



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:55 AM UTC

PDB ID : 6HK6 / pdb_00006hk6
Title : Human RIOK2 bound to inhibitor
Authors : Wang, J.; Krojer, T.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.; Knapp, S.; Elkins, J.M.
Deposited on : 2018-09-05
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

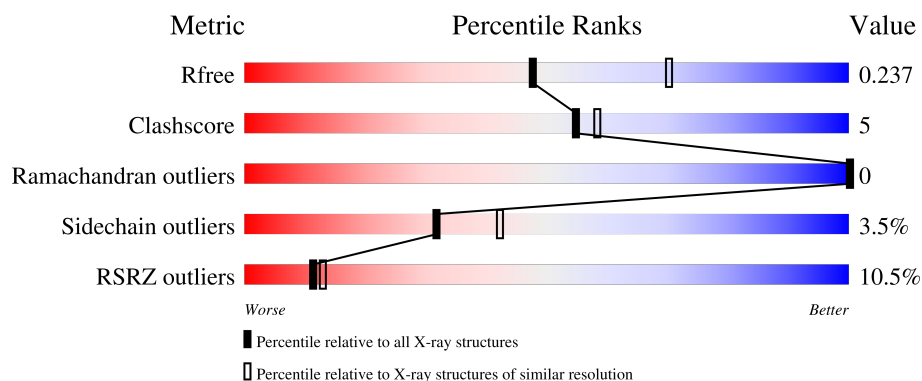
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	 4% 75% 11% • 12%
1	B	330	 3% 75% 11% • 12%
1	C	330	 6% 76% 11% • 12%
1	D	330	 10% 77% 10% • 12%
1	E	330	 12% 78% 8% • 12%

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Mol	Chain	Length	Quality of chain
1	F	330	10% 78% 8% 12%
1	G	330	15% 73% 8% 18%
1	H	330	11% 76% 8% 15%
1	I	330	5% 78% 8% 13%
1	J	330	15% 75% 11% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23349 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2336	1496	400	426	14			
1	B	290	Total	C	N	O	S	0	0	0
			2323	1487	397	425	14			
1	C	290	Total	C	N	O	S	0	0	0
			2314	1482	395	423	14			
1	D	290	Total	C	N	O	S	0	0	0
			2272	1457	383	418	14			
1	E	289	Total	C	N	O	S	0	0	0
			2262	1457	379	412	14			
1	F	289	Total	C	N	O	S	0	0	0
			2268	1456	378	419	15			
1	G	271	Total	C	N	O	S	0	0	0
			2141	1380	351	396	14			
1	H	282	Total	C	N	O	S	0	0	0
			2241	1438	374	416	13			
1	I	288	Total	C	N	O	S	0	0	0
			2288	1470	384	420	14			
1	J	290	Total	C	N	O	S	0	0	0
			2236	1438	369	415	14			

There are 20 discrepancies between the modelled and reference sequences:

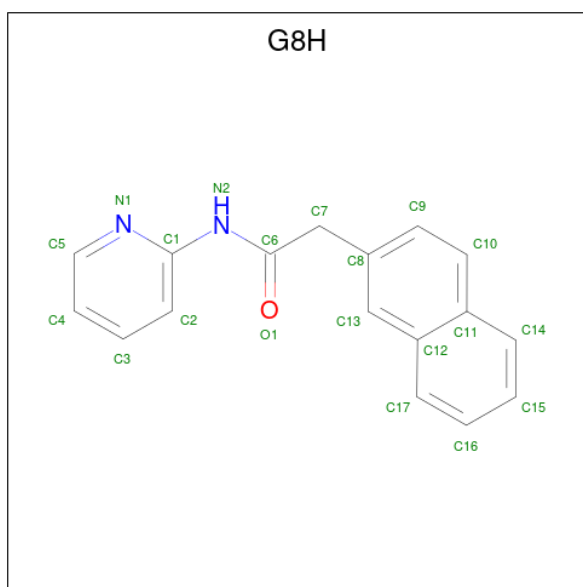
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9BVS4
A	144	TYR	HIS	conflict	UNP Q9BVS4
B	0	SER	-	expression tag	UNP Q9BVS4
B	144	TYR	HIS	conflict	UNP Q9BVS4
C	0	SER	-	expression tag	UNP Q9BVS4
C	144	TYR	HIS	conflict	UNP Q9BVS4
D	0	SER	-	expression tag	UNP Q9BVS4
D	144	TYR	HIS	conflict	UNP Q9BVS4
E	0	SER	-	expression tag	UNP Q9BVS4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	144	TYR	HIS	conflict	UNP Q9BVS4
F	0	SER	-	expression tag	UNP Q9BVS4
F	144	TYR	HIS	conflict	UNP Q9BVS4
G	0	SER	-	expression tag	UNP Q9BVS4
G	144	TYR	HIS	conflict	UNP Q9BVS4
H	0	SER	-	expression tag	UNP Q9BVS4
H	144	TYR	HIS	conflict	UNP Q9BVS4
I	0	SER	-	expression tag	UNP Q9BVS4
I	144	TYR	HIS	conflict	UNP Q9BVS4
J	0	SER	-	expression tag	UNP Q9BVS4
J	144	TYR	HIS	conflict	UNP Q9BVS4

- Molecule 2 is 2-naphthalen-2-yl- {N}-pyridin-2-yl-ethanamide (CCD ID: G8H) (formula: C₁₇H₁₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	17	2	1		
2	B	1	Total	C	N	O	0	0
			20	17	2	1		
2	C	1	Total	C	N	O	0	0
			20	17	2	1		
2	D	1	Total	C	N	O	0	0
			20	17	2	1		
2	E	1	Total	C	N	O	0	0
			20	17	2	1		

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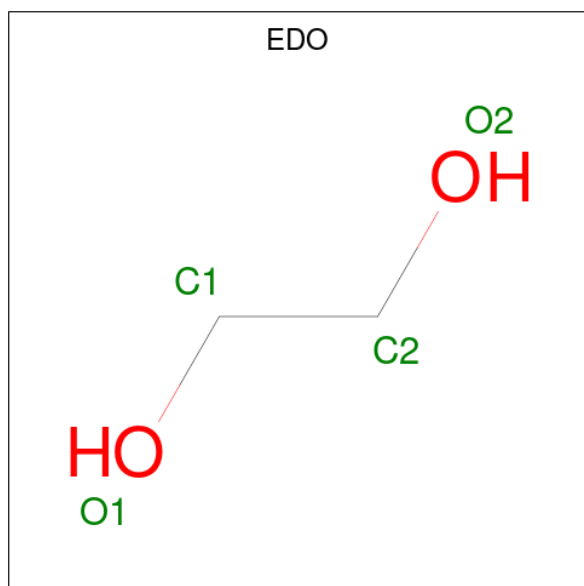
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			20	17	2	1		
2	G	1	Total	C	N	O	0	0
			20	17	2	1		
2	H	1	Total	C	N	O	0	0
			20	17	2	1		
2	I	1	Total	C	N	O	0	0
			20	17	2	1		
2	J	1	Total	C	N	O	0	0
			20	17	2	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



