Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:51 AM GMT

PDB ID	:	3CCH
Title	:	H-2Db complex with murine gp100
Authors	:	Badia-Martinez, D.; Achour, A.
Deposited on	:	2008-02-25
Resolution	:	2.60 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:

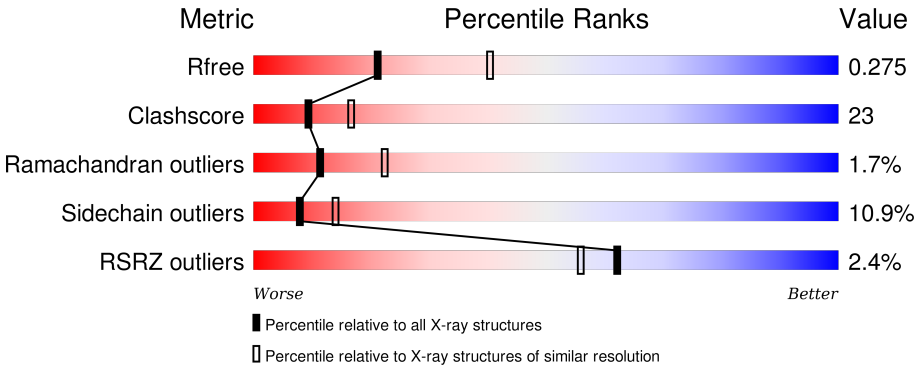
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	276	60% 33% 7%
1	D	276	58% 34% 8%
1	G	276	4% 54% 36% 7%
1	J	276	5% 53% 39% 7%
2	B	99	67% 31%

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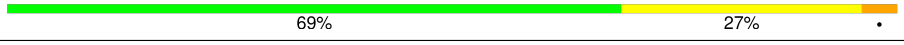
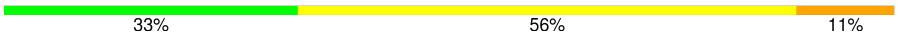
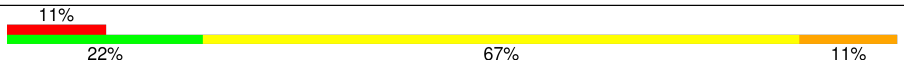
Mol	Chain	Length	Quality of chain
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

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
4	SO4	H	102	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12836 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	2	0
			2276	1438	400	428	10			
1	D	276	Total	C	N	O	S	0	2	0
			2275	1437	400	428	10			
1	G	272	Total	C	N	O	S	0	0	0
			2232	1410	395	418	9			
1	J	272	Total	C	N	O	S	0	0	0
			2232	1410	395	418	9			

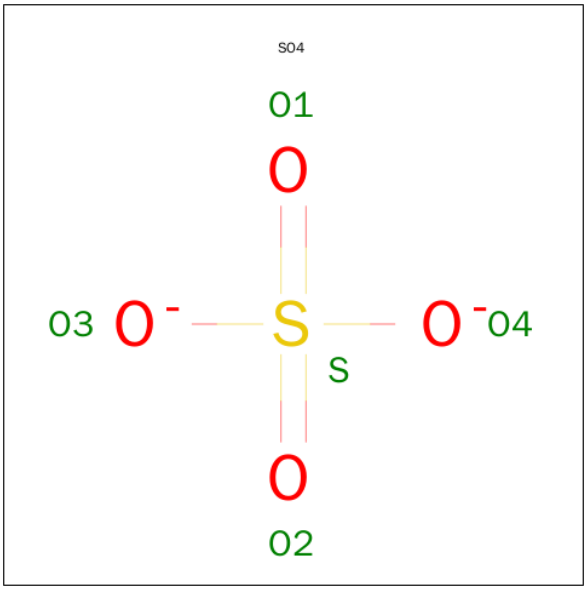
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	1	0
			828	529	140	152	7			
2	K	99	Total	C	N	O	S	0	1	0
			828	529	140	152	7			

- Molecule 3 is a protein called nonameric peptide murine gp100.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			78	46	15	17			
3	F	9	Total	C	N	O	0	0	0
			78	46	15	17			
3	I	9	Total	C	N	O	0	0	0
			78	46	15	17			
3	L	9	Total	C	N	O	0	0	0
			78	46	15	17			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

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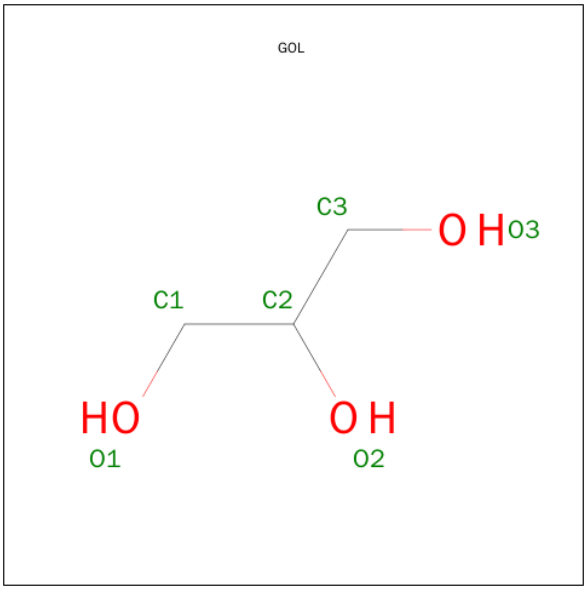
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

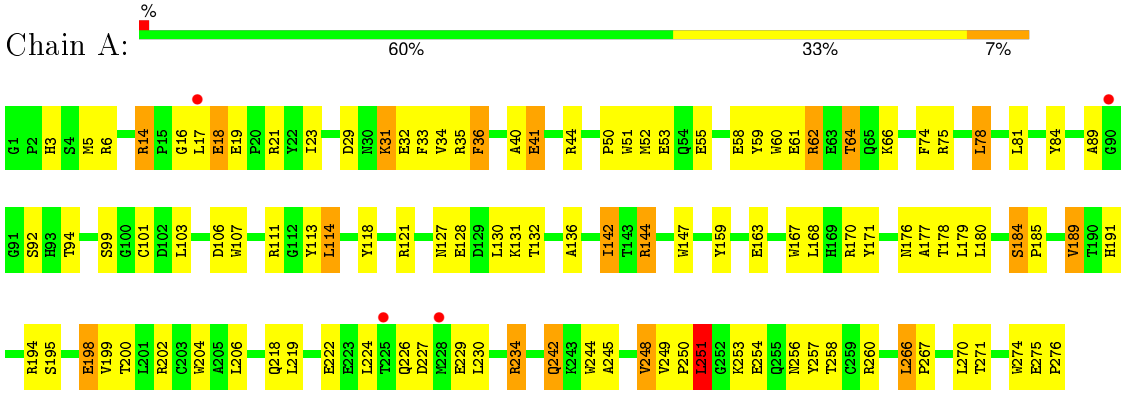
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	13	Total	O	0	0
			13	13		
6	C	1	Total	O	0	0
			1	1		
6	D	14	Total	O	0	0
			14	14		
6	E	9	Total	O	0	0
			9	9		
6	F	1	Total	O	0	0
			1	1		
6	G	8	Total	O	0	0
			8	8		
6	H	3	Total	O	0	0
			3	3		
6	I	1	Total	O	0	0
			1	1		
6	J	10	Total	O	0	0
			10	10		
6	K	5	Total	O	0	0
			5	5		
6	L	1	Total	O	0	0
			1	1		

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.

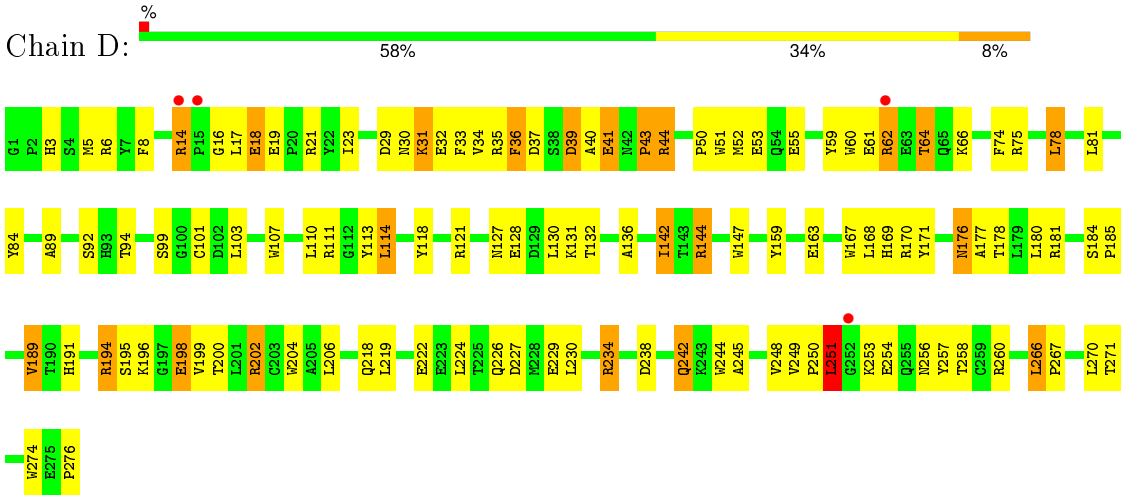
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



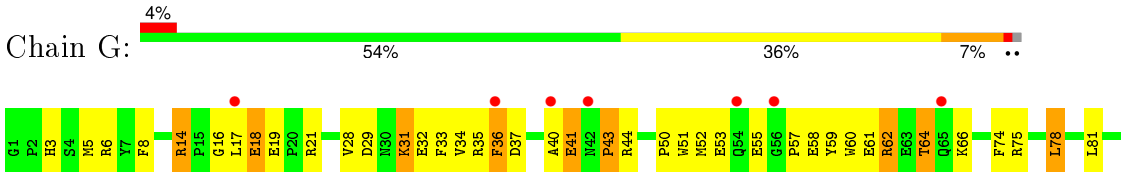
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

