLU:H	1:B:382:THR:HG21	1.53	0.72
1:F:231:LYS:HG2	1:F:251:THR:HG21	1.71	0.72
1:D:374:GLU:H	1:D:382:THR:HG21	1.54	0.72
1:G:231:LYS:HG2	1:G:251:THR:HG21	1.72	0.71
1:H:374:GLU:H	1:H:382:THR:HG21	1.55	0.71
1:G:374:GLU:H	1:G:382:THR:HG21	1.56	0.71
1:D:231:LYS:HG2	1:D:251:THR:HG21	1.73	0.70
1:A:231:LYS:HG2	1:A:251:THR:HG21	1.74	0.69
1:H:231:LYS:HG2	1:H:251:THR:HG21	1.75	0.69
1:C:305:ARG:HG3	1:C:305:ARG:HH11	1.59	0.68
1:F:374:GLU:H	1:F:382:THR:HG21	1.57	0.68
1:E:231:LYS:HG2	1:E:251:THR:HG21	1.77	0.67
1:B:231:LYS:HG2	1:B:251:THR:HG21	1.76	0.67
1:C:374:GLU:H	1:C:382:THR:HG21	1.59	0.67
1:C:305:ARG:HG3	1:C:305:ARG:NH1	2.08	0.67
1:H:105:VAL:HG22	1:H:182:KCX:HG2	1.76	0.67
1:E:374:GLU:H	1:E:382:THR:HG21	1.60	0.66
1:F:105:VAL:HG22	1:F:182:KCX:HG2	1.77	0.65
1:A:374:GLU:H	1:A:382:THR:HG21	1.62	0.65
1:G:105:VAL:HG22	1:G:182:KCX:HG2	1.81	0.63
1:C:105:VAL:HG22	1:C:182:KCX:HG2	1.79	0.63
1:C:231:LYS:HG2	1:C:251:THR:HG21	1.79	0.62
1:E:305:ARG:CG	1:E:305:ARG:NH2	2.50	0.62
1:A:105:VAL:HG22	1:A:182:KCX:HG2	1.80	0.62
1:E:105:VAL:HG22	1:E:182:KCX:HG2	1.82	0.61
1:D:105:VAL:HG22	1:D:182:KCX:HG2	1.85	0.59
1:B:140:GLY:O	1:H:174:ARG:NH2	2.37	0.58
1:E:305:ARG:HG2	1:E:305:ARG:NH2	1.99	0.56
1:C:167[A]:ARG:NH2	1:C:211:ASP:OD2	2.38	0.56
1:E:5:ASP:HB2	1:E:44:ALA:HB3	1.89	0.55
1:F:266:ILE:O	1:F:297:ARG:NH1	2.40	0.54
1:D:5:ASP:N	1:D:44:ALA:CB	2.71	0.54
1:B:321:HIS:H	4:B:432:GOL:H12	1.72	0.54
1:H:266:ILE:O	1:H:297:ARG:NH1	2.40	0.54
1:C:305:ARG:CG	1:C:305:ARG:HH11	2.21	0.53
1:G:247:ILE:HG12	1:G:252:ILE:HG13	1.90	0.53
1:B:27:LEU:HD23	1:B:35:GLU:HG3	1.90	0.52
1:F:27:LEU:HB3	1:F:35:GLU:HB2	1.92	0.52
1:G:36:ILE:HG13	1:G:363:GLU:HG3	1.90	0.52
1:D:200:GLN:O	1:D:201:PHE:HB2	2.09	0.52
1:B:247:ILE:HG12	1:B:252:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:GLN:O	1:G:201:PHE:HB2	2.09	0.51
1:H:200:GLN:O	1:H:201:PHE:HB2	2.10	0.50
1:G:266:ILE:O	1:G:297:ARG:NH1	2.43	0.50
1:B:167:ARG:HH21	1:B:212:GLU:HB2	1.76	0.50
1:C:301:MET:O	1:C:305:ARG:HG2	2.12	0.50
1:C:200:GLN:O	1:C:201:PHE:HB2	2.11	0.50
1:F:200:GLN:O	1:F:201:PHE:HB2	2.11	0.50
1:E:266:ILE:O	1:E:297:ARG:NH1	2.45	0.50
1:A:200:GLN:O	1:A:201:PHE:HB2	2.12	0.50
1:H:301:MET:O	1:H:305:ARG:CG	2.60	0.50
1:B:138:ILE:HB	1:H:171:ARG:HD3	1.94	0.50
1:A:247:ILE:HG12	1:A:252:ILE:HG13	1.94	0.50
1:B:21:ILE:HG21	1:B:375:ASN:HD21	1.77	0.49
1:E:200:GLN:O	1:E:201:PHE:HB2	2.12	0.49
1:D:247:ILE:HG12	1:D:252:ILE:HG13	1.93	0.49
1:C:247:ILE:HG12	1:C:252:ILE:HG13	1.94	0.49
1:E:247:ILE:HG12	1:E:252:ILE:HG13	1.95	0.49
1:D:9:LYS:HB2	1:D:48:SER:HA	1.94	0.49
1:E:167:ARG:NH2	1:E:211:ASP:OD2	2.46	0.48
