



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:47 pm GMT

PDB ID : 1FDU  
Title : HUMAN 17-BETA-HYDROXYSTEROID-DEHYDROGENASE TYPE 1  
MUTANT H221L COMPLEXED WITH ESTRADIOL AND NADP+  
Authors : Mazza, C.; Breton, R.; Housset, D.; Fontecilla-Camps, J.-C.  
Deposited on : 1998-01-14  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

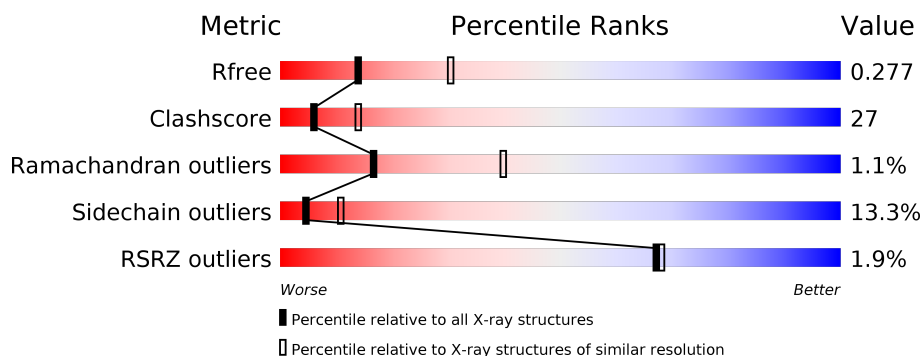
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>39%</div> <div>7%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	327	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>37%</div> <div>8%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	327	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>33%</div> <div>11%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	327	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>32%</div> <div>6%</div> <div>•</div> <div>14%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	401	-	-	-	X
2	SO4	C	403	-	-	X	-
2	SO4	D	402	-	-	X	-
3	EST	A	351	-	-	X	X
3	EST	B	354	-	-	-	X
3	EST	C	353	-	-	-	X
3	EST	D	352	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9114 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 17-BETA-HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2148	1366	380	390	12			
1	B	280	Total	C	N	O	S	0	0	0
			2144	1364	379	389	12			
1	C	285	Total	C	N	O	S	0	0	0
			2179	1384	384	399	12			
1	D	281	Total	C	N	O	S	0	0	0
			2153	1369	380	392	12			

There are 8 discrepancies between the modelled and reference sequences:

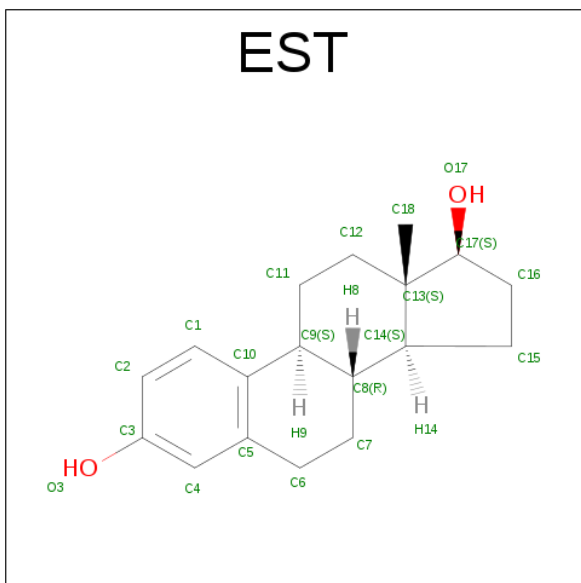
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	LEU	HIS	ENGINEERED	UNP P14061
A	301	ARG	ALA	CONFLICT	UNP P14061
B	221	LEU	HIS	ENGINEERED	UNP P14061
B	301	ARG	ALA	CONFLICT	UNP P14061
C	221	LEU	HIS	ENGINEERED	UNP P14061
C	301	ARG	ALA	CONFLICT	UNP P14061
D	221	LEU	HIS	ENGINEERED	UNP P14061
D	301	ARG	ALA	CONFLICT	UNP P14061