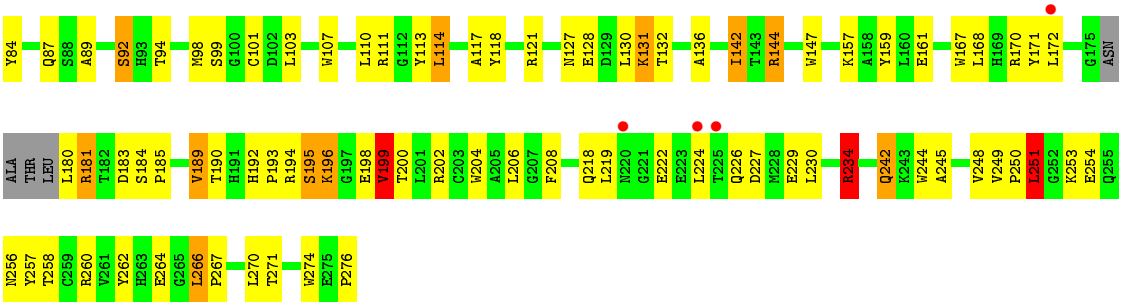
Chain D:



- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

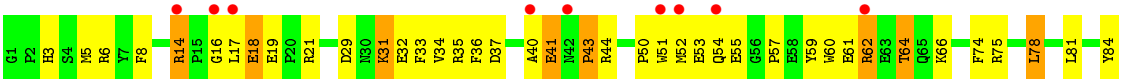
Chain G:

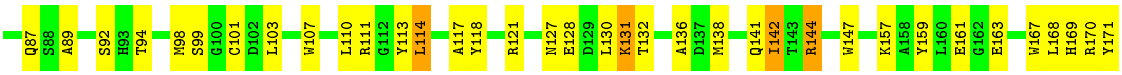


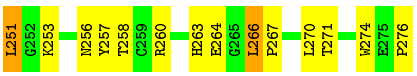


• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain J:

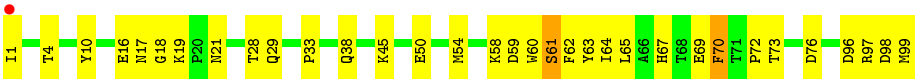






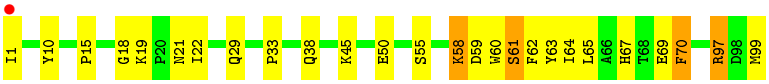
• Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin

Chain E:

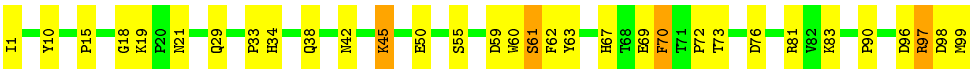


• Molecule 2: Beta-2-microglobulin

Chain H:

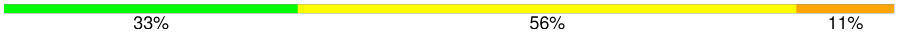
• Molecule 2: Beta-2-microglobulin

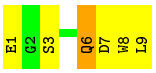
Chain K:



- Molecule 3: nonameric peptide murine gp100

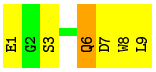
Chain C:





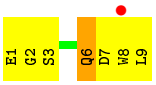
- Molecule 3: nonameric peptide murine gp100

Chain F:



- Molecule 3: nonameric peptide murine gp100

Chain I:



- Molecule 3: nonameric peptide murine gp100

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.50Å 176.60Å 85.50Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	19.60 – 2.60 19.61 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.60-2.60) 99.7 (19.61-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.279 0.239 , 0.275	Depositor DCC
R_{free} test set	3378 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.4	EDS
Estimated twinning fraction	0.019 for -h-l,k,h 0.019 for l,k,-h-l 0.026 for h,-k,-h-l 0.026 for -h-l,-k,l 0.477 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 66893 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12836	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 9.59% 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, SO4

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	0.66	1/2349 (0.0%)	0.86	6/3188 (0.2%)
1	D	0.65	1/2348 (0.0%)	0.78	6/3187 (0.2%)
1	G	0.64	1/2298 (0.0%)	0.80	7/3117 (0.2%)
1	J	0.64	1/2298 (0.0%)	0.79	5/3117 (0.2%)
2	B	0.64	0/847	0.75	0/1148
2	E	0.66	0/847	0.76	0/1148
2	H	0.70	0/858	0.74	0/1163
2	K	0.69	0/858	0.74	0/1163
3	C	0.48	0/79	0.50	0/104
3	F	0.51	0/79	0.49	0/104
3	I	0.57	0/79	0.49	0/104
3	L	0.53	0/79	0.51	0/104
All	All	0.65	4/13019 (0.0%)	0.79	24/17647 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	CYS	CB-SG	-7.84	1.69	1.82
1	D	101	CYS	CB-SG	-7.51	1.69	1.82
1	G	101	CYS	CB-SG	-5.57	1.72	1.81
1	J	101	CYS	CB-SG	-5.29	1.73	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ARG	NE-CZ-NH1	-14.02	113.29	120.30
1	A	44	ARG	NE-CZ-NH2	13.30	126.95	120.30
1	J	62	ARG	NE-CZ-NH1	-11.17	114.72	120.30
1	A	62	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	J	62	ARG	NE-CZ-NH2	10.48	125.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	62	ARG	NE-CZ-NH1	-10.43	115.08	120.30
1	G	62	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	62	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	G	62	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	D	62	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	G	251	LEU	CA-CB-CG	7.95	133.58	115.30
1	D	251	LEU	CA-CB-CG	7.54	132.63	115.30
1	A	251	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	44	ARG	CD-NE-CZ	7.34	133.88	123.60
1	D	44	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	G	44	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	234	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	J	44	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	G	44	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	G	234	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	44	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	44	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	J	234	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	D	202	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	2276	0	2151	103	0
1	D	2275	0	2149	107	0
1	G	2232	0	2101	135	0
1	J	2232	0	2101	137	0
2	B	821	0	796	25	0
2	E	821	0	796	23	0
2	H	828	0	803	41	1
2	K	828	0	803	40	1
3	C	78	0	68	5	0
3	F	78	0	68	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	78	0	68	8	0
3	L	78	0	68	6	0
4	B	20	0	0	1	0
4	D	10	0	0	0	1
4	E	25	0	0	0	0
4	G	5	0	0	0	0
4	H	20	0	0	0	0
4	J	10	0	0	0	0
4	K	15	0	0	0	0
5	A	6	0	8	0	0
5	D	6	0	8	3	0
5	G	6	0	8	0	0
5	J	6	0	8	0	0
6	A	16	0	0	0	1
6	B	13	0	0	0	0
6	C	1	0	0	0	0
6	D	14	0	0	1	0
6	E	9	0	0	0	0
6	F	1	0	0	0	0
6	G	8	0	0	1	0
6	H	3	0	0	0	0
6	I	1	0	0	3	0
6	J	10	0	0	0	0
6	K	5	0	0	1	0
6	L	1	0	0	0	0
All	All	12836	0	12004	561	2

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 23.