1:F:247:ILE:HG12	1:F:252:ILE:HG13	1.95	0.48
1:C:145:HIS:CE1	1:C:147:LEU:HB2	2.48	0.48
1:C:240:SER:HB3	1:C:352:LEU:HD11	1.96	0.48
1:F:63:VAL:HG12	1:F:316:ALA:HB3	1.96	0.48
1:B:200:GLN:O	1:B:201:PHE:HB2	2.14	0.48
1:G:63:VAL:HG12	1:G:316:ALA:HB3	1.95	0.47
1:G:167:ARG:HD2	1:G:212:GLU:HB2	1.96	0.47
1:H:301:MET:O	1:H:305:ARG:HG2	2.14	0.47
1:A:305:ARG:HH21	1:A:305:ARG:HG2	1.79	0.47
1:A:167:ARG:HH21	1:A:212:GLU:HB2	1.78	0.47
1:A:174:ARG:NH2	1:C:140:GLY:O	2.47	0.47
1:H:167:ARG:HH21	1:H:212:GLU:HB2	1.78	0.47
1:G:6:PHE:HB2	1:G:28:ILE:HB	1.96	0.47
1:H:247:ILE:HG12	1:H:252:ILE:HG13	1.95	0.47
1:B:171:ARG:HD3	1:D:138:ILE:HB	1.97	0.47
1:H:371:GLY:HA3	1:H:388:PHE:HB3	1.97	0.47
1:D:5:ASP:O	1:D:44:ALA:HB3	2.15	0.47
1:F:167:ARG:HH21	1:F:212:GLU:HB2	1.79	0.47
1:F:297:ARG:H	1:F:297:ARG:HG2	1.54	0.46
1:D:189:VAL:HB	3:D:429:ARG:HG2	1.97	0.46
1:D:103:ARG:HD2	1:D:180:LEU:HD13	1.97	0.46
1:G:9:LYS:HB2	1:G:48:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:SER:HB3	1:H:352:LEU:HD11	1.99	0.45
1:A:219:LYS:HD3	1:A:352:LEU:O	2.16	0.45
1:B:7:LEU:HB3	1:B:46:VAL:HG13	1.99	0.45
1:A:67:GLY:HA3	4:A:430:GOL:H32	1.99	0.45
1:G:21:ILE:HG13	1:G:375:ASN:HD21	1.81	0.45
1:B:59:MET:HG2	1:B:101:THR:HB	1.98	0.45
1:F:171:ARG:HD3	1:G:138:ILE:HB	1.98	0.45
1:D:63:VAL:HG12	1:D:316:ALA:HB3	1.98	0.45
1:E:375:ASN:HA	1:E:376:PRO:HD3	1.83	0.44
1:G:297:ARG:HG2	1:G:297:ARG:H	1.48	0.44
1:D:167:ARG:HD2	1:D:212:GLU:HB2	1.99	0.44
1:F:174:ARG:NH2	1:G:140:GLY:O	2.50	0.44
1:E:297:ARG:H	1:E:297:ARG:HG2	1.52	0.44
1:A:245:SER:HA	1:A:296:GLN:HG3	2.00	0.44
1:E:63:VAL:HG12	1:E:316:ALA:HB3	1.99	0.44
1:B:371:GLY:HA3	1:B:388:PHE:HB3	1.99	0.44
1:D:375:ASN:HA	1:D:376:PRO:HD3	1.84	0.44
1:E:29:ARG:HG2	1:E:34:ALA:HB2	2.00	0.44
1:E:7:LEU:HB3	1:E:46:VAL:HG22	1.98	0.44
1:D:371:GLY:HA3	1:D:388:PHE:HB3	1.98	0.44
1:B:210:VAL:HA	1:B:220:VAL:HG21	1.99	0.43
1:B:63:VAL:HG12	1:B:316:ALA:HB3	2.00	0.43
1:A:240:SER:HB3	1:A:352:LEU:HD11	2.01	0.43
1:D:240:SER:HB3	1:D:352:LEU:HD11	2.00	0.43
1:C:63:VAL:HG12	1:C:316:ALA:HB3	2.00	0.43
1:B:9:LYS:HD2	1:B:9:LYS:HA	1.84	0.43
1:A:137:GLY:HA3	1:A:143:CYS:HB2	2.01	0.43
1:A:36:ILE:HD12	1:A:363:GLU:HG3	2.01	0.43
1:D:245:SER:HA	1:D:296:GLN:HG3	2.01	0.43
1:G:371:GLY:HA3	1:G:388:PHE:HB3	2.00	0.43
1:A:171:ARG:HD3	1:C:138:ILE:HB	2.01	0.43
1:B:375:ASN:HA	1:B:376:PRO:HD3	1.83	0.42
1:C:371:GLY:HA3	1:C:388:PHE:HB3	2.01	0.42
1:H:63:VAL:HG12	1:H:316:ALA:HB3	2.01	0.42
1:G:8:ILE:HG12	1:G:47:ILE:HD12	2.01	0.42
1:H:297:ARG:H	1:H:297:ARG:HG2	1.47	0.42
1:D:167:ARG:HH21	1:D:212:GLU:HB2	1.85	0.42
1:H:261:VAL:HG11	1:H:352:LEU:HD22	2.01	0.42