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



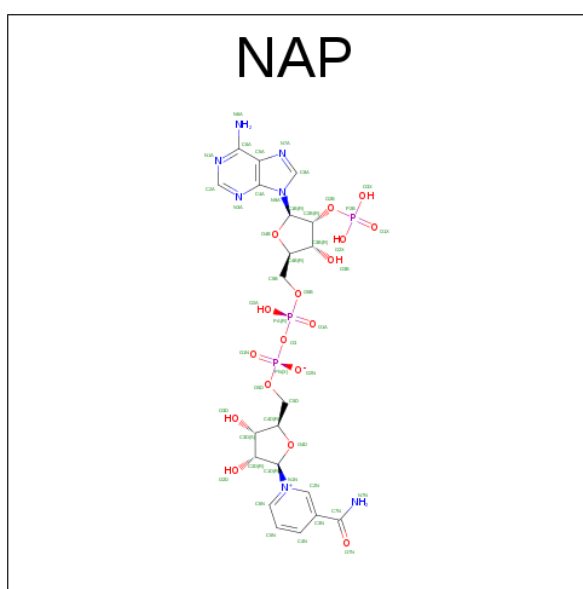
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ESTRADIOL (three-letter code: EST) (formula:  $C_{18}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		
3	C	1	Total	C	O	0	0
			20	18	2		
3	D	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		

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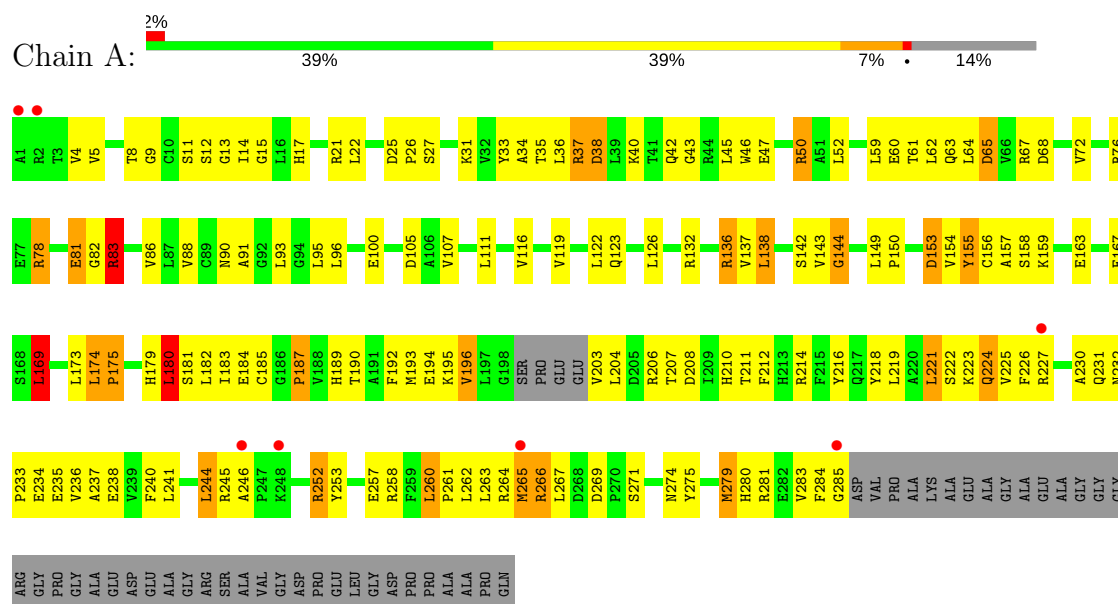
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	53	Total 53	O 53	0	0
5	C	48	Total 48	O 48	0	0
5	D	46	Total 46	O 46	0	0