All (561) 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:G:57:PRO:CG	2:K:19:LYS:HE3	1.60	1.31
2:H:19:LYS:HE3	1:J:57:PRO:CG	1.62	1.30
2:H:19:LYS:CE	1:J:57:PRO:CG	2.19	1.21
1:D:51:TRP:CZ3	1:D:52:MET:HE2	1.77	1.18
1:G:57:PRO:CG	2:K:19:LYS:CE	2.20	1.18
1:A:51:TRP:CZ3	1:A:52:MET:HE2	1.77	1.17
1:G:57:PRO:HD3	2:K:19:LYS:CE	1.74	1.16
1:G:57:PRO:HD3	2:K:19:LYS:HE2	1.17	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:HE2	1:J:57:PRO:HD3	1.18	1.14
1:G:195:SER:HB3	1:G:196:LYS:HE2	1.29	1.14
1:G:57:PRO:HG3	2:K:19:LYS:HE3	1.18	1.13
2:H:19:LYS:CE	1:J:57:PRO:HD3	1.77	1.12
1:G:57:PRO:CD	2:K:19:LYS:CE	2.27	1.12
2:H:19:LYS:HE3	1:J:57:PRO:HG3	1.20	1.11
2:H:19:LYS:CE	1:J:57:PRO:CD	2.29	1.10
2:H:19:LYS:HE2	1:J:57:PRO:CD	1.84	1.07
1:G:144:ARG:HH11	1:G:144:ARG:HG2	1.12	1.06
1:J:144:ARG:HG2	1:J:144:ARG:HH11	1.13	1.06
1:G:57:PRO:CD	2:K:19:LYS:HE2	1.85	1.06
1:D:144:ARG:HH11	1:D:144:ARG:HG2	1.13	1.05
1:J:14:ARG:HG2	1:J:14:ARG:NH2	1.62	1.04
1:J:199:VAL:HG22	1:J:251:LEU:HB3	1.39	1.03
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.17	1.03
1:G:195:SER:HB3	1:G:196:LYS:CE	1.89	1.02
1:G:51:TRP:CZ3	1:G:52:MET:HE2	1.95	1.02
1:G:14:ARG:HG2	1:G:14:ARG:NH2	1.61	1.01
2:H:19:LYS:CE	1:J:57:PRO:HG3	1.86	1.01
1:G:14:ARG:CG	1:G:14:ARG:HH21	1.74	1.00
1:A:14:ARG:CG	1:A:14:ARG:HH21	1.74	1.00
1:G:57:PRO:HG3	2:K:19:LYS:CE	1.87	1.00
1:D:14:ARG:HH21	1:D:14:ARG:HG2	0.83	1.00
1:J:14:ARG:HH21	1:J:14:ARG:CG	1.75	0.98
1:G:14:ARG:HG2	1:G:14:ARG:HH21	0.81	0.97
1:A:14:ARG:HG2	1:A:14:ARG:HH21	0.80	0.96
1:D:14:ARG:CG	1:D:14:ARG:HH21	1.77	0.96
1:A:14:ARG:HG2	1:A:14:ARG:NH2	1.60	0.96
1:D:14:ARG:NH2	1:D:14:ARG:HG2	1.64	0.96
1:J:234:ARG:HD2	1:J:242:GLN:HE21	1.31	0.95
1:J:14:ARG:HG2	1:J:14:ARG:HH21	0.81	0.94
1:G:195:SER:CB	1:G:196:LYS:HE2	1.97	0.94
1:J:60:TRP:O	1:J:64:THR:HG22	1.67	0.94
1:J:196:LYS:H	1:J:196:LYS:HD3	1.34	0.93
1:J:51:TRP:CZ3	1:J:52:MET:HE3	2.05	0.92
1:D:249:VAL:HG11	1:D:257:TYR:CE2	2.05	0.91
1:G:181:ARG:HG3	1:G:181:ARG:HH11	1.34	0.91
1:D:60:TRP:O	1:D:64:THR:HG22	1.72	0.90
1:J:234:ARG:HD2	1:J:242:GLN:NE2	1.85	0.90
1:G:60:TRP:O	1:G:64:THR:HG22	1.71	0.89
1:J:249:VAL:HG11	1:J:257:TYR:CE2	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:HG11	1:G:257:TYR:CE2	2.07	0.89
1:A:60:TRP:O	1:A:64:THR:HG22	1.73	0.88
1:J:60:TRP:O	1:J:64:THR:CG2	2.22	0.87
1:A:249:VAL:HG11	1:A:257:TYR:CE2	2.09	0.87
1:G:57:PRO:HG2	2:K:19:LYS:HE3	1.58	0.84
1:A:234:ARG:HD3	2:B:10:TYR:CE1	2.13	0.84
1:D:60:TRP:O	1:D:64:THR:CG2	2.25	0.84
1:G:60:TRP:O	1:G:64:THR:CG2	2.25	0.83
2:H:19:LYS:HE3	1:J:57:PRO:HG2	1.58	0.83
1:A:60:TRP:O	1:A:64:THR:CG2	2.26	0.83
1:J:50:PRO:O	1:J:53:GLU:HG2	1.79	0.82
1:D:234:ARG:HD2	1:D:242:GLN:NE2	1.93	0.82
1:G:195:SER:CB	1:G:196:LYS:CE	2.56	0.82
1:J:199:VAL:HG22	1:J:251:LEU:CB	2.09	0.82
1:G:144:ARG:CG	1:G:144:ARG:HH11	1.91	0.82
1:J:144:ARG:CG	1:J:144:ARG:HH11	1.92	0.81
1:D:234:ARG:HD2	1:D:242:GLN:HE21	1.44	0.81
1:A:234:ARG:HD2	1:A:242:GLN:NE2	1.95	0.81
1:G:234:ARG:HD3	2:H:10:TYR:CE1	2.15	0.80
1:G:50:PRO:O	1:G:53:GLU:HG2	1.81	0.80
1:G:199:VAL:HG22	1:G:251:LEU:HB3	1.63	0.80
1:G:234:ARG:HD2	1:G:242:GLN:HE21	1.47	0.79
1:A:144:ARG:HH11	1:A:144:ARG:CG	1.95	0.78
1:D:234:ARG:HD3	2:E:10:TYR:CE1	2.19	0.78
1:G:57:PRO:CD	2:K:19:LYS:NZ	2.47	0.77
1:G:234:ARG:HD2	1:G:242:GLN:NE2	1.97	0.77
1:G:196:LYS:O	1:G:198:GLU:HG3	1.85	0.77
2:H:19:LYS:NZ	1:J:57:PRO:CD	2.47	0.77
1:D:51:TRP:CZ3	1:D:52:MET:CE	2.66	0.77
1:A:51:TRP:CZ3	1:A:52:MET:CE	2.65	0.77
1:D:51:TRP:HZ3	1:D:52:MET:HE2	1.44	0.76
1:D:144:ARG:CG	1:D:144:ARG:HH11	1.93	0.76
1:J:234:ARG:HD3	2:K:10:TYR:CE1	2.20	0.76
1:A:234:ARG:HD2	1:A:242:GLN:HE21	1.47	0.76
1:G:57:PRO:HD3	2:K:19:LYS:NZ	1.99	0.76
2:H:19:LYS:NZ	1:J:57:PRO:HD3	2.01	0.75
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.21	0.75
1:D:249:VAL:HB	1:D:250:PRO:HD2	1.69	0.75
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.22	0.75
1:A:218:GLN:NE2	1:A:260:ARG:NH1	2.34	0.74
1:J:52:MET:HE1	1:J:171:TYR:CD1	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:ARG:HG2	1:J:144:ARG:NH1	1.94	0.73
1:D:50:PRO:O	1:D:53:GLU:HG2	1.87	0.73
1:D:8:PHE:CE1	5:D:279:GOL:H12	2.24	0.73
1:G:234:ARG:HD3	2:H:10:TYR:CZ	2.23	0.73
1:A:50:PRO:O	1:A:53:GLU:HG2	1.88	0.73
1:A:249:VAL:HB	1:A:250:PRO:HD2	1.71	0.72
2:E:29:GLN:HA	2:E:61:SER:OG	1.89	0.72
1:A:51:TRP:HZ3	1:A:52:MET:HE2	1.44	0.72
1:D:234:ARG:HH11	1:D:242:GLN:NE2	1.87	0.72
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.23	0.72
1:J:159:TYR:CE2	3:L:3:SER:HB3	2.24	0.72
1:A:66:LYS:NZ	3:C:1:GLU:HG3	2.04	0.72
1:J:194:ARG:HB2	1:J:198:GLU:O	1.90	0.72
1:G:159:TYR:CE2	3:I:3:SER:HB3	2.25	0.71
1:D:66:LYS:NZ	3:F:1:GLU:HG3	2.05	0.71
2:E:50:GLU:CB	2:E:67:HIS:CE1	2.73	0.71
2:B:50:GLU:CB	2:B:67:HIS:CE1	2.74	0.71
1:G:144:ARG:NH1	1:G:144:ARG:HG2	1.94	0.70
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.26	0.70
2:H:29:GLN:HA	2:H:61:SER:OG	1.91	0.70
2:B:29:GLN:HA	2:B:61:SER:OG	1.92	0.69
1:D:144:ARG:NH1	1:D:144:ARG:HG2	1.94	0.69
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.27	0.69
1:G:184:SER:HB2	1:G:266:LEU:CD1	2.23	0.69
1:D:218:GLN:NE2	1:D:260:ARG:NH1	2.40	0.69
1:G:111:ARG:NE	6:G:280:HOH:O	2.20	0.68
1:A:194:ARG:HB2	1:A:198:GLU:HB2	1.74	0.68
1:J:234:ARG:HH11	1:J:242:GLN:NE2	1.92	0.68
1:J:249:VAL:HB	1:J:250:PRO:HD2	1.76	0.67
1:J:274:TRP:CZ2	1:J:276:PRO:HA	2.30	0.67
1:G:274:TRP:CZ2	1:G:276:PRO:HA	2.29	0.67
1:A:234:ARG:HH11	1:A:242:GLN:NE2	1.92	0.67
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.29	0.67
1:J:51:TRP:CZ3	1:J:52:MET:CE	2.78	0.67
1:G:181:ARG:HH11	1:G:181:ARG:CG	2.08	0.66
1:G:249:VAL:HB	1:G:250:PRO:HD2	1.77	0.65
1:A:219:LEU:HB3	1:A:224:LEU:HD11	1.79	0.65
1:D:249:VAL:CG1	1:D:257:TYR:CE2	2.80	0.65
2:B:4:THR:N	4:B:101:SO4:O2	2.20	0.65
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.31	0.65
2:K:29:GLN:HA	2:K:61:SER:OG	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:TRP:CH2	1:J:276:PRO:HA	2.32	0.65
1:A:144:ARG:HG2	1:A:144:ARG:NH1	1.98	0.64
1:G:274:TRP:CH2	1:G:276:PRO:HA	2.33	0.64
1:G:234:ARG:HH11	1:G:242:GLN:NE2	1.96	0.64
1:J:219:LEU:HB3	1:J:224:LEU:HD11	1.79	0.64
1:A:121:ARG:HH21	2:B:1:ILE:HG22	1.63	0.64
1:D:219:LEU:HB3	1:D:224:LEU:HD11	1.80	0.63
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.33	0.63
1:G:51:TRP:CZ3	1:G:52:MET:CE	2.79	0.63
1:A:194:ARG:HD2	1:A:248:VAL:CG1	2.28	0.63
2:K:50:GLU:HB2	2:K:67:HIS:CE1	2.34	0.63
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.33	0.63
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.81	0.62
3:I:6:GLN:HE21	3:I:7:ASP:H	1.46	0.62
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.34	0.62
1:A:51:TRP:HZ3	1:A:52:MET:CE	2.07	0.62
1:G:194:ARG:HB2	1:G:198:GLU:O	1.98	0.62
1:G:219:LEU:HB3	1:G:224:LEU:HD11	1.80	0.62
2:H:18:GLY:C	2:H:19:LYS:HD3	2.21	0.61
1:A:195:SER:O	1:A:198:GLU:HG3	1.99	0.61
1:A:3:HIS:HD2	1:A:29:ASP:OD1	1.82	0.61
3:L:6:GLN:HE21	3:L:7:ASP:H	1.47	0.61
1:D:147:TRP:CZ2	3:F:9:LEU:HD23	2.36	0.61
2:H:19:LYS:HE2	1:J:57:PRO:CG	2.14	0.61
1:G:52:MET:HE3	1:G:171:TYR:CD1	2.35	0.61
1:D:234:ARG:NH2	2:E:99:MET:O	2.33	0.61
1:A:224:LEU:C	1:A:226:GLN:H	2.04	0.60
1:G:218:GLN:HG2	1:G:222:GLU:O	2.01	0.60
1:A:16:GLY:C	1:A:18:GLU:H	2.05	0.60
2:H:50:GLU:HB2	2:H:67:HIS:CE1	2.36	0.60
1:J:55:GLU:HG2	1:J:59:TYR:CG	2.36	0.60
1:G:249:VAL:CG1	1:G:257:TYR:CE2	2.83	0.60
2:B:59:ASP:OD2	2:B:61:SER:HB2	2.01	0.60
1:A:218:GLN:HE22	1:A:260:ARG:NH1	1.99	0.60
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.36	0.60
1:J:234:ARG:NH2	2:K:99:MET:O	2.33	0.60
1:J:249:VAL:CG1	1:J:257:TYR:CE2	2.84	0.60
1:D:224:LEU:C	1:D:226:GLN:H	2.04	0.60
1:J:185:PRO:HD2	1:J:266:LEU:HD13	1.83	0.60
1:J:224:LEU:C	1:J:226:GLN:H	2.03	0.60
1:J:33:PHE:CD2	1:J:34:VAL:HG13	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:CD	1:A:75:ARG:HH21	2.04	0.60
2:H:19:LYS:N	2:H:19:LYS:HD3	2.17	0.59
1:G:224:LEU:C	1:G:226:GLN:H	2.05	0.59
1:A:66:LYS:HZ3	3:C:1:GLU:HG3	1.67	0.59
2:E:50:GLU:HB3	2:E:67:HIS:CE1	2.38	0.59
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.85	0.59
1:G:19:GLU:CD	1:G:75:ARG:HH21	2.05	0.59
2:E:38:GLN:OE1	2:E:45:LYS:HG3	2.02	0.59
1:D:51:TRP:HZ3	1:D:52:MET:CE	2.10	0.59
2:K:50:GLU:CB	2:K:67:HIS:CE1	2.86	0.58
1:D:16:GLY:C	1:D:18:GLU:H	2.04	0.58
1:D:55:GLU:HG2	1:D:59:TYR:CG	2.38	0.58
1:G:234:ARG:NH2	2:H:99:MET:O	2.36	0.58
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.38	0.58