1:E:240:SER:HB3	1:E:352:LEU:HD11	2.00	0.42
1:H:210:VAL:HA	1:H:220:VAL:HG21	2.01	0.42
1:C:247:ILE:HD13	1:C:262:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:VAL:HA	1:F:220:VAL:HG21	2.01	0.42
1:G:210:VAL:HA	1:G:220:VAL:HG21	2.01	0.42
1:C:69:ASP:HB2	1:C:86:TRP:CD2	2.54	0.42
1:A:35:GLU:HB3	1:A:39:ILE:HD12	2.02	0.42
1:A:375:ASN:HA	1:A:376:PRO:HD3	1.84	0.42
1:E:137:GLY:HA3	1:E:143:CYS:HB2	2.01	0.42
1:A:63:VAL:HG12	1:A:316:ALA:HB3	2.00	0.41
1:F:5:ASP:HB2	1:F:44:ALA:HB3	2.02	0.41
1:H:301:MET:O	1:H:305:ARG:HG3	2.21	0.41
1:E:371:GLY:HA3	1:E:388:PHE:HB3	2.02	0.41
1:E:189:VAL:HB	3:E:429:ARG:HG2	2.03	0.41
1:D:137:GLY:HA3	1:D:143:CYS:HB2	2.03	0.41
1:A:138:ILE:HB	1:G:171:ARG:HD3	2.02	0.41
1:E:69:ASP:HB2	1:E:86:TRP:CD2	2.56	0.41
1:G:69:ASP:HB2	1:G:86:TRP:CD2	2.56	0.41
1:F:35:GLU:HB3	1:F:39:ILE:HG12	2.03	0.40
1:F:223:HIS:HE1	3:F:429:ARG:O	2.03	0.40
1:D:327:GLN:NE2	5:D:434:HOH:O	2.53	0.40
1:B:219:LYS:HG3	4:B:433:GOL:H2	2.03	0.40
1:A:371:GLY:HA3	1:A:388:PHE:HB3	2.04	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	393/408 (96%)	379 (96%)	14 (4%)	0	100 100
1	B	393/408 (96%)	377 (96%)	16 (4%)	0	100 100
1	C	394/408 (97%)	375 (95%)	18 (5%)	1 (0%)	46 70
1	D	391/408 (96%)	374 (96%)	17 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	391/408 (96%)	370 (95%)	20 (5%)	1 (0%)	46 70
1	F	394/408 (97%)	376 (95%)	18 (5%)	0	100 100
1	G	391/408 (96%)	375 (96%)	16 (4%)	0	100 100
1	H	395/408 (97%)	378 (96%)	17 (4%)	0	100 100
All	All	3142/3264 (96%)	3004 (96%)	136 (4%)	2 (0%)	56 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	ASN
1	E	40	ASN

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	A	318/329 (97%)	297 (93%)	21 (7%)	21 39
1	B	318/329 (97%)	295 (93%)	23 (7%)	18 34
1	C	319/329 (97%)	296 (93%)	23 (7%)	18 34
1	D	316/329 (96%)	298 (94%)	18 (6%)	25 48
1	E	316/329 (96%)	296 (94%)	20 (6%)	22 43
1	F	319/329 (97%)	302 (95%)	17 (5%)	28 52
1	G	316/329 (96%)	294 (93%)	22 (7%)	19 36
1	H	320/329 (97%)	302 (94%)	18 (6%)	26 49
All	All	2542/2632 (97%)	2380 (94%)	162 (6%)	22 42

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	35	GLU
1	A	39	ILE
1	A	40	ASN
1	A	41	THR
1	A	51	ASP
1	A	66	VAL
1	A	105	VAL
1	A	113	VAL
1	A	120	GLU
1	A	153	ASN
1	A	167	ARG
1	A	180	LEU
1	A	278	LYS
1	A	283	GLU
1	A	297	ARG
1	A	331	MET
1	A	372	VAL
1	A	382	THR
1	A	398	ARG
1	B	7	LEU
1	B	16	ILE
1	B	21	ILE
1	B	32	LYS
1	B	39	ILE
1	B	41	THR
1	B	43	ASP
1	B	66	VAL
1	B	105	VAL
1	B	113	VAL
1	B	120	GLU
1	B	136	LEU
1	B	167	ARG
1	B	180	LEU
1	B	262	LEU
1	B	283	GLU
1	B	297	ARG
1	B	305	ARG
1	B	331	MET
1	B	356	GLU
1	B	372	VAL