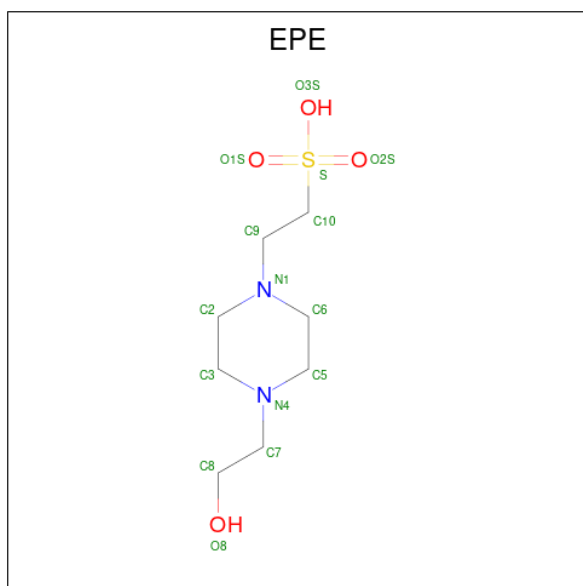
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

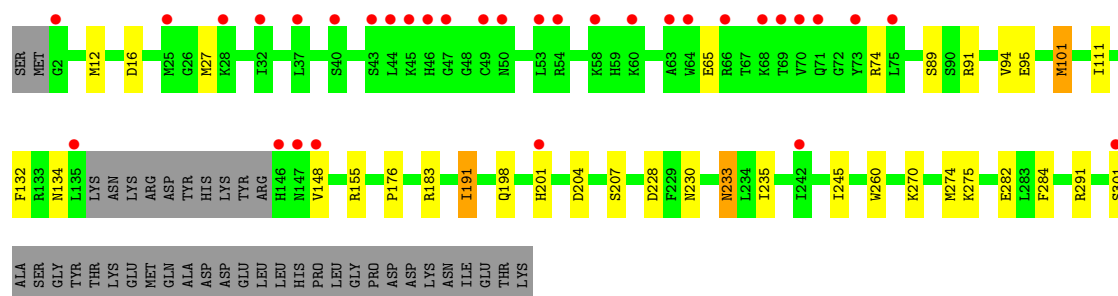
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	59	Total 59	O 59	0	0
6	C	55	Total 55	O 55	0	0
6	D	17	Total 17	O 17	0	0
6	E	26	Total 26	O 26	0	0
6	F	44	Total 44	O 44	0	0
6	G	3	Total 3	O 3	0	0
6	H	51	Total 51	O 51	0	0
6	I	35	Total 35	O 35	0	0
6	J	7	Total 7	O 7	0	0

HIS
PRO
LEU
GLY
PRO
ASP
ASP
LYS
ASN
ILE
GLU
THR
LYS

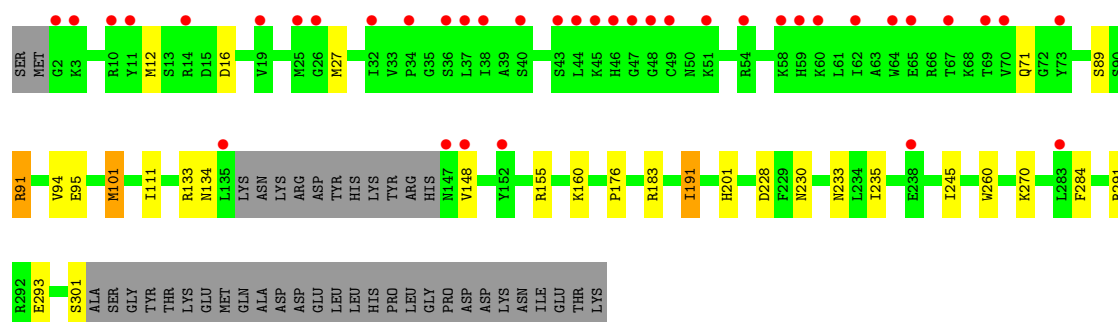
• Molecule 1: Serine/threonine-protein kinase RIO2

Chain D: 10% 77% 10% 12%



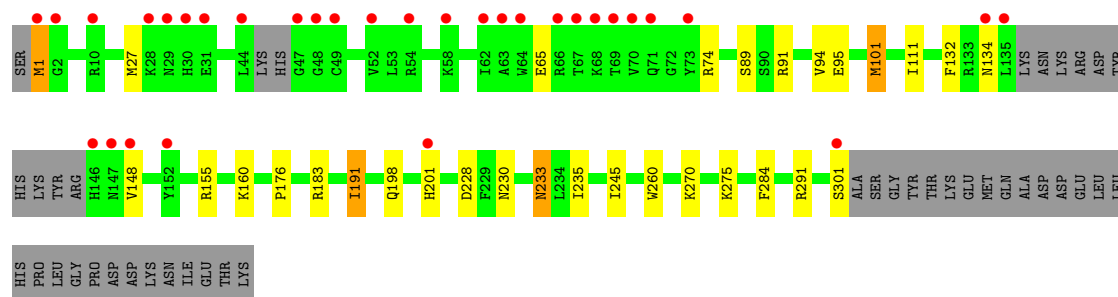
• Molecule 1: Serine/threonine-protein kinase RIO2

Chain E: 12% 78% 8% 12%



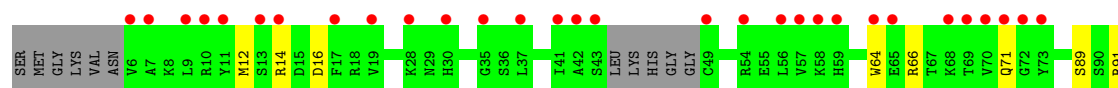
• Molecule 1: Serine/threonine-protein kinase RIO2

Chain F: 10% 78% 8% 12%



• Molecule 1: Serine/threonine-protein kinase RIO2

Chain G: 15% 73% 8% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.01Å 92.86Å 237.65Å 90.00° 99.10° 90.00°	Depositor
Resolution (Å)	78.34 – 2.35 78.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.34-2.35) 99.7 (78.34-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.215 , 0.235 0.217 , 0.237	Depositor DCC
R_{free} test set	8217 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23349	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, EPE, CL, G8H

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	1.03	0/2388	1.41	3/3225 (0.1%)
1	B	1.00	0/2375	1.39	3/3210 (0.1%)
1	C	1.01	0/2365	1.39	1/3197 (0.0%)
1	D	0.99	0/2322	1.37	1/3147 (0.0%)
1	E	0.98	0/2313	1.37	0/3134
1	F	0.99	0/2317	1.38	3/3137 (0.1%)
1	G	0.98	0/2188	1.38	2/2963 (0.1%)
1	H	1.01	0/2290	1.40	4/3100 (0.1%)
1	I	1.02	0/2339	1.39	1/3164 (0.0%)
1	J	1.02	1/2286 (0.0%)	1.40	4/3105 (0.1%)
All	All	1.00	1/23183 (0.0%)	1.39	22/31382 (0.1%)