### 3 Residue-property plots

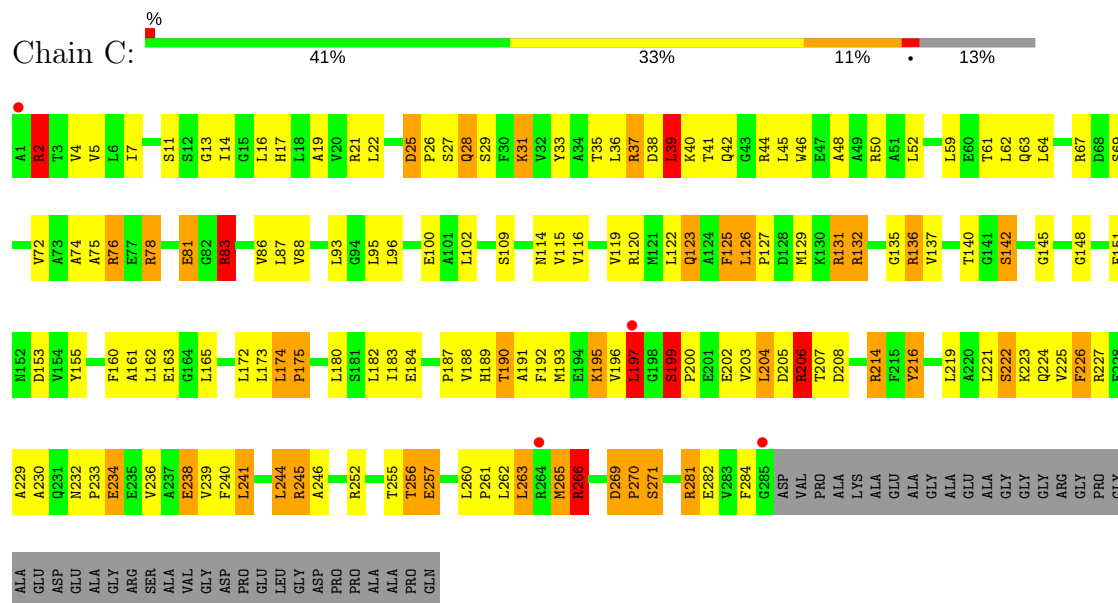
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE

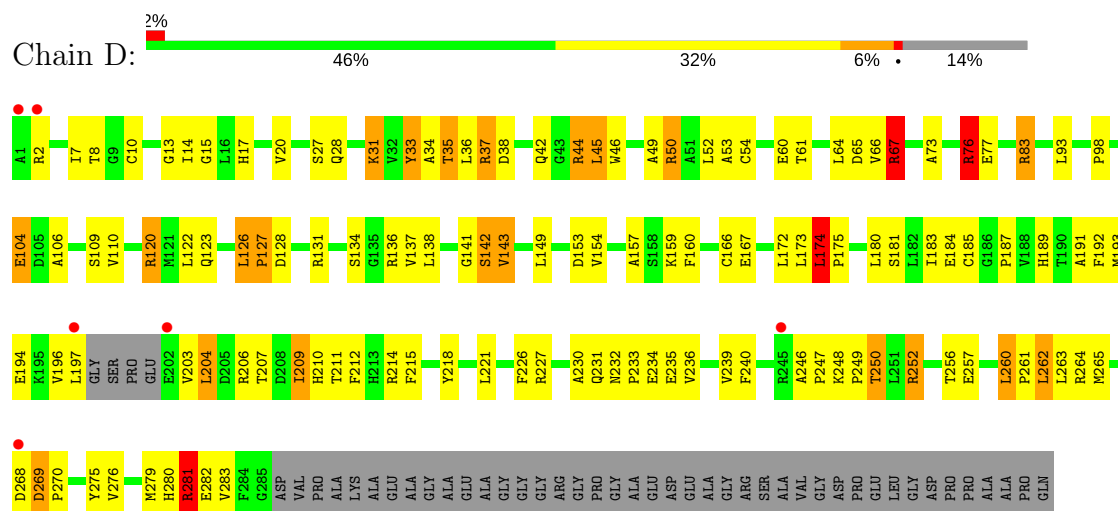




- Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



- Molecule 1: 17-BETA-HYDROXYSTEROID DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.80Å 78.78Å 121.19Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 24.09 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 89.6 (24.09-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.33 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.295 0.212 , 0.277	Depositor DCC
$R_{free}$ test set	2691 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 75.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.011 for h,-k,-l 0.109 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAP, EST, 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	0.78	0/2186	1.64	31/2963 (1.0%)
1	B	0.74	0/2182	1.66	34/2958 (1.1%)
1	C	0.79	0/2219	1.74	41/3010 (1.4%)
1	D	0.77	0/2191	1.64	28/2970 (0.9%)
All	All	0.77	0/8778	1.67	134/11901 (1.1%)

There are no bond length outliers.