1	B	382	THR
1	B	398	ARG

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Mol	Chain	Res	Type
1	C	7	LEU
1	C	17	GLN
1	C	21	ILE
1	C	32	LYS
1	C	39	ILE
1	C	41	THR
1	C	43	ASP
1	C	45	THR
1	C	51	ASP
1	C	66	VAL
1	C	79	SER
1	C	105	VAL
1	C	113	VAL
1	C	120	GLU
1	C	167[A]	ARG
1	C	167[B]	ARG
1	C	180	LEU
1	C	283	GLU
1	C	297	ARG
1	C	305	ARG
1	C	331	MET
1	C	382	THR
1	C	398	ARG
1	D	16	ILE
1	D	32	LYS
1	D	39	ILE
1	D	41	THR
1	D	45	THR
1	D	49	ILE
1	D	51	ASP
1	D	66	VAL
1	D	105	VAL
1	D	113	VAL
1	D	120	GLU
1	D	167	ARG
1	D	283	GLU
1	D	305	ARG
1	D	331	MET
1	D	372	VAL
1	D	382	THR
1	D	398	ARG
1	E	5	ASP

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Mol	Chain	Res	Type
1	E	32	LYS
1	E	41	THR
1	E	43	ASP
1	E	66	VAL
1	E	74	GLU
1	E	105	VAL
1	E	113	VAL
1	E	120	GLU
1	E	136	LEU
1	E	153	ASN
1	E	174	ARG
1	E	180	LEU
1	E	283	GLU
1	E	297	ARG
1	E	331	MET
1	E	356	GLU
1	E	372	VAL
1	E	382	THR
1	E	398	ARG
1	F	10	SER
1	F	16	ILE
1	F	41	THR
1	F	43	ASP
1	F	66	VAL
1	F	113	VAL
1	F	120	GLU
1	F	136	LEU
1	F	153	ASN
1	F	167	ARG
1	F	180	LEU
1	F	283	GLU
1	F	297	ARG
1	F	331	MET
1	F	372	VAL
1	F	382	THR
1	F	398	ARG
1	G	7	LEU
1	G	20	GLU
1	G	23	LYS
1	G	41	THR
1	G	42	LYS
1	G	47	ILE

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Mol	Chain	Res	Type
1	G	54	LEU
1	G	66	VAL
1	G	79	SER
1	G	105	VAL
1	G	113	VAL
1	G	120	GLU
1	G	153	ASN
1	G	167	ARG
1	G	180	LEU
1	G	283	GLU
1	G	297	ARG
1	G	305	ARG
1	G	331	MET
1	G	372	VAL
1	G	382	THR
1	G	398	ARG
1	H	7	LEU
1	H	32	LYS
1	H	41	THR
1	H	54	LEU
1	H	66	VAL
1	H	105	VAL
1	H	113	VAL
1	H	120	GLU
1	H	153	ASN
1	H	167	ARG
1	H	180	LEU
1	H	283	GLU
1	H	297	ARG
1	H	305	ARG
1	H	331	MET
1	H	372	VAL
1	H	382	THR
1	H	398	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	40	ASN
1	C	360	GLN
1	F	17	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	A	182	1,2	7,11,12	0.92	0	7,12,14	1.65	1 (14%)
1	KCX	B	182	1,2	7,11,12	0.56	0	7,12,14	1.66	2 (28%)
1	KCX	C	182	1	7,11,12	0.74	0	7,12,14	1.70	1 (14%)
1	KCX	D	182	1,2	7,11,12	0.71	0	7,12,14	1.82	2 (28%)
1	KCX	E	182	1,2	7,11,12	0.67	0	7,12,14	1.83	2 (28%)
1	KCX	F	182	1	7,11,12	0.59	0	7,12,14	1.56	2 (28%)
1	KCX	G	182	1,2	7,11,12	0.69	0	7,12,14	1.48	2 (28%)
1	KCX	H	182	1	7,11,12	0.72	0	7,12,14	1.35	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	182	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	182	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	182	1	-	0/6/10/12	0/0/0/0
1	KCX	D	182	1,2	-	0/6/10/12	0/0/0/0
1	KCX	E	182	1,2	-	0/6/10/12	0/0/0/0
1	KCX	F	182	1	-	0/6/10/12	0/0/0/0
1	KCX	G	182	1,2	-	0/6/10/12	0/0/0/0