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	J	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	299	GLU	N-CA	5.16	1.52	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	200	HIS	CA-CB-CG	-8.54	105.26	113.80
1	G	200	HIS	CA-CB-CG	-7.67	106.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	299	GLU	CA-C-O	-5.93	114.26	120.55
1	G	200	HIS	CB-CA-C	5.86	119.49	109.24
1	I	233	ASN	CB-CA-C	-5.75	99.89	109.55
1	J	233	ASN	CB-CA-C	-5.58	99.94	109.65
1	H	48	GLY	CA-C-N	5.51	127.66	120.28
1	H	48	GLY	C-N-CA	5.51	127.66	120.28
1	J	299	GLU	N-CA-C	5.33	117.09	111.28
1	J	299	GLU	N-CA-CB	5.28	117.88	110.12
1	C	233	ASN	CB-CA-C	-5.26	100.50	109.65
1	H	233	ASN	CB-CA-C	-5.17	100.64	109.65
1	D	233	ASN	CB-CA-C	-5.14	100.70	109.65
1	A	233	ASN	CB-CA-C	-5.14	100.71	109.65
1	B	233	ASN	CB-CA-C	-5.13	100.73	109.65
1	F	233	ASN	CB-CA-C	-5.12	100.75	109.65
1	A	20	LEU	CA-C-N	5.05	127.47	120.29
1	A	20	LEU	C-N-CA	5.05	127.47	120.29
1	F	1	MET	CA-C-N	5.04	126.54	121.35
1	F	1	MET	C-N-CA	5.04	126.54	121.35
1	B	46	HIS	CB-CA-C	5.02	117.99	109.55
1	B	148	VAL	N-CA-C	-5.00	107.59	112.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	300	VAL	Peptide