1:J:218:GLN:HG2	1:J:222:GLU:O	2.02	0.58
1:D:32:GLU:OE2	1:D:35:ARG:HD2	2.03	0.58
1:J:5:MET:HB2	1:J:168:LEU:HD13	1.86	0.58
1:J:206:LEU:HD23	1:J:242:GLN:HB3	1.84	0.58
2:H:42:ASN:ND2	2:H:76:ASP:OD2	2.35	0.58
1:J:234:ARG:HH11	1:J:242:GLN:HE22	1.52	0.58
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.38	0.58
1:D:3:HIS:HD2	1:D:29:ASP:OD1	1.87	0.58
1:G:55:GLU:HG2	1:G:59:TYR:CG	2.38	0.58
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.86	0.58
1:J:195:SER:OG	1:J:196:LYS:HD3	2.03	0.57
1:A:55:GLU:HG2	1:A:59:TYR:CG	2.39	0.57
2:H:50:GLU:CB	2:H:67:HIS:CE1	2.86	0.57
1:D:128:GLU:O	1:D:130:LEU:HD13	2.04	0.57
1:G:196:LYS:HE3	1:G:196:LYS:H	1.68	0.57
1:G:206:LEU:HD23	1:G:242:GLN:HB3	1.86	0.57
1:G:5:MET:HB2	1:G:168:LEU:HD13	1.85	0.57
1:D:159:TYR:CE2	3:F:3:SER:HB3	2.40	0.57
1:G:128:GLU:O	1:G:130:LEU:HD13	2.04	0.57
1:A:249:VAL:CG1	1:A:257:TYR:CE2	2.83	0.57
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.19	0.57
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.40	0.57
1:A:274:TRP:CZ2	1:A:276:PRO:HA	2.40	0.57
1:G:66:LYS:NZ	3:I:1:GLU:HG3	2.20	0.57
1:G:147:TRP:CZ2	3:I:9:LEU:HD23	2.39	0.57
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.40	0.57
1:G:16:GLY:C	1:G:18:GLU:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:HH11	1:D:242:GLN:HE22	1.53	0.56
1:J:147:TRP:CZ2	3:L:9:LEU:HD23	2.40	0.56
2:K:18:GLY:C	2:K:19:LYS:HD3	2.25	0.56
1:G:195:SER:CB	1:G:196:LYS:HE3	2.35	0.56
1:A:99:SER:CB	1:A:114:LEU:HD23	2.35	0.56
1:D:19:GLU:CD	1:D:75:ARG:HH21	2.08	0.56
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.88	0.56
1:J:19:GLU:CD	1:J:75:ARG:HH21	2.07	0.56
1:D:60:TRP:O	1:D:64:THR:HG23	2.06	0.56
1:A:128:GLU:O	1:A:130:LEU:HD13	2.05	0.56
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.05	0.56
1:J:52:MET:HE1	1:J:171:TYR:CE1	2.40	0.56
1:D:274:TRP:CZ2	1:D:276:PRO:HA	2.40	0.56
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.41	0.56
1:D:30:ASN:HA	5:D:279:GOL:H31	1.86	0.56
2:E:59:ASP:OD2	2:E:61:SER:HB2	2.06	0.56
2:B:50:GLU:HB3	2:B:67:HIS:CE1	2.40	0.56
1:J:16:GLY:C	1:J:18:GLU:H	2.07	0.56
1:G:51:TRP:HZ3	1:G:52:MET:HE2	1.66	0.55
1:A:99:SER:HB3	1:A:114:LEU:HD23	1.88	0.55
1:A:176:ASN:HD22	1:D:181:ARG:HA	1.70	0.55
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.41	0.55
1:D:218:GLN:HE22	1:D:260:ARG:NH1	2.04	0.55
1:A:159:TYR:CE2	3:C:3:SER:HB3	2.40	0.55
3:C:6:GLN:HE21	3:C:7:ASP:H	1.52	0.55
1:A:199:VAL:CG1	1:A:251:LEU:HB3	2.36	0.55
2:K:42:ASN:ND2	2:K:76:ASP:OD2	2.36	0.55
1:A:234:ARG:NH2	2:B:99:MET:O	2.37	0.55
1:G:183:ASP:O	1:G:208:PHE:HA	2.07	0.55
2:H:19:LYS:HE2	1:J:57:PRO:HG3	1.81	0.55
1:G:185:PRO:HD2	1:G:266:LEU:HD13	1.88	0.55
1:G:218:GLN:NE2	1:G:260:ARG:NH1	2.55	0.55
1:D:99:SER:CB	1:D:114:LEU:HD23	2.37	0.55
1:G:52:MET:CE	1:G:171:TYR:CD1	2.89	0.55
2:B:38:GLN:OE1	2:B:45:LYS:HG3	2.07	0.55
1:D:121:ARG:HH21	2:E:1:ILE:HG22	1.72	0.55
2:K:19:LYS:N	2:K:19:LYS:HD3	2.21	0.55
1:J:60:TRP:O	1:J:64:THR:HG23	2.05	0.55
1:A:218:GLN:HG2	1:A:222:GLU:O	2.07	0.55
1:D:249:VAL:HG11	1:D:257:TYR:CD2	2.41	0.54
1:G:234:ARG:HD3	2:H:10:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:LEU:HB3	1:G:224:LEU:CD1	2.38	0.54
1:J:128:GLU:O	1:J:130:LEU:HD13	2.07	0.54
2:H:38:GLN:OE1	2:H:45:LYS:HG3	2.08	0.54
1:A:219:LEU:HB3	1:A:224:LEU:CD1	2.37	0.54
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.42	0.54
1:J:52:MET:CE	1:J:171:TYR:CD1	2.90	0.54
1:D:218:GLN:HG2	1:D:222:GLU:O	2.07	0.54
1:D:99:SER:HB3	1:D:114:LEU:HD23	1.90	0.54
1:D:194:ARG:CG	1:D:198:GLU:HB2	2.37	0.54
1:A:249:VAL:HG11	1:A:257:TYR:CD2	2.42	0.54
1:J:219:LEU:HB3	1:J:224:LEU:CD1	2.38	0.53
1:J:14:ARG:NH2	1:J:14:ARG:CG	2.46	0.53
2:H:59:ASP:OD2	2:H:61:SER:HB2	2.09	0.53
1:D:36:PHE:C	1:D:36:PHE:CD1	2.81	0.53
1:D:219:LEU:HB3	1:D:224:LEU:CD1	2.39	0.53
1:J:167:TRP:CZ3	1:J:170:ARG:HD3	2.43	0.53
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.43	0.53
1:A:191:HIS:CE1	1:A:199:VAL:HG21	2.43	0.53
3:F:6:GLN:HE21	3:F:7:ASP:H	1.55	0.53
1:A:36:PHE:C	1:A:36:PHE:CD1	2.82	0.53
1:G:127:ASN:HD22	1:G:132:THR:C	2.11	0.53
1:D:66:LYS:HZ3	3:F:1:GLU:HG3	1.74	0.53
2:K:21:ASN:HB3	2:K:70:PHE:CE1	2.43	0.53
1:A:31:LYS:HA	1:A:31:LYS:HE2	1.90	0.53
1:D:167:TRP:CZ3	1:D:170:ARG:HD3	2.44	0.53
1:G:57:PRO:O	1:G:61:GLU:HG2	2.09	0.53
1:J:196:LYS:HD3	1:J:196:LYS:N	2.14	0.53
1:G:60:TRP:O	1:G:64:THR:HG23	2.06	0.53
1:J:103:LEU:CD1	1:J:168:LEU:HD23	2.39	0.53
2:K:38:GLN:OE1	2:K:45:LYS:HG3	2.09	0.52
1:G:219:LEU:H	1:G:224:LEU:HD13	1.75	0.52
1:J:218:GLN:NE2	1:J:260:ARG:NH1	2.57	0.52
1:A:163:GLU:N	1:A:163:GLU:OE1	2.29	0.52
2:K:33:PRO:HG3	2:K:62:PHE:CE1	2.45	0.52
1:G:99:SER:HB3	1:G:114:LEU:CD2	2.40	0.52
1:A:274:TRP:CH2	1:A:276:PRO:HA	2.45	0.52
1:J:19:GLU:OE2	1:J:75:ARG:NE	2.43	0.52
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.45	0.52
1:J:57:PRO:O	1:J:61:GLU:HG2	2.09	0.52
1:A:60:TRP:O	1:A:64:THR:HG23	2.06	0.52
1:G:14:ARG:CG	1:G:14:ARG:NH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ARG:HH11	1:G:242:GLN:HE22	1.58	0.52
1:G:99:SER:HB3	1:G:114:LEU:HD23	1.92	0.52
1:D:274:TRP:CH2	1:D:276:PRO:HA	2.45	0.52
1:A:234:ARG:HD3	2:B:10:TYR:CD1	2.45	0.51
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.25	0.51
1:A:99:SER:HB3	1:A:114:LEU:CD2	2.40	0.51
1:D:144:ARG:NH1	1:D:144:ARG:CG	2.61	0.51
1:D:266:LEU:HD21	1:D:270:LEU:HG	1.93	0.51
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.46	0.51
1:G:229:GLU:O	1:G:245:ALA:HA	2.11	0.51
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.78	0.51
1:D:19:GLU:OE2	1:D:75:ARG:NE	2.44	0.51
2:K:59:ASP:OD2	2:K:61:SER:HB2	2.11	0.51
1:J:202:ARG:HG2	1:J:204:TRP:NE1	2.25	0.51
1:D:99:SER:HB3	1:D:114:LEU:CD2	2.41	0.51
1:J:190:THR:OG1	1:J:202:ARG:HB3	2.10	0.51
1:J:111:ARG:HD3	1:J:113:TYR:CZ	2.46	0.51
1:D:199:VAL:HB	1:D:251:LEU:HB3	1.92	0.51
1:A:19:GLU:OE1	1:A:75:ARG:NH2	2.36	0.51
1:G:195:SER:HB2	1:G:196:LYS:CE	2.40	0.51
1:D:206:LEU:HD23	1:D:242:GLN:HB3	1.93	0.51
1:G:99:SER:CB	1:G:114:LEU:HD23	2.41	0.51
1:A:199:VAL:HB	1:A:251:LEU:HB3	1.93	0.51
1:J:66:LYS:NZ	3:L:1:GLU:HG3	2.26	0.51
1:J:99:SER:CB	1:J:114:LEU:HD23	2.40	0.51
1:D:238:ASP:OD2	6:D:282:HOH:O	2.19	0.51
1:G:167:TRP:CZ3	1:G:170:ARG:HD3	2.46	0.50
1:G:19:GLU:OE2	1:G:75:ARG:NE	2.43	0.50
1:G:36:PHE:CD1	1:G:36:PHE:C	2.85	0.50
1:J:191:HIS:CE1	1:J:199:VAL:HG11	2.46	0.50
1:J:191:HIS:NE2	1:J:199:VAL:HG11	2.27	0.50
1:A:144:ARG:NH1	1:A:144:ARG:CG	2.63	0.50
1:G:249:VAL:HG11	1:G:257:TYR:CD2	2.44	0.50
1:A:234:ARG:HH11	1:A:242:GLN:HE22	1.56	0.50
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.25	0.50
1:J:167:TRP:NE1	3:L:1:GLU:OE2	2.44	0.50
1:J:74:PHE:O	1:J:78:LEU:HB2	2.11	0.50
1:G:111:ARG:HD3	1:G:113:TYR:CZ	2.47	0.50
1:D:195:SER:O	1:D:198:GLU:HG3	2.11	0.50
1:G:74:PHE:O	1:G:78:LEU:HB2	2.11	0.50
1:J:121:ARG:HH21	2:K:1:ILE:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:PRO:HD3	2:K:19:LYS:HZ3	1.74	0.49
1:J:99:SER:HB3	1:J:114:LEU:HD23	1.94	0.49
1:D:127:ASN:HD22	1:D:132:THR:C	2.15	0.49
1:J:36:PHE:CD1	1:J:36:PHE:C	2.86	0.49
1:A:229:GLU:O	1:A:245:ALA:HA	2.13	0.49
1:D:251:LEU:HB2	1:D:254:GLU:OE1	2.12	0.49
1:J:3:HIS:HD2	1:J:29:ASP:OD1	1.96	0.49
1:A:251:LEU:HB2	1:A:254:GLU:OE1	2.12	0.49
2:K:33:PRO:HG3	2:K:62:PHE:CZ	2.48	0.49
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.47	0.49
1:G:195:SER:HB2	1:G:196:LYS:HE3	1.94	0.49
1:J:266:LEU:HD21	1:J:270:LEU:HG	1.95	0.49
1:J:249:VAL:HG11	1:J:257:TYR:CD2	2.46	0.49
1:J:6:ARG:NH2	1:J:113:TYR:CE1	2.81	0.49
1:D:37:ASP:OD1	1:D:39[A]:ASP:HB2	2.12	0.49
1:D:40:ALA:O	1:D:41:GLU:C	2.52	0.49
1:J:51:TRP:HZ3	1:J:52:MET:CE	2.25	0.48
1:A:19:GLU:OE2	1:A:75:ARG:NE	2.45	0.48
1:D:191:HIS:CE1	1:D:199:VAL:HG21	2.47	0.48
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.48	0.48
1:D:229:GLU:O	1:D:245:ALA:HA	2.13	0.48
1:D:21:ARG:NE	1:D:23:ILE:HD11	2.28	0.48
1:J:199:VAL:CG2	1:J:251:LEU:HB3	2.27	0.48
3:I:3:SER:N	6:I:62:HOH:O	2.46	0.48
1:J:219:LEU:H	1:J:224:LEU:HD13	1.78	0.48
1:A:52:MET:HE3	1:A:171:TYR:CD1	2.49	0.48
1:J:144:ARG:CG	1:J:144:ARG:NH1	2.60	0.48
1:A:219:LEU:H	1:A:224:LEU:HD13	1.78	0.48
1:D:55:GLU:HG2	1:D:59:TYR:CD2	2.48	0.48
1:J:99:SER:HB3	1:J:114:LEU:CD2	2.42	0.48
1:D:52:MET:CE	1:D:171:TYR:CD1	2.96	0.48
1:G:190:THR:OG1	1:G:192:HIS:CE1	2.65	0.48
1:J:196:LYS:CD	1:J:196:LYS:H	2.15	0.48
1:A:21:ARG:NE	1:A:23:ILE:HD11	2.29	0.48
1:J:234:ARG:HD3	2:K:10:TYR:CD1	2.48	0.48