1	KCX	H	182	1	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	182	KCX	CE-NZ-CX	-4.13	118.81	123.49
1	D	182	KCX	CE-NZ-CX	-4.10	118.85	123.49
1	C	182	KCX	CE-NZ-CX	-3.88	119.09	123.49
1	A	182	KCX	CE-NZ-CX	-3.70	119.31	123.49
1	B	182	KCX	CE-NZ-CX	-3.66	119.35	123.49
1	F	182	KCX	CE-NZ-CX	-3.28	119.78	123.49
1	G	182	KCX	CE-NZ-CX	-2.94	120.17	123.49
1	H	182	KCX	CE-NZ-CX	-2.59	120.56	123.49
1	G	182	KCX	O-C-CA	-2.19	119.79	125.49
1	D	182	KCX	O-C-CA	-2.17	119.83	125.49
1	E	182	KCX	O-C-CA	-2.15	119.90	125.49
1	H	182	KCX	O-C-CA	-2.12	119.95	125.49
1	F	182	KCX	O-C-CA	-2.08	120.06	125.49
1	B	182	KCX	O-C-CA	-2.02	120.23	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	182	KCX	1	0
1	B	182	KCX	1	0
1	C	182	KCX	1	0
1	D	182	KCX	1	0
1	E	182	KCX	1	0
1	F	182	KCX	1	0
1	G	182	KCX	1	0
1	H	182	KCX	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 32 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
3	ARG	A	429	-	5,11,11	0.18	0	3,13,13	0.44	0
4	GOL	A	430	-	5,5,5	0.43	0	5,5,5	0.13	0
3	ARG	B	429	-	5,11,11	0.22	0	3,13,13	0.41	0
4	GOL	B	430	-	5,5,5	0.34	0	5,5,5	0.26	0
4	GOL	B	431	-	5,5,5	0.42	0	5,5,5	0.21	0
4	GOL	B	432	-	5,5,5	0.27	0	5,5,5	0.33	0
4	GOL	B	433	-	5,5,5	0.32	0	5,5,5	0.43	0
3	ARG	C	429	-	5,11,11	0.21	0	3,13,13	0.35	0
3	ARG	D	429	-	5,11,11	0.23	0	3,13,13	0.27	0
4	GOL	D	430	-	5,5,5	0.30	0	5,5,5	0.32	0
3	ARG	E	429	-	5,11,11	0.23	0	3,13,13	0.19	0
4	GOL	E	430	-	5,5,5	0.33	0	5,5,5	0.30	0
4	GOL	E	431	-	5,5,5	0.35	0	5,5,5	0.16	0
3	ARG	F	429	-	5,11,11	0.14	0	3,13,13	0.61	0
3	ARG	G	429	-	5,11,11	0.16	0	3,13,13	0.63	0
4	GOL	G	430	-	5,5,5	0.44	0	5,5,5	0.58	0
3	ARG	H	429	-	5,11,11	0.21	0	3,13,13	0.37	0
4	GOL	H	430	-	5,5,5	0.40	0	5,5,5	0.49	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	ARG	A	429	-	-	0/5/11/11	0/0/0/0
4	GOL	A	430	-	-	0/4/4/4	0/0/0/0
3	ARG	B	429	-	-	0/5/11/11	0/0/0/0
4	GOL	B	430	-	-	0/4/4/4	0/0/0/0
4	GOL	B	431	-	-	0/4/4/4	0/0/0/0
4	GOL	B	432	-	-	0/4/4/4	0/0/0/0
4	GOL	B	433	-	-	0/4/4/4	0/0/0/0
3	ARG	C	429	-	-	0/5/11/11	0/0/0/0
3	ARG	D	429	-	-	0/5/11/11	0/0/0/0
4	GOL	D	430	-	-	0/4/4/4	0/0/0/0
3	ARG	E	429	-	-	0/5/11/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	430	-	-	0/4/4/4	0/0/0/0
4	GOL	E	431	-	-	0/4/4/4	0/0/0/0
3	ARG	F	429	-	-	0/5/11/11	0/0/0/0
3	ARG	G	429	-	-	0/5/11/11	0/0/0/0
4	GOL	G	430	-	-	0/4/4/4	0/0/0/0
3	ARG	H	429	-	-	0/5/11/11	0/0/0/0
4	GOL	H	430	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	430	GOL	1	0
4	B	432	GOL	1	0
4	B	433	GOL	1	0
3	D	429	ARG	1	0
3	E	429	ARG	1	0
3	F	429	ARG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	393/408 (96%)	0.18	18 (4%) 36 29	45, 73, 104, 136	0