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	2336	0	2276	35	0
1	B	2323	0	2266	32	0
1	C	2314	0	2247	26	0
1	D	2272	0	2167	26	0
1	E	2262	0	2166	22	0
1	F	2268	0	2175	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2141	0	2046	22	0
1	H	2241	0	2153	18	0
1	I	2288	0	2200	25	0
1	J	2236	0	2106	32	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	1	0
2	E	20	0	0	0	0
2	F	20	0	0	1	0
2	G	20	0	0	0	0
2	H	20	0	0	1	0
2	I	20	0	0	1	0
2	J	20	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	18	0	0
4	B	12	0	18	0	0
4	F	4	0	6	0	0
5	B	15	0	18	1	0
5	D	15	0	18	0	0
5	E	15	0	18	2	0
5	H	15	0	18	0	0
6	A	79	0	0	3	0
6	B	59	0	0	1	0
6	C	55	0	0	0	0
6	D	17	0	0	0	0
6	E	26	0	0	0	0
6	F	44	0	0	0	0
6	G	3	0	0	0	0
6	H	51	0	0	0	0
6	I	35	0	0	0	0
6	J	7	0	0	0	0
All	All	23349	0	21916	217	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 (217) 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:J:296:LEU:O	1:J:300:VAL:HG22	1.52	1.08
1:D:301:SER:HA	1:E:134:ASN:HB3	1.51	0.92
1:J:297:ASP:O	1:J:301:SER:HA	1.70	0.91
1:C:301:SER:HA	1:F:134:ASN:HB3	1.57	0.85
1:J:222:HIS:HB3	1:J:296:LEU:HD12	1.62	0.80
1:G:153:LEU:HD11	1:J:156:LEU:HD21	1.67	0.75
1:I:228:ASP:O	1:I:233:ASN:ND2	2.24	0.71
1:D:228:ASP:O	1:D:233:ASN:ND2	2.24	0.71
1:H:228:ASP:O	1:H:233:ASN:ND2	2.25	0.70
1:A:228:ASP:O	1:A:233:ASN:ND2	2.24	0.70
1:C:228:ASP:O	1:C:233:ASN:ND2	2.25	0.70
1:E:228:ASP:O	1:E:233:ASN:ND2	2.25	0.70
1:B:228:ASP:O	1:B:233:ASN:ND2	2.24	0.70
1:J:228:ASP:O	1:J:233:ASN:ND2	2.24	0.70
1:F:101:MET:HE3	1:F:111:ILE:HG13	1.74	0.69
1:F:228:ASP:O	1:F:233:ASN:ND2	2.25	0.69
1:G:228:ASP:O	1:G:233:ASN:ND2	2.24	0.69
1:B:101:MET:HE3	1:B:111:ILE:HG13	1.75	0.69
1:A:11:TYR:OH	1:H:238:GLU:OE1	2.07	0.68
1:I:101:MET:HE3	1:I:111:ILE:HG13	1.74	0.68
1:A:90:SER:OG	1:H:203:GLU:HG2	1.92	0.68
1:H:101:MET:HE3	1:H:111:ILE:HG13	1.76	0.68
1:D:101:MET:HE3	1:D:111:ILE:HG13	1.76	0.68
1:J:164:TYR:CE1	1:J:300:VAL:HB	2.28	0.68
1:A:50:ASN:HB3	6:A:501:HOH:O	1.93	0.68
1:G:101:MET:HE3	1:G:111:ILE:HG13	1.76	0.68
1:D:134:ASN:HB3	1:E:301:SER:HA	1.76	0.67
1:A:54:ARG:NH2	6:A:501:HOH:O	2.26	0.66
1:A:159:MET:HE2	1:B:146:HIS:CE1	2.30	0.66
1:C:101:MET:HE3	1:C:111:ILE:HG13	1.75	0.66
1:B:69:THR:HB	1:B:70:VAL:HG23	1.76	0.66
1:J:215:LEU:HD21	1:J:244:MET:SD	2.36	0.66
1:J:101:MET:HE3	1:J:111:ILE:HG13	1.77	0.66
1:A:101:MET:HE3	1:A:111:ILE:HG13	1.76	0.66
1:I:215:LEU:HD21	1:I:244:MET:SD	2.36	0.65
1:J:226:HIS:HA	1:J:250:MET:HE3	1.79	0.65
1:E:101:MET:HE3	1:E:111:ILE:HG13	1.77	0.65
1:A:148:VAL:HG12	1:A:148:VAL:O	1.97	0.64
1:C:134:ASN:HB3	1:F:301:SER:HA	1.80	0.63
1:I:226:HIS:HA	1:I:250:MET:HE3	1.78	0.63
1:C:148:VAL:HG12	1:C:148:VAL:O	1.97	0.63
1:C:64:TRP:CH2	1:C:71:GLN:HG3	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:VAL:HG12	1:H:148:VAL:O	2.00	0.61
1:E:148:VAL:HG12	1:E:148:VAL:O	2.01	0.61
1:H:27:MET:O	1:H:148:VAL:HG11	2.02	0.60
1:A:13:SER:HA	1:H:238:GLU:OE1	2.02	0.60
1:I:219:LEU:HD22	1:I:250:MET:HE1	1.84	0.60
1:A:134:ASN:HB3	1:B:301:SER:HA	1.83	0.59
1:B:194:TYR:HE2	1:I:198:GLN:O	1.86	0.59
1:D:148:VAL:HG12	1:D:148:VAL:O	2.02	0.59
1:A:27:MET:O	1:A:148:VAL:HG11	2.03	0.59
1:I:224:LEU:HB3	1:I:250:MET:HE2	1.84	0.59
1:C:27:MET:O	1:C:148:VAL:HG11	2.03	0.58
1:J:219:LEU:HD22	1:J:250:MET:HE1	1.84	0.58
1:A:160:LYS:HG2	1:B:132:PHE:CZ	2.37	0.58
1:G:301:SER:HA	1:J:134:ASN:HB3	1.85	0.58
1:D:27:MET:O	1:D:148:VAL:HG11	2.04	0.57
1:E:27:MET:O	1:E:148:VAL:HG11	2.04	0.57
1:J:296:LEU:O	1:J:300:VAL:CG2	2.41	0.57
1:J:224:LEU:HB3	1:J:250:MET:HE2	1.87	0.57
1:J:27:MET:O	1:J:148:VAL:HG11	2.06	0.56
1:F:27:MET:O	1:F:148:VAL:HG11	2.05	0.56
1:A:74:ARG:NH1	6:A:503:HOH:O	2.34	0.56
1:F:148:VAL:HG12	1:F:148:VAL:O	2.04	0.56
1:G:260:TRP:CZ2	1:J:230:ASN:HB3	2.40	0.56
1:I:27:MET:O	1:I:148:VAL:HG11	2.06	0.56
1:A:132:PHE:CZ	1:B:160:LYS:HG2	2.41	0.56
1:J:148:VAL:HG12	1:J:148:VAL:O	2.06	0.55
1:E:91:ARG:O	1:G:14:ARG:NH1	2.40	0.55
1:A:301:SER:HA	1:B:134:ASN:HB3	1.89	0.54
1:A:146:HIS:ND1	1:A:146:HIS:C	2.65	0.54
1:F:235:ILE:HD12	1:F:245:ILE:HG21	1.89	0.54
1:C:155:ARG:HG3	1:C:183:ARG:HA	1.90	0.53
1:C:64:TRP:HH2	1:C:71:GLN:HG3	1.73	0.53
1:B:198:GLN:O	1:I:194:TYR:HE2	1.92	0.53
1:B:155:ARG:HG3	1:B:183:ARG:HA	1.90	0.53
1:E:235:ILE:HD12	1:E:245:ILE:HG21	1.91	0.53
1:J:235:ILE:HD12	1:J:245:ILE:HG21	1.90	0.53
1:A:155:ARG:HG3	1:A:183:ARG:HA	1.91	0.53
1:B:27:MET:O	1:B:148:VAL:HG11	2.08	0.53
1:I:148:VAL:HG12	1:I:148:VAL:O	2.08	0.53
1:G:156:LEU:HD21	1:J:153:LEU:HD11	1.91	0.53
1:A:12:MET:HE2	1:A:17:PHE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:ARG:HG3	1:J:183:ARG:HA	1.92	0.52
1:F:155:ARG:HG3	1:F:183:ARG:HA	1.92	0.52
1:A:12:MET:CE	1:A:20:LEU:HD23	2.40	0.51
1:A:284:PHE:O	1:I:60:LYS:HE3	2.10	0.51
1:I:224:LEU:HB3	1:I:250:MET:CE	2.41	0.51
1:B:235:ILE:CD1	1:B:245:ILE:HG12	2.41	0.51
1:I:235:ILE:CD1	1:I:245:ILE:HG12	2.41	0.51
1:H:65:GLU:OE2	1:H:74:ARG:NE	2.38	0.51
1:A:235:ILE:HD12	1:A:245:ILE:HG21	1.92	0.51
1:C:132:PHE:CZ	1:F:160:LYS:HG2	2.45	0.50
1:G:235:ILE:CD1	1:G:245:ILE:HG12	2.41	0.50
1:A:65:GLU:OE2	1:A:74:ARG:NE	2.37	0.50
1:I:235:ILE:HD12	1:I:245:ILE:HG12	1.94	0.50
1:B:148:VAL:O	1:B:148:VAL:HG12	2.11	0.50
1:B:235:ILE:HD12	1:B:245:ILE:HG12	1.93	0.50
1:G:155:ARG:HG3	1:G:183:ARG:HA	1.94	0.50
1:I:235:ILE:HD12	1:I:245:ILE:HG21	1.93	0.50
1:C:235:ILE:HD12	1:C:245:ILE:HG21	1.92	0.50
1:E:155:ARG:HG3	1:E:183:ARG:HA	1.94	0.50
1:C:235:ILE:CD1	1:C:245:ILE:HG12	2.42	0.50
1:D:235:ILE:HD12	1:D:245:ILE:HG21	1.93	0.50
1:G:235:ILE:HD12	1:G:245:ILE:HG21	1.94	0.49
1:E:235:ILE:CD1	1:E:245:ILE:HG12	2.42	0.49
1:F:235:ILE:CD1	1:F:245:ILE:HG12	2.42	0.49
1:G:64:TRP:CH2	1:G:66:ARG:CB	2.94	0.49
1:H:235:ILE:CD1	1:H:245:ILE:HG12	2.42	0.49
1:J:224:LEU:HB3	1:J:250:MET:CE	2.42	0.49