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH1	-15.57	112.52	120.30
1	B	214	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	C	37	ARG	NE-CZ-NH1	-13.82	113.39	120.30
1	D	67	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	D	214	ARG	NE-CZ-NH2	-12.99	113.80	120.30
1	D	67	ARG	CD-NE-CZ	12.42	140.99	123.60
1	C	83	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	D	44	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	A	83	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	C	266	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	B	214	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	C	245	ARG	CD-NE-CZ	9.29	136.61	123.60
1	A	50	ARG	CD-NE-CZ	8.96	136.15	123.60
1	C	67	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	B	252	ARG	NE-CZ-NH1	-8.43	116.08	120.30
1	D	76	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	216	TYR	CA-CB-CG	-8.27	97.68	113.40
1	C	245	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	65	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	C	83	ARG	CD-NE-CZ	7.92	134.69	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ARG	CD-NE-CZ	7.84	134.58	123.60
1	C	281	ARG	CD-NE-CZ	7.75	134.45	123.60
1	B	132	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	155	TYR	CB-CG-CD2	7.69	125.61	121.00
1	C	281	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	37	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	258	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	D	33	TYR	CB-CG-CD1	-7.51	116.49	121.00
1	B	132	ARG	CD-NE-CZ	7.32	133.85	123.60
1	D	37	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	C	76	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	269	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	C	208	ASP	CB-CG-OD2	7.24	124.81	118.30
1	D	131	ARG	CD-NE-CZ	7.21	133.70	123.60
1	A	216	TYR	CB-CG-CD1	-7.19	116.68	121.00
1	C	67	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	D	37	ARG	CD-NE-CZ	-7.16	113.58	123.60
1	B	2	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	C	50	ARG	N-CA-CB	7.13	123.44	110.60
1	A	155	TYR	CB-CG-CD1	7.11	125.27	121.00
1	B	68	ASP	CB-CG-OD1	7.10	124.69	118.30
1	B	67	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	185	CYS	CB-CA-C	-7.08	96.24	110.40
1	C	33	TYR	CB-CG-CD1	7.07	125.24	121.00
1	C	216	TYR	CB-CA-C	7.05	124.49	110.40
1	D	214	ARG	NH1-CZ-NH2	7.05	127.15	119.40
1	B	44	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	D	36	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	83	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	C	76	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	33	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	A	258	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	252	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	36	LEU	CA-CB-CG	6.69	130.69	115.30
1	A	214	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	37	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	68	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	136	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	C	265	MET	CB-CA-C	6.49	123.38	110.40
1	A	37	ARG	NH1-CZ-NH2	6.39	126.43	119.40
1	D	37	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	D	184	GLU	OE1-CD-OE2	-6.28	115.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	LEU	CB-CA-C	-6.26	98.30	110.20
1	B	184	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	C	190	THR	CA-C-N	6.19	130.82	117.20
1	D	227	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	B	120	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	227	ARG	CA-CB-CG	6.04	126.69	113.40
1	C	93	LEU	CB-CA-C	-6.03	98.74	110.20