1	B	393/408 (96%)	0.30	18 (4%) 36 29	45, 74, 111, 136	0
1	C	394/408 (96%)	0.43	46 (11%) 6 4	47, 76, 114, 136	0
1	D	393/408 (96%)	0.39	28 (7%) 19 13	43, 75, 113, 142	0
1	E	393/408 (96%)	0.29	23 (5%) 26 19	45, 74, 110, 143	0
1	F	394/408 (96%)	0.60	49 (12%) 5 3	46, 72, 106, 136	0
1	G	393/408 (96%)	0.33	30 (7%) 17 12	39, 74, 110, 136	0
1	H	393/408 (96%)	0.30	29 (7%) 17 12	45, 69, 104, 136	0
All	All	3146/3264 (96%)	0.35	241 (7%) 16 11	39, 73, 110, 143	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	279	ALA	8.9
1	F	280	GLY	8.9
1	F	268	VAL	8.3
1	F	285	SER	7.9
1	F	286	LEU	7.4
1	F	271	TYR	7.2
1	H	277	ALA	7.2
1	F	277	ALA	7.1
1	F	276	GLY	6.9
1	F	281	ILE	6.4
1	F	291	LEU	6.3
1	F	287	ASN	6.3
1	D	44	ALA	6.2
1	C	280	GLY	6.1
1	F	292	VAL	6.0
1	G	291	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	279	ALA	5.7
1	H	281	ILE	5.6
1	C	28	ILE	5.5
1	F	275	GLU	5.5
1	C	272	ILE	5.5
1	C	279	ALA	5.4
1	C	276	GLY	5.4
1	F	283	GLU	5.4
1	G	292	VAL	5.4
1	C	47	ILE	5.3
1	C	39	ILE	5.2
1	C	6	PHE	5.1
1	C	286	LEU	5.1
1	E	40	ASN	5.0
1	D	43	ASP	5.0
1	G	47	ILE	4.9
1	F	44	ALA	4.9
1	E	280	GLY	4.9
1	F	272	ILE	4.9
1	H	286	LEU	4.9
1	A	278	LYS	4.9
1	F	267	PHE	4.8
1	F	284	GLU	4.8
1	G	276	GLY	4.7
1	C	271	TYR	4.6
1	D	40	ASN	4.6
1	C	278	LYS	4.6
1	A	280	GLY	4.5
1	E	275	GLU	4.5
1	D	39	ILE	4.4
1	B	292	VAL	4.4
1	G	275	GLU	4.3
1	B	6	PHE	4.3
1	C	273	LEU	4.2
1	C	275	GLU	4.2
1	G	273	LEU	4.2
1	F	282	ARG	4.2
1	B	280	GLY	4.2
1	D	7	LEU	4.1
1	H	280	GLY	4.1
1	C	277	ALA	4.1
1	G	39	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	4.0
1	E	273	LEU	4.0
1	F	8	ILE	4.0
1	C	26	LEU	3.9
1	F	398	ARG	3.9
1	D	385	GLU	3.9
1	H	268	VAL	3.8
1	F	289	GLU	3.8
1	D	29	ARG	3.8
1	F	195	ASP	3.8
1	B	47	ILE	3.8
1	F	278	LYS	3.8
1	G	281	ILE	3.8
1	E	42	LYS	3.7
1	H	282[A]	ARG	3.7
1	H	267	PHE	3.7
1	D	278	LYS	3.6
1	E	278	LYS	3.6
1	G	282	ARG	3.6
1	H	287	ASN	3.6
1	G	286	LEU	3.5
1	E	43	ASP	3.5
1	C	284	GLU	3.5
1	C	46	VAL	3.5
1	C	292	VAL	3.5
1	G	48	SER	3.5
1	C	43	ASP	3.5
1	D	47	ILE	3.5
1	G	278	LYS	3.4
1	F	9	LYS	3.4
1	D	28	ILE	3.4
1	A	276	GLY	3.4
1	G	46	VAL	3.4
1	E	6	PHE	3.3
1	E	277	ALA	3.3
1	E	39	ILE	3.3
1	C	270	ASP	3.3
1	A	42	LYS	3.3
1	B	45	THR	3.3
1	H	275	GLU	3.3
1	F	290	ARG	3.3
1	B	295	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	285	SER	3.3
1	D	46	VAL	3.3
1	H	330	TYR	3.3
1	H	270	ASP	3.3
1	F	40	ASN	3.3
1	H	279	ALA	3.3
1	C	40	ASN	3.2
1	H	292	VAL	3.2
1	D	378	ALA	3.2
1	C	7	LEU	3.2
1	F	6	PHE	3.2
1	A	279	ALA	3.1
1	G	279	ALA	3.1
1	H	192	ARG	3.1
1	D	300	PHE	3.1
1	C	293	GLY	3.1
1	E	47	ILE	3.1
1	F	47	ILE	3.1
1	F	246	PHE	3.1