1:J:235:ILE:CD1	1:J:245:ILE:HG12	2.42	0.49
1:E:235:ILE:HD12	1:E:245:ILE:HG12	1.94	0.49
1:D:132:PHE:CZ	1:E:160:LYS:HG2	2.47	0.49
1:C:260:TRP:CZ2	1:F:230:ASN:HB3	2.47	0.49
1:D:235:ILE:CD1	1:D:245:ILE:HG12	2.42	0.49
1:A:12:MET:HB2	1:A:82:TYR:OH	2.12	0.49
1:F:235:ILE:HD12	1:F:245:ILE:HG12	1.94	0.49
1:H:235:ILE:HD12	1:H:245:ILE:HG21	1.94	0.49
1:A:194:TYR:HE2	1:F:198:GLN:O	1.95	0.49
1:J:235:ILE:HD12	1:J:245:ILE:HG12	1.94	0.49
1:H:155:ARG:HG3	1:H:183:ARG:HA	1.94	0.49
1:F:101:MET:HB2	2:F:401:G8H:C17	2.42	0.49
1:A:201:HIS:HB3	1:F:1:MET:SD	2.53	0.48
1:A:235:ILE:CD1	1:A:245:ILE:HG12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ARG:HG2	5:B:402:EPE:H71	1.96	0.48
1:B:65:GLU:OE2	1:B:74:ARG:NE	2.38	0.48
1:B:235:ILE:HD12	1:B:245:ILE:HG21	1.95	0.48
1:H:235:ILE:HD12	1:H:245:ILE:HG12	1.95	0.48
1:C:89:SER:HA	1:C:94:VAL:O	2.13	0.48
1:C:160:LYS:HG2	1:F:132:PHE:CZ	2.49	0.48
1:H:148:VAL:O	1:H:148:VAL:CG1	2.62	0.48
1:I:155:ARG:HG3	1:I:183:ARG:HA	1.94	0.48
1:D:155:ARG:HG3	1:D:183:ARG:HA	1.94	0.48
1:A:260:TRP:CZ2	1:B:230:ASN:HB3	2.49	0.48
1:G:235:ILE:HD12	1:G:245:ILE:HG12	1.95	0.48
1:H:89:SER:HA	1:H:94:VAL:O	2.14	0.47
1:G:89:SER:HA	1:G:94:VAL:O	2.14	0.47
1:I:14:ARG:HE	1:I:14:ARG:HB2	1.68	0.47
1:A:89:SER:HA	1:A:94:VAL:O	2.14	0.47
1:D:89:SER:HA	1:D:94:VAL:O	2.15	0.47
1:F:89:SER:HA	1:F:94:VAL:O	2.14	0.47
1:H:176:PRO:HG3	1:H:191:ILE:CD1	2.45	0.47
1:D:235:ILE:HD12	1:D:245:ILE:HG12	1.96	0.47
1:J:89:SER:HA	1:J:94:VAL:O	2.14	0.47
1:E:89:SER:HA	1:E:94:VAL:O	2.14	0.47
1:E:148:VAL:O	1:E:148:VAL:CG1	2.63	0.47
1:I:89:SER:HA	1:I:94:VAL:O	2.14	0.47
1:C:235:ILE:HD12	1:C:245:ILE:HG12	1.96	0.47
1:B:8:LYS:HE3	1:B:95:GLU:OE2	2.15	0.47
1:A:230:ASN:HB3	1:B:260:TRP:CZ2	2.51	0.46
1:D:148:VAL:O	1:D:148:VAL:CG1	2.64	0.46
1:E:176:PRO:HG3	1:E:191:ILE:CD1	2.46	0.46
1:A:148:VAL:O	1:A:148:VAL:CG1	2.63	0.46
1:A:176:PRO:HG3	1:A:191:ILE:CD1	2.46	0.46
1:G:176:PRO:HG3	1:G:191:ILE:CD1	2.46	0.46
1:B:176:PRO:HG3	1:B:191:ILE:CD1	2.46	0.45
1:B:126:ARG:NH1	6:B:507:HOH:O	2.49	0.45
1:C:148:VAL:O	1:C:148:VAL:CG1	2.62	0.45
1:I:148:VAL:O	1:I:148:VAL:CG1	2.65	0.45
1:F:148:VAL:O	1:F:148:VAL:CG1	2.64	0.45
1:B:89:SER:HA	1:B:94:VAL:O	2.15	0.45
1:D:176:PRO:HG3	1:D:191:ILE:CD1	2.46	0.45
1:E:12:MET:HG3	1:E:16:ASP:HB2	1.99	0.45
1:B:99:ASN:ND2	1:I:275:LYS:HG2	2.32	0.45
1:F:176:PRO:HG3	1:F:191:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:176:PRO:HG3	1:I:191:ILE:CD1	2.47	0.44
1:A:235:ILE:HD12	1:A:245:ILE:HG12	1.98	0.44
1:A:156:LEU:HD21	1:B:153:LEU:HD11	1.99	0.44
1:E:293:GLU:O	5:E:402:EPE:H92	2.18	0.44
1:D:65:GLU:OE2	1:D:74:ARG:NE	2.38	0.44
1:J:148:VAL:O	1:J:148:VAL:CG1	2.65	0.44
1:C:198:GLN:HB2	1:D:198:GLN:NE2	2.33	0.44
1:C:198:GLN:NE2	1:D:198:GLN:HB2	2.32	0.44
1:F:65:GLU:OE2	1:F:74:ARG:NE	2.38	0.44
1:F:101:MET:CE	1:F:111:ILE:HG13	2.47	0.44
1:C:176:PRO:HG3	1:C:191:ILE:CD1	2.48	0.44
1:C:230:ASN:HB3	1:F:260:TRP:CZ2	2.53	0.44
1:G:153:LEU:HD11	1:J:156:LEU:CD2	2.40	0.44
1:B:198:GLN:HB3	1:I:198:GLN:NE2	2.33	0.43
1:C:12:MET:HG3	1:C:16:ASP:HB2	2.00	0.43
1:C:99:ASN:ND2	1:D:275:LYS:HG2	2.32	0.43
1:D:230:ASN:HB3	1:E:260:TRP:CZ2	2.53	0.43
1:G:12:MET:HG3	1:G:16:ASP:HB2	2.01	0.43
1:I:296:LEU:HA	1:I:296:LEU:HD23	1.81	0.43
1:G:153:LEU:HD21	1:J:156:LEU:HD23	2.00	0.42
1:B:148:VAL:O	1:B:148:VAL:CG1	2.67	0.42
1:D:12:MET:HG3	1:D:16:ASP:HB2	2.01	0.42
1:I:101:MET:HB2	2:I:600:G8H:C17	2.50	0.42
1:J:176:PRO:HG3	1:J:191:ILE:CD1	2.50	0.42
1:G:230:ASN:HB3	1:J:260:TRP:CZ2	2.54	0.42
1:D:101:MET:HB2	2:D:401:G8H:C17	2.49	0.42
1:E:101:MET:CE	1:E:111:ILE:HG13	2.49	0.42
1:C:204:ASP:OD2	1:C:207:SER:HB2	2.20	0.42
1:B:195:PRO:HG2	1:B:198:GLN:HG3	2.01	0.41
1:G:270:LYS:HE3	1:G:284:PHE:CG	2.55	0.41
1:C:5:ASN:HB2	1:D:274:MET:O	2.20	0.41
1:D:270:LYS:HE3	1:D:284:PHE:CG	2.55	0.41
1:J:204:ASP:OD2	1:J:207:SER:HB2	2.21	0.41
1:D:204:ASP:OD2	1:D:207:SER:HB2	2.21	0.41
1:H:235:ILE:HD13	2:H:401:G8H:C6	2.50	0.41
1:H:204:ASP:OD2	1:H:207:SER:HB2	2.21	0.41
1:B:101:MET:CE	1:B:111:ILE:HG13	2.48	0.41
1:J:270:LYS:HE3	1:J:284:PHE:CG	2.55	0.41
1:D:260:TRP:CZ2	1:E:230:ASN:HB3	2.56	0.41
1:B:204:ASP:OD2	1:B:207:SER:HB2	2.21	0.41
1:A:12:MET:SD	1:A:17:PHE:HB2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:MET:CE	1:G:111:ILE:HG13	2.49	0.40
1:G:204:ASP:OD2	1:G:207:SER:HB2	2.21	0.40
1:E:270:LYS:HE3	1:E:284:PHE:CG	2.56	0.40
1:F:270:LYS:HE3	1:F:284:PHE:CG	2.56	0.40
1:C:194:TYR:HE2	1:D:198:GLN:O	2.03	0.40
1:G:153:LEU:HD21	1:J:156:LEU:CD2	2.51	0.40
1:H:270:LYS:HE3	1:H:284:PHE:CG	2.56	0.40
1:A:16:ASP:O	1:A:20:LEU:HB2	2.22	0.40
1:B:198:GLN:NE2	1:I:198:GLN:HB2	2.37	0.40
1:E:293:GLU:O	5:E:402:EPE:H21	2.22	0.40
1:J:12:MET:HG3	1:J:16:ASP:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/330 (87%)	279 (98%)	7 (2%)	0	100	100
1	B	286/330 (87%)	281 (98%)	5 (2%)	0	100	100
1	C	286/330 (87%)	280 (98%)	6 (2%)	0	100	100
1	D	286/330 (87%)	279 (98%)	7 (2%)	0	100	100
1	E	285/330 (86%)	281 (99%)	4 (1%)	0	100	100
1	F	283/330 (86%)	279 (99%)	4 (1%)	0	100	100
1	G	265/330 (80%)	262 (99%)	3 (1%)	0	100	100
1	H	278/330 (84%)	272 (98%)	6 (2%)	0	100	100
1	I	284/330 (86%)	276 (97%)	8 (3%)	0	100	100
1	J	286/330 (87%)	278 (97%)	8 (3%)	0	100	100
All	All	2825/3300 (86%)	2767 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	247/294 (84%)	237 (96%)	10 (4%)	28	37
1	B	248/294 (84%)	238 (96%)	10 (4%)	28	37
1	C	244/294 (83%)	232 (95%)	12 (5%)	22	28
1	D	234/294 (80%)	227 (97%)	7 (3%)	36	48
1	E	232/294 (79%)	224 (97%)	8 (3%)	32	43
1	F	236/294 (80%)	229 (97%)	7 (3%)	36	48
1	G	221/294 (75%)	216 (98%)	5 (2%)	44	58
1	H	233/294 (79%)	224 (96%)	9 (4%)	28	39
1	I	237/294 (81%)	230 (97%)	7 (3%)	36	48
1	J	228/294 (78%)	221 (97%)	7 (3%)	35	47
All	All	2360/2940 (80%)	2278 (96%)	82 (4%)	32	42