1:J:229:GLU:O	1:J:245:ALA:HA	2.12	0.48
1:A:40:ALA:O	1:A:41:GLU:C	2.52	0.48
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.49	0.48
1:D:219:LEU:H	1:D:224:LEU:HD13	1.77	0.48
1:J:87:GLN:NE2	1:J:118:TYR:OH	2.29	0.48
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:CE	1:A:171:TYR:CD1	2.97	0.48
1:G:196:LYS:O	1:G:198:GLU:CG	2.60	0.48
1:A:14:ARG:CG	1:A:14:ARG:NH2	2.45	0.48
1:G:189:VAL:HG23	1:G:202:ARG:O	2.14	0.48
1:D:74:PHE:O	1:D:78:LEU:HB2	2.14	0.48
2:E:33:PRO:HG3	2:E:62:PHE:CE1	2.49	0.48
1:A:189:VAL:HA	1:A:202:ARG:O	2.14	0.47
1:J:55:GLU:HG2	1:J:59:TYR:CD2	2.49	0.47
1:D:199:VAL:CG1	1:D:251:LEU:HB3	2.44	0.47
2:K:55:SER:HB3	2:K:63:TYR:CZ	2.49	0.47
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.96	0.47
2:H:21:ASN:HB3	2:H:70:PHE:CE1	2.49	0.47
1:G:144:ARG:CG	1:G:144:ARG:NH1	2.59	0.47
1:D:253:LYS:HD3	1:D:256:ASN:HD21	1.79	0.47
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.82	0.47
2:E:18:GLY:C	2:E:19:LYS:HD3	2.35	0.47
1:J:53:GLU:HA	1:J:53:GLU:OE1	2.15	0.47
1:G:251:LEU:HB2	1:G:254:GLU:OE1	2.14	0.47
1:A:184:SER:HB3	1:A:266:LEU:CD1	2.44	0.47
1:J:40:ALA:O	1:J:41:GLU:C	2.53	0.47
1:G:121:ARG:HH21	2:H:1:ILE:HG22	1.80	0.47
3:I:2:GLY:CA	6:I:62:HOH:O	2.63	0.47
1:A:55:GLU:HG2	1:A:59:TYR:CD2	2.50	0.47
1:A:74:PHE:O	1:A:78:LEU:HB2	2.15	0.47
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.31	0.47
1:A:177:ALA:O	1:A:180:LEU:HB2	2.15	0.47
1:G:81:LEU:HD13	1:G:118:TYR:CD1	2.50	0.47
1:G:21:ARG:NH2	1:G:37:ASP:OD2	2.34	0.47
1:D:234:ARG:HD3	2:E:10:TYR:CD1	2.50	0.46
1:G:266:LEU:HD21	1:G:270:LEU:HG	1.96	0.46
1:D:103:LEU:CD1	1:D:168:LEU:HD23	2.45	0.46
1:A:266:LEU:HD21	1:A:270:LEU:HG	1.98	0.46
1:D:176:ASN:HB3	1:D:177:ALA:H	1.46	0.46
1:A:127:ASN:HD22	1:A:132:THR:C	2.19	0.46
1:J:196:LYS:O	1:J:198:GLU:HG3	2.16	0.46
1:G:103:LEU:CD1	1:G:168:LEU:HD23	2.45	0.46
1:D:249:VAL:HB	1:D:250:PRO:CD	2.44	0.46
1:G:266:LEU:HA	1:G:267:PRO:HD2	1.73	0.46
1:J:19:GLU:HA	1:J:19:GLU:OE1	2.16	0.46
1:G:3:HIS:HD2	1:G:29:ASP:OD1	1.98	0.46
1:J:127:ASN:HD22	1:J:132:THR:C	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LYS:CE	1:J:57:PRO:HG2	2.26	0.46
1:D:163:GLU:N	1:D:163:GLU:OE1	2.32	0.46
1:A:103:LEU:CD1	1:A:168:LEU:HD23	2.46	0.46
1:G:19:GLU:OE1	1:G:19:GLU:HA	2.15	0.46
1:G:131:LYS:HB3	1:G:131:LYS:HE3	1.81	0.46
1:D:111:ARG:HD3	1:D:113:TYR:CZ	2.52	0.45
2:B:18:GLY:C	2:B:19:LYS:HD3	2.37	0.45
1:G:31:LYS:HA	1:G:31:LYS:HE2	1.97	0.45
1:J:103:LEU:HD11	1:J:168:LEU:HD23	1.97	0.45
1:A:58:GLU:O	1:A:62:ARG:HD3	2.16	0.45
1:G:8:PHE:CD2	1:G:98:MET:HG2	2.51	0.45
1:G:40:ALA:O	1:G:41:GLU:C	2.53	0.45
2:K:19:LYS:O	2:K:72:PRO:HD2	2.17	0.45
1:A:253:LYS:HD3	1:A:256:ASN:HD21	1.81	0.45
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.51	0.45
2:K:73:THR:OG1	2:K:76:ASP:HB2	2.17	0.45
1:G:58:GLU:O	1:G:62:ARG:HD3	2.16	0.45
1:G:92:SER:OG	2:H:34[A]:HIS:HE1	1.99	0.45
1:G:87:GLN:NE2	1:G:118:TYR:OH	2.32	0.45
1:J:183:ASP:O	1:J:208:PHE:HA	2.17	0.45
1:D:189:VAL:HA	1:D:202:ARG:O	2.16	0.45
1:J:266:LEU:HA	1:J:267:PRO:HD2	1.73	0.45
1:D:14:ARG:CG	1:D:14:ARG:NH2	2.48	0.45
1:G:6:ARG:NH2	1:G:113:TYR:CE1	2.85	0.45
1:A:99:SER:HB2	1:A:114:LEU:HD23	1.99	0.45
2:H:21:ASN:OD1	2:H:22:ILE:N	2.45	0.45
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.17	0.45
1:G:41:GLU:O	1:G:43:PRO:HD3	2.16	0.45
2:H:33:PRO:HG3	2:H:62:PHE:CE1	2.51	0.45
1:G:84:TYR:CZ	1:G:142:ILE:HD11	2.52	0.45
1:A:35:ARG:NH2	2:B:54:MET:O	2.43	0.44
2:H:33:PRO:HG3	2:H:62:PHE:CZ	2.52	0.44
2:K:96:ASP:O	2:K:98:ASP:N	2.50	0.44
1:J:185:PRO:HD2	1:J:266:LEU:CD1	2.47	0.44
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.99	0.44
1:D:61:GLU:HA	1:D:61:GLU:OE1	2.18	0.44
1:J:131:LYS:HB3	1:J:131:LYS:HE3	1.83	0.44
1:G:196:LYS:HD3	1:G:196:LYS:N	2.31	0.44
1:J:31:LYS:HE2	1:J:31:LYS:HA	2.00	0.44
1:A:198:GLU:O	1:A:251:LEU:HD12	2.18	0.44
1:D:266:LEU:HA	1:D:267:PRO:HD2	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:MET:HE3	1:D:171:TYR:CD1	2.53	0.44
1:G:53:GLU:OE1	1:G:53:GLU:HA	2.18	0.44
1:J:84:TYR:CZ	1:J:142:ILE:HD11	2.53	0.44
1:D:31:LYS:HE2	1:D:31:LYS:HA	1.99	0.44
1:G:51:TRP:HZ3	1:G:52:MET:CE	2.26	0.44
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.52	0.44
2:H:55:SER:HB3	2:H:63:TYR:CZ	2.53	0.44
2:H:19:LYS:HZ1	1:J:57:PRO:CD	2.30	0.44
1:G:196:LYS:HE3	1:G:196:LYS:N	2.31	0.44
1:G:55:GLU:HG2	1:G:59:TYR:CD2	2.53	0.43
1:J:32:GLU:OE2	1:J:35:ARG:HD2	2.17	0.43
1:J:107:TRP:HB3	1:J:169:HIS:NE2	2.32	0.43
1:A:177:ALA:O	1:A:178:THR:C	2.57	0.43
2:H:19:LYS:HD2	2:H:19:LYS:HA	1.60	0.43
1:J:41:GLU:O	1:J:43:PRO:HD3	2.18	0.43
2:B:19:LYS:N	2:B:19:LYS:HD3	2.33	0.43
1:A:107:TRP:CD1	1:A:107:TRP:N	2.86	0.43
1:G:196:LYS:CD	1:G:196:LYS:N	2.82	0.43
1:D:66:LYS:HZ2	3:F:1:GLU:HG3	1.81	0.43
1:D:194:ARG:CD	1:D:198:GLU:HB2	2.48	0.43
3:I:2:GLY:HA3	6:I:62:HOH:O	2.18	0.43
2:K:59:ASP:O	2:K:60:TRP:HB2	2.19	0.43
2:H:73:THR:OG1	2:H:76:ASP:HB2	2.19	0.43
2:B:64:ILE:HG22	2:B:65:LEU:N	2.34	0.43
1:A:249:VAL:HB	1:A:250:PRO:CD	2.46	0.43
1:G:253:LYS:HD3	1:G:256:ASN:HD21	1.84	0.43
1:A:224:LEU:C	1:A:226:GLN:N	2.72	0.43
1:J:237:GLY:HA3	6:K:103:HOH:O	2.19	0.43
1:J:8:PHE:CD2	1:J:98:MET:HG2	2.54	0.43
1:D:19:GLU:OE1	1:D:19:GLU:HA	2.19	0.42
2:B:19:LYS:O	2:B:72:PRO:HD2	2.19	0.42
1:J:138:MET:O	1:J:141:GLN:HG2	2.18	0.42
1:D:107:TRP:HB3	1:D:169:HIS:NE2	2.34	0.42
1:G:52:MET:HE3	1:G:171:TYR:CE1	2.54	0.42
1:G:181:ARG:NH1	1:G:181:ARG:CG	2.74	0.42
1:J:224:LEU:C	1:J:226:GLN:N	2.71	0.42
1:D:99:SER:HB2	1:D:114:LEU:HD23	2.00	0.42
1:D:195:SER:HB2	1:D:196:LYS:HG3	2.01	0.42
2:B:19:LYS:HA	2:B:19:LYS:HD2	1.66	0.42
1:A:61:GLU:OE1	1:A:61:GLU:HA	2.19	0.42
1:J:19:GLU:OE1	1:J:75:ARG:NH2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASP:O	2:B:60:TRP:HB2	2.20	0.42
2:H:50:GLU:HB3	2:H:67:HIS:CE1	2.54	0.42
2:E:55:SER:HB3	2:E:63:TYR:CZ	2.54	0.42
1:J:157:LYS:O	1:J:161:GLU:HB2	2.20	0.42
1:G:57:PRO:HG3	2:K:19:LYS:HE2	1.85	0.42
1:G:181:ARG:NH2	1:J:181:ARG:CB	2.82	0.42
1:G:19:GLU:OE1	1:G:75:ARG:NH2	2.42	0.42
1:J:253:LYS:HD3	1:J:256:ASN:HD21	1.85	0.42
2:H:96:ASP:O	2:H:98:ASP:N	2.52	0.42
1:D:180:LEU:O	1:D:181:ARG:C	2.57	0.42
1:G:99:SER:HA	1:G:113:TYR:O	2.18	0.42
2:B:33:PRO:HG3	2:B:62:PHE:CE1	2.55	0.42
1:J:163:GLU:OE1	1:J:163:GLU:N	2.25	0.42
1:J:99:SER:HA	1:J:113:TYR:O	2.20	0.41
2:E:21:ASN:OD1	2:E:22:ILE:N	2.46	0.41
2:E:19:LYS:N	2:E:19:LYS:HD3	2.33	0.41
1:A:106:ASP:O	1:G:262:TYR:HD2	2.03	0.41
2:B:73:THR:OG1	2:B:76:ASP:HB2	2.20	0.41
1:G:157:LYS:O	1:G:161:GLU:HB2	2.20	0.41
1:G:184:SER:CB	1:G:266:LEU:CD1	2.95	0.41
1:A:84:TYR:CE2	1:A:142:ILE:HD11	2.55	0.41
1:D:176:ASN:HA	1:D:176:ASN:HD22	1.65	0.41
2:E:58:LYS:H	2:E:58:LYS:HZ1	1.68	0.41
1:J:14:ARG:HD2	2:K:34[A]:HIS:NE2	2.35	0.41
1:G:8:PHE:CE2	1:G:98:MET:HG2	2.56	0.41
1:J:107:TRP:CD1	1:J:107:TRP:N	2.89	0.41
1:D:84:TYR:CE2	1:D:142:ILE:HD11	2.55	0.41
2:B:96:ASP:O	2:B:98:ASP:N	2.53	0.41
2:H:59:ASP:O	2:H:60:TRP:HB2	2.21	0.41
1:G:28:VAL:HG23	1:G:33:PHE:CD1	2.56	0.41
1:G:84:TYR:CE2	1:G:142:ILE:HD11	2.56	0.41
1:D:107:TRP:N	1:D:107:TRP:CD1	2.86	0.41
2:E:58:LYS:H	2:E:58:LYS:NZ	2.18	0.41
1:J:263:HIS:O	1:J:264:GLU:C	2.59	0.41
1:J:249:VAL:HB	1:J:250:PRO:CD	2.48	0.41
2:E:59:ASP:O	2:E:60:TRP:HB2	2.21	0.41
1:A:275:GLU:HA	1:A:276:PRO:HD2	1.90	0.41
1:A:266:LEU:HA	1:A:267:PRO:HD2	1.74	0.41
2:E:64:ILE:HG22	2:E:65:LEU:N	2.36	0.41
2:K:15:PRO:HG3	2:K:97:ARG:HB2	2.03	0.41
1:J:201:LEU:O	1:J:246:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:TRP:NE1	3:I:1:GLU:OE2	2.54	0.41
1:J:167:TRP:CE2	3:L:1:GLU:OE2	2.74	0.41
2:K:19:LYS:HA	2:K:19:LYS:HD2	1.64	0.40
1:J:84:TYR:CE2	1:J:142:ILE:HD11	2.55	0.40
2:H:19:LYS:O	2:H:72:PRO:HD2	2.22	0.40
1:D:8:PHE:CZ	5:D:279:GOL:H12	2.55	0.40
2:B:16:GLU:O	2:B:17:ASN:C	2.58	0.40
1:G:107:TRP:CD1	1:G:107:TRP:N	2.89	0.40
1:J:197:GLY:C	1:J:251:LEU:HD23	2.42	0.40
1:J:16:GLY:C	1:J:18:GLU:N	2.74	0.40
2:E:19:LYS:HA	2:E:19:LYS:HD2	1.66	0.40
1:D:52:MET:HE1	1:D:171:TYR:CD1	2.56	0.40
1:J:194:ARG:HB3	1:J:195:SER:H	1.54	0.40
1:D:19:GLU:OE1	1:D:75:ARG:NH2	2.42	0.40
1:J:57:PRO:HA	1:J:60:TRP:HD1	1.87	0.40
1:A:194:ARG:HD2	1:A:248:VAL:HG11	2.04	0.40
1:D:41:GLU:O	1:D:43:PRO:HD3	2.22	0.40
2:K:83:LYS:HG2	2:K:90:PRO:HG3	2.02	0.40
2:E:15:PRO:HG3	2:E:97:ARG:HB2	2.03	0.40
1:J:54:GLN:HB3	1:J:54:GLN:HE21	1.60	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:GLU:OE2	6:A:290:HOH:O[1_656]	1.99	0.21
2:K:81:ARG:NH1	4:D:278:SO4:O4[1_656]	2.06	0.14