1	H	289	GLU	3.1
1	E	7	LEU	3.1
1	B	395	VAL	3.1
1	C	287	ASN	3.1
1	H	278	LYS	3.0
1	G	373	ILE	3.0
1	F	293	GLY	3.0
1	F	29	ARG	3.0
1	B	291	LEU	3.0
1	G	280	GLY	3.0
1	H	272	ILE	2.9
1	C	37	GLY	2.9
1	F	46	VAL	2.9
1	G	44	ALA	2.9
1	D	6	PHE	2.9
1	E	378	ALA	2.8
1	C	42	LYS	2.8
1	A	291	LEU	2.8
1	C	8	ILE	2.8
1	F	288	LYS	2.8
1	A	250	GLU	2.8
1	A	292	VAL	2.8
1	C	274	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	41	THR	2.7
1	F	244	ALA	2.7
1	C	27	LEU	2.7
1	C	246	PHE	2.7
1	D	26	LEU	2.7
1	G	313	GLY	2.7
1	E	23	LYS	2.7
1	F	294	LYS	2.7
1	F	189	VAL	2.7
1	C	369	ILE	2.6
1	D	42	LYS	2.6
1	C	281	ILE	2.6
1	D	36	ILE	2.6
1	G	290	ARG	2.6
1	F	7	LEU	2.6
1	F	192	ARG	2.6
1	F	42	LYS	2.5
1	F	28	ILE	2.5
1	C	45	THR	2.5
1	F	191	SER	2.5
1	H	276	GLY	2.5
1	C	4	GLU	2.5
1	B	27	LEU	2.5
1	C	38	LYS	2.5
1	D	294	LYS	2.5
1	D	27	LEU	2.5
1	E	26	LEU	2.5
1	C	48	SER	2.5
1	D	37	GLY	2.5
1	A	388	PHE	2.5
1	D	375	ASN	2.5
1	G	272	ILE	2.4
1	D	20	GLU	2.4
1	A	277	ALA	2.4
1	F	318	ILE	2.4
1	H	271	TYR	2.4
1	E	28	ILE	2.4
1	F	45	THR	2.4
1	G	45	THR	2.4
1	G	43	ASP	2.4
1	G	6	PHE	2.4
1	D	398	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	9	LYS	2.4
1	H	357	ASN	2.4
1	C	395	VAL	2.4
1	C	398	ARG	2.4
1	E	281	ILE	2.4
1	E	45	THR	2.4
1	G	287	ASN	2.4
1	B	273	LEU	2.3
1	H	293	GLY	2.3
1	H	381	ARG	2.3
1	F	49	ILE	2.3
1	E	73	GLU	2.3
1	B	371	GLY	2.3
1	D	227	LEU	2.3
1	G	29	ARG	2.3
1	C	13	TYR	2.3
1	D	291	LEU	2.3
1	H	290	ARG	2.3
1	A	395	VAL	2.2
1	H	189	VAL	2.2
1	A	282[A]	ARG	2.2
1	C	29	ARG	2.2
1	B	43	ASP	2.2
1	B	388	PHE	2.2
1	C	363	GLU	2.2
1	A	398	ARG	2.2
1	B	282[A]	ARG	2.2
1	G	331	MET	2.2
1	A	61	SER	2.1
1	D	55	ILE	2.1
1	G	335	GLY	2.1
1	C	41	THR	2.1
1	H	274	GLY	2.1
1	D	145	HIS	2.1
1	A	48	SER	2.1
1	F	300	PHE	2.1
1	E	271	TYR	2.1
1	B	385	GLU	2.1
1	C	290	ARG	2.1
1	H	283	GLU	2.1
1	A	41	THR	2.1
1	F	190	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	302	ASN	2.0
1	G	311	THR	2.0
1	B	278	LYS	2.0
1	B	73	GLU	2.0
1	F	385	GLU	2.0
1	H	73	GLU	2.0
1	G	277	ALA	2.0
1	F	273	LEU	2.0
1	H	285	SER	2.0
1	B	283	GLU	2.0
1	G	31	GLY	2.0
1	C	36	ILE	2.0
1	D	317	GLY	2.0
1	H	269[A]	SER	2.0
1	E	27	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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, 95^{th} 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
1	KCX	G	182	12/13	0.94	0.21	-	57,66,103,109	0
1	KCX	A	182	12/13	0.93	0.26	-	56,66,102,108	0
1	KCX	C	182	12/13	0.95	0.23	-	55,66,102,108	0
1	KCX	F	182	12/13	0.93	0.18	-	54,63,103,111	0
1	KCX	H	182	12/13	0.93	0.21	-	56,65,102,109	0
1	KCX	B	182	12/13	0.95	0.19	-	55,64,104,109	0
1	KCX	D	182	12/13	0.92	0.25	-	54,63,103,107	0