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	71	GLN
1	A	91	ARG
1	A	95	GLU
1	A	101	MET
1	A	146	HIS
1	A	160	LYS
1	A	191	ILE
1	A	201	HIS
1	A	291	ARG
1	B	8	LYS
1	B	71	GLN
1	B	91	ARG
1	B	95	GLU

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Mol	Chain	Res	Type
1	B	101	MET
1	B	191	ILE
1	B	198	GLN
1	B	201	HIS
1	B	288	LYS
1	B	291	ARG
1	C	60	LYS
1	C	65	GLU
1	C	66	ARG
1	C	67	THR
1	C	71	GLN
1	C	91	ARG
1	C	95	GLU
1	C	101	MET
1	C	133	ARG
1	C	191	ILE
1	C	201	HIS
1	C	291	ARG
1	D	91	ARG
1	D	95	GLU
1	D	101	MET
1	D	191	ILE
1	D	201	HIS
1	D	282	GLU
1	D	291	ARG
1	E	71	GLN
1	E	91	ARG
1	E	95	GLU
1	E	101	MET
1	E	133	ARG
1	E	191	ILE
1	E	201	HIS
1	E	291	ARG
1	F	91	ARG
1	F	95	GLU
1	F	101	MET
1	F	191	ILE
1	F	201	HIS
1	F	275	LYS
1	F	291	ARG
1	G	71	GLN
1	G	91	ARG

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Mol	Chain	Res	Type
1	G	95	GLU
1	G	101	MET
1	G	191	ILE
1	H	3	LYS
1	H	18	ARG
1	H	31	GLU
1	H	71	GLN
1	H	91	ARG
1	H	95	GLU
1	H	101	MET
1	H	191	ILE
1	H	291	ARG
1	I	14	ARG
1	I	71	GLN
1	I	91	ARG
1	I	95	GLU
1	I	101	MET
1	I	191	ILE
1	I	201	HIS
1	J	18	ARG
1	J	91	ARG
1	J	95	GLU
1	J	101	MET
1	J	191	ILE
1	J	201	HIS
1	J	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	71	GLN
1	A	99	ASN
1	A	118	GLN
1	A	200	HIS
1	B	71	GLN
1	B	99	ASN
1	B	118	GLN
1	B	146	HIS
1	B	198	GLN
1	C	30	HIS
1	C	71	GLN

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Mol	Chain	Res	Type
1	C	99	ASN
1	C	118	GLN
1	C	200	HIS
1	C	257	ASN
1	D	99	ASN
1	D	200	HIS
1	E	30	HIS
1	E	71	GLN
1	F	118	GLN
1	F	200	HIS
1	G	118	GLN
1	H	71	GLN
1	H	118	GLN
1	I	71	GLN
1	I	118	GLN
1	I	198	GLN
1	J	118	GLN
1	J	257	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	G8H	D	401	-	22,22,22	0.48	0	29,29,29	0.29	0
4	EDO	B	403	-	3,3,3	0.10	0	2,2,2	0.08	0
5	EPE	D	402	-	15,15,15	2.02	1 (6%)	19,20,20	1.33	2 (10%)
2	G8H	C	401	-	22,22,22	0.45	0	29,29,29	0.29	0
4	EDO	B	405	-	3,3,3	0.10	0	2,2,2	0.11	0
2	G8H	H	401	-	22,22,22	0.50	0	29,29,29	0.33	0
2	G8H	I	600	-	22,22,22	0.48	0	29,29,29	0.30	0
2	G8H	F	401	-	22,22,22	0.47	0	29,29,29	0.33	0
2	G8H	B	401	-	22,22,22	0.47	0	29,29,29	0.32	0
4	EDO	F	402	-	3,3,3	0.11	0	2,2,2	0.13	0
2	G8H	J	600	-	22,22,22	0.47	0	29,29,29	0.32	0
4	EDO	A	406	-	3,3,3	0.12	0	2,2,2	0.16	0
5	EPE	E	402	-	15,15,15	1.87	1 (6%)	19,20,20	1.39	2 (10%)
5	EPE	H	402	-	15,15,15	1.90	1 (6%)	19,20,20	1.26	1 (5%)
2	G8H	E	401	-	22,22,22	0.49	0	29,29,29	0.32	0
4	EDO	B	404	-	3,3,3	0.11	0	2,2,2	0.08	0
2	G8H	A	401	-	22,22,22	0.49	0	29,29,29	0.35	0
4	EDO	A	404	-	3,3,3	0.09	0	2,2,2	0.06	0
4	EDO	A	405	-	3,3,3	0.15	0	2,2,2	0.16	0
5	EPE	B	402	-	15,15,15	1.95	1 (6%)	19,20,20	1.37	2 (10%)
2	G8H	G	600	-	22,22,22	0.46	0	29,29,29	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G8H	D	401	-	-	0/8/8/8	0/3/3/3
4	EDO	B	403	-	-	1/1/1/1	-
5	EPE	D	402	-	-	4/9/19/19	0/1/1/1
2	G8H	C	401	-	-	0/8/8/8	0/3/3/3
4	EDO	B	405	-	-	1/1/1/1	-
2	G8H	H	401	-	-	0/8/8/8	0/3/3/3
2	G8H	I	600	-	-	0/8/8/8	0/3/3/3
2	G8H	F	401	-	-	0/8/8/8	0/3/3/3
2	G8H	B	401	-	-	0/8/8/8	0/3/3/3
4	EDO	F	402	-	-	1/1/1/1	-
2	G8H	J	600	-	-	0/8/8/8	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	406	-	-	1/1/1/1	-
5	EPE	E	402	-	-	4/9/19/19	0/1/1/1
5	EPE	H	402	-	-	4/9/19/19	0/1/1/1
2	G8H	E	401	-	-	0/8/8/8	0/3/3/3
4	EDO	B	404	-	-	0/1/1/1	-
2	G8H	A	401	-	-	0/8/8/8	0/3/3/3
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
5	EPE	B	402	-	-	4/9/19/19	0/1/1/1
2	G8H	G	600	-	-	0/8/8/8	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	402	EPE	C10-S	-7.45	1.67	1.77
5	B	402	EPE	C10-S	-6.98	1.67	1.77
5	H	402	EPE	C10-S	-6.78	1.68	1.77
5	E	402	EPE	C10-S	-6.69	1.68	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	402	EPE	O2S-S-C10	3.69	112.30	106.73
5	B	402	EPE	O1S-S-C10	3.50	112.01	106.73
5	H	402	EPE	O3S-S-C10	3.01	111.89	106.00
5	D	402	EPE	O1S-S-C10	2.81	110.97	106.73
5	D	402	EPE	C6-N1-C2	2.44	114.10	108.84
5	B	402	EPE	C5-N4-C3	2.42	114.05	108.84
5	E	402	EPE	C6-N1-C2	2.39	114.00	108.84