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	276/276 (100%)	258 (94%)	15 (5%)	3 (1%)	17 36
1	D	276/276 (100%)	255 (92%)	16 (6%)	5 (2%)	11 21
1	G	268/276 (97%)	244 (91%)	16 (6%)	8 (3%)	5 8
1	J	268/276 (97%)	244 (91%)	19 (7%)	5 (2%)	10 19
2	B	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19 39
2	E	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19 39
2	H	98/99 (99%)	94 (96%)	3 (3%)	1 (1%)	19 39
2	K	98/99 (99%)	94 (96%)	3 (3%)	1 (1%)	19 39
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
All	All	1506/1536 (98%)	1399 (93%)	82 (5%)	25 (2%)	11 22

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	D	89	ALA
1	G	195	SER
1	G	199	VAL
1	A	89	ALA
1	D	41	GLU
1	G	41	GLU
1	G	89	ALA
1	G	136	ALA
1	J	41	GLU
2	K	97	ARG
2	B	97	ARG
2	H	97	ARG
1	J	89	ALA
1	J	136	ALA
1	A	136	ALA
1	D	136	ALA
1	D	178	THR
2	E	97	ARG
1	G	43	PRO
1	G	264	GLU
1	J	43	PRO

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Mol	Chain	Res	Type
1	G	193	PRO
1	D	43	PRO
1	J	193	PRO