1	KCX	E	182	12/13	0.94	0.32	-	54,67,103,108	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95^{th} 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
4	GOL	E	431	6/6	0.85	0.42	15.04	87,94,97,105	0
4	GOL	B	433	6/6	0.72	0.45	10.58	93,96,98,99	0
4	GOL	B	430	6/6	0.91	0.29	10.47	95,100,103,106	0
4	GOL	H	430	6/6	0.91	0.29	8.68	67,81,86,100	0
2	ZN	B	427	1/1	0.96	0.37	7.30	80,80,80,80	1
4	GOL	G	430	6/6	0.82	0.29	5.86	58,70,74,77	0
2	ZN	E	427	1/1	0.95	0.33	4.90	76,76,76,76	1
4	GOL	A	430	6/6	0.75	0.32	4.17	77,89,90,93	0
4	GOL	B	432	6/6	0.78	0.32	3.84	75,92,94,95	0
2	ZN	G	427	1/1	0.71	0.20	3.78	74,74,74,74	1
2	ZN	D	427	1/1	0.93	0.31	3.62	78,78,78,78	1
2	ZN	F	427	1/1	0.87	0.24	1.46	113,113,113,113	0
4	GOL	E	430	6/6	0.87	0.23	1.10	84,89,93,101	0
4	GOL	B	431	6/6	0.86	0.25	0.93	60,75,79,84	0
2	ZN	C	427	1/1	0.92	0.21	0.78	67,67,67,67	1
2	ZN	H	428	1/1	0.81	0.19	0.74	127,127,127,127	1
3	ARG	A	429	12/12	0.79	0.26	0.57	81,84,86,87	0
3	ARG	G	429	12/12	0.89	0.25	0.52	87,95,102,103	0
2	ZN	C	428	1/1	0.92	0.15	0.43	106,106,106,106	1
3	ARG	C	429	12/12	0.83	0.24	0.39	85,92,100,105	0
3	ARG	F	429	12/12	0.77	0.26	-0.22	98,108,130,132	0
3	ARG	B	429	12/12	0.89	0.17	-0.26	61,74,94,95	0
2	ZN	F	428	1/1	0.64	0.15	-0.27	127,127,127,127	1
3	ARG	H	429	12/12	0.86	0.21	-0.40	68,82,106,108	0
3	ARG	E	429	12/12	0.90	0.17	-0.41	66,71,76,77	0
3	ARG	D	429	12/12	0.87	0.17	-0.43	78,84,85,85	0
2	ZN	H	427	1/1	0.92	0.08	-2.49	118,118,118,118	0
2	ZN	A	427	1/1	0.84	0.10	-3.04	122,122,122,122	0
2	ZN	G	428	1/1	0.95	0.21	-	101,101,101,101	1
2	ZN	C	426	1/1	0.89	0.19	-	117,117,117,117	0
2	ZN	E	426	1/1	0.96	0.17	-	102,102,102,102	0
2	ZN	F	426	1/1	0.97	0.22	-	98,98,98,98	0
2	ZN	E	428	1/1	0.93	0.21	-	91,91,91,91	1
2	ZN	G	426	1/1	0.94	0.37	-	78,78,78,78	1
2	ZN	A	428	1/1	0.89	0.28	-	106,106,106,106	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	425	1/1	0.97	0.23	-	92,92,92,92	0
4	GOL	D	430	6/6	0.81	0.27	-	85,95,99,100	0
2	ZN	B	426	1/1	0.95	0.35	-	77,77,77,77	1
2	ZN	D	425	1/1	0.98	0.19	-	88,88,88,88	0
2	ZN	B	428	1/1	0.94	0.15	-	87,87,87,87	1
2	ZN	C	425	1/1	0.97	0.18	-	93,93,93,93	0
2	ZN	A	426	1/1	0.95	0.15	-	104,104,104,104	0
2	ZN	H	426	1/1	0.98	0.11	-	95,95,95,95	0
2	ZN	B	425	1/1	0.97	0.22	-	85,85,85,85	0
2	ZN	F	425	1/1	0.95	0.16	-	93,93,93,93	0
2	ZN	H	425	1/1	0.98	0.15	-	93,93,93,93	0
2	ZN	D	428	1/1	0.95	0.20	-	89,89,89,89	1
2	ZN	G	425	1/1	0.97	0.22	-	93,93,93,93	0
2	ZN	E	425	1/1	0.97	0.22	-	88,88,88,88	0
2	ZN	D	426	1/1	0.92	0.18	-	128,128,128,128	0

6.5 Other polymers (i)

There are no such residues in this entry.