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	402	EPE	C9-C10-S-O1S
5	E	402	EPE	C9-C10-S-O3S
5	H	402	EPE	C9-C10-S-O1S
5	H	402	EPE	C9-C10-S-O2S
5	B	402	EPE	N4-C7-C8-O8
5	B	402	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
5	D	402	EPE	C9-C10-S-O3S
5	H	402	EPE	C9-C10-S-O3S
4	B	405	EDO	O1-C1-C2-O2
5	D	402	EPE	N4-C7-C8-O8
5	E	402	EPE	N4-C7-C8-O8
5	B	402	EPE	C9-C10-S-O1S
5	B	402	EPE	C9-C10-S-O2S
5	D	402	EPE	C9-C10-S-O1S
5	D	402	EPE	C9-C10-S-O2S
5	E	402	EPE	C9-C10-S-O2S
4	A	404	EDO	O1-C1-C2-O2
4	B	403	EDO	O1-C1-C2-O2
5	H	402	EPE	N4-C7-C8-O8
4	A	406	EDO	O1-C1-C2-O2
4	F	402	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	G8H	1	0
2	H	401	G8H	1	0
2	I	600	G8H	1	0
2	F	401	G8H	1	0
5	E	402	EPE	2	0
5	B	402	EPE	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	290/330 (87%)	0.07	13 (4%)	38 44	23, 36, 66, 106	0
1	B	290/330 (87%)	0.20	10 (3%)	48 55	27, 41, 73, 99	0
1	C	290/330 (87%)	0.39	21 (7%)	21 24	29, 45, 95, 139	0
1	D	290/330 (87%)	0.64	33 (11%)	10 11	40, 57, 119, 152	0
1	E	289/330 (87%)	0.72	39 (13%)	7 8	34, 56, 126, 155	0
1	F	289/330 (87%)	0.57	32 (11%)	10 12	34, 51, 112, 140	0
1	G	271/330 (82%)	1.28	51 (18%)	3 3	56, 85, 117, 128	0
1	H	282/330 (85%)	0.45	35 (12%)	8 9	25, 42, 99, 124	0
1	I	288/330 (87%)	0.51	18 (6%)	26 29	34, 51, 84, 106	0
1	J	290/330 (87%)	1.21	50 (17%)	4 4	54, 76, 117, 142	0
All	All	2869/3300 (86%)	0.60	302 (10%)	11 13	23, 54, 110, 155	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	146	HIS	6.9
1	C	146	HIS	6.7
1	H	47	GLY	5.7
1	F	44	LEU	5.5
1	B	148	VAL	5.3
1	J	283	LEU	5.2
1	A	146	HIS	5.2
1	J	146	HIS	5.2
1	B	146	HIS	5.2
1	F	47	GLY	5.1
1	J	152	TYR	5.0
1	F	147	ASN	4.9
1	H	148	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	298	VAL	4.8
1	H	302	ALA	4.8
1	D	146	HIS	4.7
1	E	48	GLY	4.7
1	E	147	ASN	4.6
1	D	46	HIS	4.6
1	E	46	HIS	4.5
1	E	69	THR	4.4
1	H	46	HIS	4.4
1	G	6	VAL	4.3
1	E	47	GLY	4.2
1	E	135	LEU	4.2
1	C	45	LYS	4.2
1	E	51	LYS	4.2
1	F	2	GLY	4.1
1	G	201	HIS	4.1
1	D	45	LYS	4.1
1	H	69	THR	4.1
1	I	147	ASN	4.1
1	I	298	VAL	4.1
1	F	146	HIS	4.0
1	C	70	VAL	4.0
1	D	148	VAL	4.0
1	F	69	THR	3.9
1	B	2	GLY	3.9
1	C	135	LEU	3.8
1	G	149	SER	3.8
1	I	2	GLY	3.8
1	H	13	SER	3.8
1	E	70	VAL	3.8
1	E	148	VAL	3.8
1	G	128	GLY	3.8
1	J	135	LEU	3.8
1	D	69	THR	3.7
1	D	44	LEU	3.7
1	H	11	TYR	3.7
1	J	46	HIS	3.7
1	F	64	TRP	3.7
1	E	11	TYR	3.7
1	I	201	HIS	3.6
1	E	37	LEU	3.6
1	J	156	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	147	ASN	3.6
1	G	70	VAL	3.6
1	G	43	SER	3.6
1	E	26	GLY	3.6
1	E	2	GLY	3.5
1	I	299	GLU	3.5
1	D	47	GLY	3.5
1	H	4	VAL	3.5
1	H	48	GLY	3.5
1	B	135	LEU	3.5
1	G	283	LEU	3.5
1	J	147	ASN	3.5
1	C	148	VAL	3.4
1	G	49	CYS	3.4
1	D	135	LEU	3.4
1	J	90	SER	3.4
1	D	147	ASN	3.4
1	A	69	THR	3.4
1	C	2	GLY	3.4
1	H	149	SER	3.3
1	E	34	PRO	3.3
1	I	148	VAL	3.3
1	G	58	LYS	3.3
1	D	71	GLN	3.3
1	C	147	ASN	3.3
1	J	64	TRP	3.3
1	E	25	MET	3.2
1	H	70	VAL	3.2
1	J	2	GLY	3.2
1	C	47	GLY	3.2
1	J	50	ASN	3.2
1	D	64	TRP	3.2
1	E	14	ARG	3.1
1	G	54	ARG	3.1
1	G	7	ALA	3.1
1	F	148	VAL	3.1
1	I	70	VAL	3.1
1	E	73	TYR	3.1
1	F	152	TYR	3.1
1	E	60	LYS	3.1
1	F	58	LYS	3.1
1	F	66	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	151	LEU	3.1
1	B	69	THR	3.0
1	A	147	ASN	3.0
1	G	11	TYR	3.0
1	C	69	THR	3.0
1	G	150	TRP	3.0
1	A	68	LYS	3.0
1	H	17	PHE	3.0
1	E	44	LEU	3.0
1	J	148	VAL	3.0
1	G	71	GLN	3.0
1	D	301	SER	3.0
1	A	135	LEU	3.0
1	J	67	THR	3.0
1	D	2	GLY	3.0
1	G	30	HIS	2.9
1	G	68	LYS	2.9
1	G	69	THR	2.9
1	H	67	THR	2.9
1	G	73	TYR	2.9
1	G	59	HIS	2.9
1	J	288	LYS	2.9
1	G	64	TRP	2.9
1	H	8	LYS	2.9
1	I	66	ARG	2.9
1	G	127	LEU	2.9
1	J	63	ALA	2.9
1	E	64	TRP	2.9
1	E	65	GLU	2.9
1	C	44	LEU	2.8
1	C	201	HIS	2.8
1	F	201	HIS	2.8
1	H	44	LEU	2.8
1	J	282	GLU	2.8
1	J	70	VAL	2.8
1	H	45	LYS	2.8
1	E	283	LEU	2.8
1	E	19	VAL	2.8
1	F	70	VAL	2.8
1	G	196	LEU	2.8
1	F	1	MET	2.8
1	I	291	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	129	ARG	2.8