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	236/234 (101%)	209 (89%)	27 (11%)	7 12
1	D	236/234 (101%)	203 (86%)	33 (14%)	4 7
1	G	230/234 (98%)	200 (87%)	30 (13%)	5 9
1	J	230/234 (98%)	200 (87%)	30 (13%)	5 9
2	B	94/94 (100%)	90 (96%)	4 (4%)	35 64
2	E	94/94 (100%)	90 (96%)	4 (4%)	35 64
2	H	95/94 (101%)	88 (93%)	7 (7%)	17 34
2	K	95/94 (101%)	91 (96%)	4 (4%)	36 65
3	C	8/8 (100%)	6 (75%)	2 (25%)	1 1
3	F	8/8 (100%)	6 (75%)	2 (25%)	1 1
3	I	8/8 (100%)	6 (75%)	2 (25%)	1 1
3	L	8/8 (100%)	6 (75%)	2 (25%)	1 1
All	All	1342/1344 (100%)	1195 (89%)	147 (11%)	8 14

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	18	GLU
1	A	31	LYS
1	A	36	PHE
1	A	64	THR
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	92	SER
1	A	94	THR
1	A	114	LEU
1	A	131	LYS
1	A	142	ILE
1	A	144	ARG
1	A	179	LEU
1	A	184	SER
1	A	189	VAL
1	A	198	GLU
1	A	200	THR
1	A	227	ASP
1	A	230	LEU
1	A	234	ARG
1	A	242	GLN
1	A	248	VAL
1	A	251	LEU
1	A	258	THR
1	A	266	LEU
1	A	271	THR
2	B	58	LYS
2	B	61	SER
2	B	69	GLU
2	B	70	PHE
3	C	6	GLN
3	C	8	TRP
1	D	14	ARG
1	D	17	LEU
1	D	18	GLU
1	D	31	LYS
1	D	36	PHE
1	D	39[A]	ASP
1	D	39[B]	ASP
1	D	44	ARG
1	D	62	ARG
1	D	64	THR
1	D	78	LEU
1	D	92	SER
1	D	94	THR
1	D	110	LEU
1	D	114	LEU
1	D	131	LYS

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Mol	Chain	Res	Type
1	D	142	ILE
1	D	144	ARG
1	D	176	ASN
1	D	184	SER
1	D	189	VAL
1	D	194	ARG
1	D	198	GLU
1	D	200	THR
1	D	227	ASP
1	D	230	LEU
1	D	234	ARG
1	D	242	GLN
1	D	248	VAL
1	D	251	LEU
1	D	258	THR
1	D	266	LEU
1	D	271	THR
2	E	58	LYS
2	E	61	SER
2	E	69	GLU
2	E	70	PHE
3	F	6	GLN
3	F	8	TRP
1	G	14	ARG
1	G	17	LEU
1	G	18	GLU
1	G	31	LYS
1	G	36	PHE
1	G	64	THR
1	G	78	LEU
1	G	92	SER
1	G	94	THR
1	G	110	LEU
1	G	114	LEU
1	G	131	LYS
1	G	142	ILE
1	G	144	ARG
1	G	172	LEU
1	G	180	LEU
1	G	181	ARG
1	G	189	VAL
1	G	196	LYS

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Mol	Chain	Res	Type
1	G	199	VAL
1	G	200	THR
1	G	227	ASP
1	G	230	LEU
1	G	234	ARG
1	G	242	GLN
1	G	248	VAL
1	G	251	LEU
1	G	258	THR
1	G	266	LEU
1	G	271	THR
2	H	34[A]	HIS
2	H	34[B]	HIS
2	H	45	LYS
2	H	58	LYS
2	H	61	SER
2	H	69	GLU
2	H	70	PHE
3	I	6	GLN
3	I	8	TRP
1	J	14	ARG
1	J	17	LEU
1	J	18	GLU
1	J	31	LYS
1	J	62	ARG
1	J	64	THR
1	J	78	LEU
1	J	92	SER
1	J	94	THR
1	J	110	LEU
1	J	114	LEU
1	J	131	LYS
1	J	142	ILE
1	J	144	ARG
1	J	180	LEU
1	J	181	ARG
1	J	186	LYS
1	J	194	ARG
1	J	196	LYS
1	J	199	VAL
1	J	200	THR
1	J	227	ASP

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Mol	Chain	Res	Type
1	J	230	LEU
1	J	234	ARG
1	J	242	GLN
1	J	248	VAL
1	J	251	LEU
1	J	258	THR
1	J	266	LEU
1	J	271	THR
2	K	45	LYS
2	K	61	SER
2	K	69	GLU
2	K	70	PHE
3	L	6	GLN
3	L	8	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	54	GLN
1	A	86	ASN
1	A	87	GLN
1	A	127	ASN
1	A	176	ASN
1	A	191	HIS
1	A	218	GLN
1	A	242	GLN
1	A	256	ASN
2	B	8	GLN
2	B	67	HIS
3	C	6	GLN
1	D	3	HIS
1	D	54	GLN
1	D	86	ASN
1	D	87	GLN
1	D	127	ASN
1	D	176	ASN
1	D	191	HIS
1	D	192	HIS
1	D	218	GLN
1	D	242	GLN
1	D	256	ASN