1	B	257	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	B	131	ARG	CD-NE-CZ	5.97	131.95	123.60
1	C	125	PHE	CA-C-N	5.92	130.22	117.20
1	C	136	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	83	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	180	LEU	CA-CB-CG	5.89	128.85	115.30
1	C	214	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	142	SER	N-CA-CB	5.86	119.29	110.50
1	C	39	LEU	N-CA-CB	-5.83	98.73	110.40
1	D	252	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	245	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	76	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	142	SER	O-C-N	5.75	131.91	122.70
1	B	67	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	125	PHE	CA-C-N	5.74	129.83	117.20
1	A	38	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	125	PHE	CB-CA-C	5.68	121.77	110.40
1	D	128	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	136	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	258	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	185	CYS	CB-CA-C	-5.59	99.22	110.40
1	B	23	ALA	N-CA-CB	5.57	117.90	110.10
1	D	281	ARG	CD-NE-CZ	5.48	131.27	123.60
1	B	37	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	120	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	B	136	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	31	LYS	N-CA-C	-5.39	96.46	111.00
1	D	44	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	140	THR	CA-CB-CG2	-5.33	104.94	112.40
1	B	25	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	253	TYR	CB-CG-CD2	5.30	124.18	121.00
1	A	266	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	D	214	ARG	CD-NE-CZ	-5.30	116.19	123.60
1	D	33	TYR	CB-CG-CD2	5.27	124.16	121.00
1	A	260	LEU	CB-CA-C	5.27	120.21	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	CD-NE-CZ	5.24	130.93	123.60
1	C	21	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	50	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	C	175	PRO	CA-C-N	5.22	128.70	117.20
1	A	21	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	25	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	C	136	ARG	CD-NE-CZ	5.19	130.87	123.60
1	D	93	LEU	CB-CA-C	-5.17	100.38	110.20
1	C	265	MET	CA-CB-CG	5.16	122.07	113.30
1	A	253	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	C	238	GLU	CB-CA-C	5.14	120.68	110.40
1	C	190	THR	O-C-N	-5.14	114.48	122.70
1	D	143	VAL	O-C-N	-5.13	114.48	123.20
1	D	185	CYS	CB-CA-C	-5.13	100.14	110.40
1	A	138	LEU	O-C-N	5.12	130.89	122.70
1	C	206	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	187	PRO	O-C-N	-5.10	114.54	122.70
1	A	95	LEU	O-C-N	5.10	130.86	122.70
1	A	175	PRO	CA-C-N	5.08	128.38	117.20
1	A	76	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	144	GLY	C-N-CA	5.08	132.97	122.30
1	C	67	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	C	126	LEU	N-CA-C	5.07	124.69	111.00
1	B	136	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	143	VAL	O-C-N	-5.04	114.62	123.20
1	B	11	SER	CB-CA-C	-5.04	100.52	110.10
1	C	2	ARG	CD-NE-CZ	5.03	130.64	123.60
1	D	252	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	A	169	LEU	CA-CB-CG	5.02	126.85	115.30
1	C	78	ARG	NE-CZ-NH2	-5.01	117.80	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	2148	0	2200	126	0
1	B	2144	0	2197	117	0
1	C	2179	0	2225	132	0
1	D	2153	0	2203	121	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
3	A	20	0	24	10	0
3	B	20	0	24	6	0
3	C	20	0	23	3	0
3	D	20	0	23	6	0
4	A	48	0	25	6	0
4	B	48	0	25	5	0
4	C	48	0	25	5	0
4	D	48	0	25	5	0
5	A	51	0	0	9	0
5	B	53	0	0	3	0
5	C	48	0	0	2	0
5	D	46	0	0	3	0
All	All	9114	0	9019	483	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 27.