1	G	19	VAL	2.8
1	G	202	VAL	2.8
1	I	64	TRP	2.7
1	J	14	ARG	2.7
1	D	70	VAL	2.7
1	E	43	SER	2.7
1	D	66	ARG	2.7
1	F	73	TYR	2.7
1	D	32	ILE	2.7
1	G	41	ILE	2.7
1	G	238	GLU	2.7
1	H	12	MET	2.7
1	F	71	GLN	2.7
1	E	45	LYS	2.7
1	F	68	LYS	2.7
1	J	301	SER	2.7
1	H	9	LEU	2.7
1	C	46	HIS	2.6
1	J	58	LYS	2.6
1	D	242	ILE	2.6
1	H	128	GLY	2.6
1	E	40	SER	2.6
1	J	11	TYR	2.6
1	E	36	SER	2.6
1	H	16	ASP	2.6
1	G	72	GLY	2.6
1	J	69	THR	2.6
1	G	156	LEU	2.6
1	J	296	LEU	2.6
1	F	63	ALA	2.6
1	D	73	TYR	2.6
1	J	68	LYS	2.6
1	F	135	LEU	2.5
1	D	201	HIS	2.5
1	J	37	LEU	2.5
1	D	50	ASN	2.5
1	G	17	PHE	2.5
1	J	242	ILE	2.5
1	B	65	GLU	2.5
1	I	152	TYR	2.5
1	H	7	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	40	SER	2.5
1	J	284	PHE	2.5
1	C	42	ALA	2.5
1	E	59	HIS	2.5
1	G	203	GLU	2.4
1	E	152	TYR	2.4
1	A	70	VAL	2.4
1	D	68	LYS	2.4
1	J	201	HIS	2.4
1	B	147	ASN	2.4
1	J	133	ARG	2.4
1	D	49	CYS	2.4
1	H	3	LYS	2.4
1	H	49	CYS	2.4
1	F	29	ASN	2.4
1	H	15	ASP	2.4
1	A	2	GLY	2.4
1	A	148	VAL	2.4
1	H	6	VAL	2.4
1	H	25	MET	2.4
1	J	44	LEU	2.4
1	E	32	ILE	2.3
1	F	134	ASN	2.3
1	H	50	ASN	2.3
1	G	28	LYS	2.3
1	F	48	GLY	2.3
1	F	301	SER	2.3
1	G	13	SER	2.3
1	J	25	MET	2.3
1	C	10	ARG	2.3
1	F	54	ARG	2.3
1	G	103	VAL	2.3
1	D	75	LEU	2.3
1	G	9	LEU	2.3
1	A	289	ASP	2.3
1	G	35	GLY	2.3
1	E	54	ARG	2.3
1	G	96	SER	2.3
1	E	38	ILE	2.3
1	A	284	PHE	2.3
1	H	14	ARG	2.3
1	F	67	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	28	LYS	2.3
1	G	111	ILE	2.3
1	I	283	LEU	2.2
1	J	132	PHE	2.2
1	D	63	ALA	2.2
1	G	42	ALA	2.2
1	I	288	LYS	2.2
1	G	57	VAL	2.2
1	C	25	MET	2.2
1	C	34	PRO	2.2
1	A	201	HIS	2.2
1	F	31	GLU	2.2
1	J	71	GLN	2.2
1	D	43	SER	2.2
1	C	32	ILE	2.2
1	H	151	LEU	2.2
1	J	20	LEU	2.2
1	C	202	VAL	2.2
1	J	162	PHE	2.2
1	B	289	ASP	2.2
1	E	10	ARG	2.2
1	F	10	ARG	2.2
1	G	14	ARG	2.2
1	J	165	MET	2.2
1	H	82	TYR	2.2
1	D	53	LEU	2.2
1	I	68	LYS	2.2
1	J	59	HIS	2.2
1	F	49	CYS	2.2
1	I	69	THR	2.2
1	G	37	LEU	2.1
1	J	32	ILE	2.1
1	J	41	ILE	2.1
1	G	97	VAL	2.1
1	G	289	ASP	2.1
1	D	58	LYS	2.1
1	E	238	GLU	2.1
1	C	71	GLN	2.1
1	J	118	GLN	2.1
1	E	49	CYS	2.1
1	A	67	THR	2.1
1	J	36	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	54	ARG	2.1
1	I	164	TYR	2.1
1	F	62	ILE	2.1
1	G	56	LEU	2.1
1	B	64	TRP	2.1
1	C	133	ARG	2.1
1	E	67	THR	2.1
1	J	155	ARG	2.1
1	J	65	GLU	2.1
1	G	271	ASP	2.1
1	B	201	HIS	2.1
1	F	30	HIS	2.1
1	F	52	VAL	2.1
1	G	93	VAL	2.1
1	G	10	ARG	2.1
1	E	3	LYS	2.1
1	C	203	GLU	2.1
1	G	65	GLU	2.1
1	J	217	VAL	2.1
1	G	98	GLY	2.1
1	J	10	ARG	2.1
1	E	58	LYS	2.0
1	H	60	LYS	2.0
1	J	49	CYS	2.0
1	D	37	LEU	2.0
1	E	62	ILE	2.0
1	G	94	VAL	2.0
1	H	72	GLY	2.0
1	D	60	LYS	2.0
1	F	28	LYS	2.0
1	J	45	LYS	2.0
1	H	64	TRP	2.0
1	A	282	GLU	2.0
1	D	25	MET	2.0
1	H	65	GLU	2.0
1	J	212	ALA	2.0
1	I	296	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EPE	B	402	15/15	0.80	0.20	76,88,97,97	0
5	EPE	D	402	15/15	0.80	0.20	101,111,122,122	0
5	EPE	E	402	15/15	0.81	0.21	83,105,112,112	0
4	EDO	A	405	4/4	0.82	0.18	59,60,60,60	0
5	EPE	H	402	15/15	0.82	0.21	79,97,108,109	0
2	G8H	G	600	20/20	0.85	0.18	65,95,114,114	0
4	EDO	B	403	4/4	0.87	0.17	53,55,56,57	0
3	CL	C	402	1/1	0.88	0.15	69,69,69,69	0
4	EDO	B	405	4/4	0.90	0.14	51,52,53,54	0
3	CL	H	403	1/1	0.92	0.12	67,67,67,67	0
3	CL	A	403	1/1	0.92	0.15	78,78,78,78	0
2	G8H	E	401	20/20	0.93	0.10	39,49,56,56	0
4	EDO	A	406	4/4	0.93	0.11	42,45,47,51	0
3	CL	A	402	1/1	0.94	0.08	43,43,43,43	0
4	EDO	B	404	4/4	0.94	0.10	47,49,49,50	0
4	EDO	A	404	4/4	0.94	0.12	52,52,52,52	0
4	EDO	F	402	4/4	0.94	0.12	64,65,66,67	0
2	G8H	B	401	20/20	0.95	0.08	26,30,36,36	0
2	G8H	F	401	20/20	0.95	0.08	41,43,46,48	0
2	G8H	D	401	20/20	0.95	0.09	36,47,59,59	0
2	G8H	I	600	20/20	0.95	0.07	35,40,43,44	0
2	G8H	J	600	20/20	0.95	0.09	53,62,70,71	0
2	G8H	H	401	20/20	0.96	0.07	20,29,37,37	0
2	G8H	A	401	20/20	0.96	0.07	27,30,37,37	0
2	G8H	C	401	20/20	0.96	0.08	24,33,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.