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Mol	Chain	Res	Type
2	E	8	GLN
2	E	67	HIS
3	F	6	GLN
1	G	3	HIS
1	G	54	GLN
1	G	86	ASN
1	G	87	GLN
1	G	127	ASN
1	G	192	HIS
1	G	218	GLN
1	G	242	GLN
1	G	256	ASN
2	H	8	GLN
2	H	67	HIS
3	I	6	GLN
1	J	3	HIS
1	J	54	GLN
1	J	86	ASN
1	J	87	GLN
1	J	127	ASN
1	J	192	HIS
1	J	218	GLN
1	J	242	GLN
1	J	256	ASN
2	K	8	GLN
2	K	13	HIS
2	K	67	HIS
3	L	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	277	-	5,5,5	0.44	0	5,5,5	0.52	0
4	SO4	B	100	-	4,4,4	0.18	0	6,6,6	0.37	0
4	SO4	B	101	-	4,4,4	0.27	0	6,6,6	0.22	0
4	SO4	B	102	-	4,4,4	0.15	0	6,6,6	0.33	0
4	SO4	B	103	-	4,4,4	0.14	0	6,6,6	0.31	0
4	SO4	D	277	-	4,4,4	0.17	0	6,6,6	0.25	0
4	SO4	D	278	-	4,4,4	0.21	0	6,6,6	0.14	0
5	GOL	D	279	-	5,5,5	0.41	0	5,5,5	0.39	0
4	SO4	E	100	-	4,4,4	0.16	0	6,6,6	0.39	0
4	SO4	E	101	-	4,4,4	0.23	0	6,6,6	0.13	0
4	SO4	E	102	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	E	103	-	4,4,4	0.12	0	6,6,6	0.27	0
4	SO4	E	104	-	4,4,4	0.54	0	6,6,6	0.31	0
4	SO4	G	277	-	4,4,4	0.16	0	6,6,6	0.14	0
5	GOL	G	278	-	5,5,5	0.52	0	5,5,5	0.95	0
4	SO4	H	100	-	4,4,4	0.22	0	6,6,6	0.19	0
4	SO4	H	101	-	4,4,4	0.16	0	6,6,6	0.36	0
4	SO4	H	102	-	4,4,4	0.18	0	6,6,6	0.21	0
4	SO4	H	103	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	J	277	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	J	278	-	4,4,4	0.17	0	6,6,6	0.14	0
5	GOL	J	279	-	5,5,5	0.47	0	5,5,5	0.06	0
4	SO4	K	100	-	4,4,4	0.25	0	6,6,6	0.35	0
4	SO4	K	101	-	4,4,4	0.16	0	6,6,6	0.46	0
4	SO4	K	102	-	4,4,4	0.10	0	6,6,6	0.10	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
5	GOL	A	277	-	-	0/4/4/4	0/0/0/0
4	SO4	B	100	-	-	0/0/0/0	0/0/0/0
4	SO4	B	101	-	-	0/0/0/0	0/0/0/0
4	SO4	B	102	-	-	0/0/0/0	0/0/0/0
4	SO4	B	103	-	-	0/0/0/0	0/0/0/0
4	SO4	D	277	-	-	0/0/0/0	0/0/0/0
4	SO4	D	278	-	-	0/0/0/0	0/0/0/0
5	GOL	D	279	-	-	0/4/4/4	0/0/0/0
4	SO4	E	100	-	-	0/0/0/0	0/0/0/0
4	SO4	E	101	-	-	0/0/0/0	0/0/0/0
4	SO4	E	102	-	-	0/0/0/0	0/0/0/0
4	SO4	E	103	-	-	0/0/0/0	0/0/0/0
4	SO4	E	104	-	-	0/0/0/0	0/0/0/0
4	SO4	G	277	-	-	0/0/0/0	0/0/0/0
5	GOL	G	278	-	-	0/4/4/4	0/0/0/0
4	SO4	H	100	-	-	0/0/0/0	0/0/0/0
4	SO4	H	101	-	-	0/0/0/0	0/0/0/0
4	SO4	H	102	-	-	0/0/0/0	0/0/0/0
4	SO4	H	103	-	-	0/0/0/0	0/0/0/0
4	SO4	J	277	-	-	0/0/0/0	0/0/0/0
4	SO4	J	278	-	-	0/0/0/0	0/0/0/0
5	GOL	J	279	-	-	0/4/4/4	0/0/0/0
4	SO4	K	100	-	-	0/0/0/0	0/0/0/0
4	SO4	K	101	-	-	0/0/0/0	0/0/0/0
4	SO4	K	102	-	-	0/0/0/0	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	101	SO4	1	0
4	D	278	SO4	0	1
5	D	279	GOL	3	0

5.7 Other polymers (i)

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	276/276 (100%)	0.28	4 (1%) 78 74	37, 61, 84, 98	0
1	D	276/276 (100%)	0.26	4 (1%) 78 74	37, 61, 83, 98	0
1	G	272/276 (98%)	0.27	11 (4%) 42 34	37, 61, 85, 98	0
1	J	272/276 (98%)	0.24	14 (5%) 32 25	37, 61, 86, 98	0
2	B	99/99 (100%)	0.11	1 (1%) 84 81	33, 53, 70, 78	0
2	E	99/99 (100%)	0.12	1 (1%) 84 81	33, 53, 70, 78	0
2	H	99/99 (100%)	0.10	0 100 100	33, 53, 70, 78	0
2	K	99/99 (100%)	0.04	0 100 100	33, 53, 70, 78	0
3	C	9/9 (100%)	0.41	0 100 100	64, 72, 74, 77	0
3	F	9/9 (100%)	0.42	0 100 100	64, 72, 74, 77	0
3	I	9/9 (100%)	0.28	1 (11%) 7 4	64, 72, 74, 77	0
3	L	9/9 (100%)	-0.04	0 100 100	64, 72, 74, 77	0
All	All	1528/1536 (99%)	0.22	36 (2%) 62 56	33, 59, 82, 98	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	227	ASP	4.0
1	G	54	GLN	4.0
1	J	17	LEU	3.8
1	J	54	GLN	3.8
1	J	42	ASN	3.5
1	J	224	LEU	3.5
1	A	90	GLY	3.4
1	G	40	ALA	3.3
1	G	42	ASN	3.1
1	J	40	ALA	3.1
1	G	224	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	225	THR	3.0
2	E	1	ILE	2.9
1	J	14	ARG	2.8
2	B	1	ILE	2.7
1	G	172	LEU	2.6
1	J	51	TRP	2.6
1	G	56	GLY	2.6
1	G	17	LEU	2.6
1	A	17	LEU	2.5
1	A	225	THR	2.4
1	J	247	VAL	2.4
1	D	15	PRO	2.4
1	J	52	MET	2.3
1	D	14	ARG	2.3
1	G	220	ASN	2.3
1	J	225	THR	2.3
1	J	219	LEU	2.2
3	I	8	TRP	2.2
1	D	62	ARG	2.2
1	J	16	GLY	2.1
1	D	252	GLY	2.1
1	A	228	MET	2.1
1	J	62	ARG	2.0
1	G	36	PHE	2.0
1	G	65	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	SO4	H	102	5/5	0.81	0.24	2.40	124,124,125,125	0
4	SO4	E	104	5/5	0.80	0.25	1.86	115,115,115,115	0
4	SO4	B	100	5/5	0.83	0.21	1.72	116,116,116,117	0
4	SO4	E	100	5/5	0.81	0.20	1.21	113,114,114,114	0
5	GOL	G	278	6/6	0.93	0.20	0.43	58,60,60,61	0
5	GOL	J	279	6/6	0.93	0.19	0.20	54,56,56,57	0
5	GOL	A	277	6/6	0.92	0.19	-0.07	47,48,48,49	0
4	SO4	B	103	5/5	0.90	0.16	-0.27	106,106,107,107	0
5	GOL	D	279	6/6	0.93	0.18	-0.39	48,49,50,50	0
4	SO4	J	277	5/5	0.81	0.14	-0.84	129,129,129,129	0
4	SO4	E	102	5/5	0.96	0.14	-1.13	89,89,90,90	0
4	SO4	B	101	5/5	0.96	0.08	-	89,90,90,90	0
4	SO4	D	277	5/5	0.96	0.10	-	93,93,93,93	0
4	SO4	H	101	5/5	0.82	0.29	-	102,102,102,102	0
4	SO4	G	277	5/5	0.92	0.19	-	111,111,111,112	0
4	SO4	E	101	5/5	0.91	0.16	-	95,95,95,95	0
4	SO4	K	101	5/5	0.80	0.23	-	102,102,102,102	0
4	SO4	H	100	5/5	0.95	0.12	-	87,88,88,88	0
4	SO4	H	103	5/5	0.84	0.23	-	109,110,110,110	0
4	SO4	D	278	5/5	0.91	0.16	-	119,120,120,120	0
4	SO4	K	102	5/5	0.93	0.21	-	106,106,107,107	0
4	SO4	B	102	5/5	0.93	0.19	-	84,84,84,85	0
4	SO4	K	100	5/5	0.95	0.13	-	86,87,87,87	0
4	SO4	J	278	5/5	0.85	0.17	-	108,108,108,109	0
4	SO4	E	103	5/5	0.93	0.10	-	84,85,85,86	0

6.5 Other polymers (i)

There are no such residues in this entry.