All (483) 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:C:193:MET:HA	1:C:196:VAL:HG23	1.38	1.01
1:D:174:LEU:HB3	1:D:175:PRO:HD3	1.41	0.99
1:D:174:LEU:HB3	1:D:175:PRO:CD	1.95	0.97
1:C:100:GLU:HA	1:D:123:GLN:HG2	1.45	0.96
1:A:264:ARG:HA	1:A:267:LEU:HD12	1.51	0.93
1:A:232:ASN:HB2	1:A:235:GLU:HG3	1.54	0.87
1:A:262:LEU:HD12	1:A:265:MET:HG2	1.57	0.86
1:B:232:ASN:HB2	1:B:235:GLU:HG3	1.59	0.85
1:A:260:LEU:N	1:A:261:PRO:HD2	1.94	0.82
1:C:35:THR:HG22	1:C:62:LEU:HB2	1.61	0.82
1:A:100:GLU:HA	1:B:123:GLN:HG2	1.61	0.82
1:D:166:CYS:HB3	1:D:180:LEU:HD21	1.62	0.81
1:C:260:LEU:N	1:C:261:PRO:HD2	1.96	0.80
1:C:76:ARG:HG3	1:C:125:PHE:CE2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:THR:HG23	1:D:64:LEU:HB3	1.64	0.78
1:A:203:VAL:O	1:A:207:THR:HG22	1.83	0.78
1:C:190:THR:O	1:C:191:ALA:HB3	1.84	0.77
1:C:44:ARG:NH2	2:C:403:SO4:O2	2.18	0.77
1:D:193:MET:SD	1:D:196:VAL:HG21	2.25	0.76
1:B:31:LYS:NZ	1:B:60:GLU:HG3	2.00	0.76
1:C:219:LEU:O	1:C:223:LYS:HG3	1.85	0.76
1:C:174:LEU:HB3	1:C:175:PRO:HD3	1.65	0.75
1:B:34:ALA:HB3	1:B:61:THR:HG22	1.66	0.75
1:B:138:LEU:HD22	1:B:181:SER:HB2	1.70	0.74
1:C:64:LEU:HD21	1:C:72:VAL:HG22	1.70	0.74
1:D:142:SER:HB2	4:D:362:NAP:H6N	1.69	0.73
1:B:142:SER:HB2	4:B:364:NAP:H6N	1.70	0.73
1:A:107:VAL:HG13	1:A:154:VAL:HG11	1.69	0.73
1:B:165:LEU:O	1:B:169:LEU:HD12	1.88	0.73
1:C:189:HIS:CE1	1:C:230:ALA:HB3	2.24	0.73
1:A:111:LEU:HD23	1:A:158:SER:HB3	1.70	0.72
1:B:174:LEU:HB3	1:B:175:PRO:CD	2.19	0.72
1:C:193:MET:HA	1:C:196:VAL:CG2	2.17	0.72
1:A:42:GLN:NE2	1:A:46:TRP:HE1	1.88	0.72
1:C:13:GLY:HA2	1:C:190:THR:HG22	1.70	0.72
1:D:7:ILE:O	1:D:35:THR:HB	1.89	0.72
1:C:5:VAL:HG22	1:C:86:VAL:HB	1.70	0.72
1:D:203:VAL:O	1:D:207:THR:HG22	1.89	0.71
1:A:119:VAL:O	1:A:123:GLN:HG3	1.91	0.71
1:C:45:LEU:HD11	1:C:59:LEU:HD21	1.73	0.71
1:A:45:LEU:HD11	1:A:59:LEU:HD21	1.70	0.71
1:D:143:VAL:HB	3:D:352:EST:H121	1.71	0.70
1:B:96:LEU:HD23	1:B:196:VAL:CG1	2.22	0.70
1:D:260:LEU:N	1:D:261:PRO:HD2	2.07	0.70
1:A:8:THR:O	1:A:90:ASN:HB3	1.92	0.70
1:C:196:VAL:O	1:C:197:LEU:HB2	1.91	0.70
1:B:128:ASP:O	1:B:132:ARG:HG2	1.92	0.69
1:C:219:LEU:HD22	1:C:223:LYS:HE2	1.74	0.69
1:D:65:ASP:OD2	1:D:67:ARG:NH1	2.24	0.69
1:B:65:ASP:OD1	1:B:67:ARG:HG2	1.93	0.69
1:C:174:LEU:HB3	1:C:175:PRO:CD	2.23	0.69
1:B:20:VAL:HG23	1:B:52:LEU:HD22	1.73	0.69
1:A:43:GLY:O	1:A:47:GLU:HG3	1.93	0.68
1:A:42:GLN:HE21	1:A:46:TRP:HE1	1.40	0.68
1:C:78:ARG:NH1	1:C:78:ARG:HB3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:GLN:NE2	1:D:46:TRP:HE1	1.92	0.67
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.75	0.67
1:C:199:SER:OG	1:C:202:GLU:HB2	1.94	0.67
1:C:187:PRO:HD3	3:C:353:EST:H122	1.76	0.67
1:B:221:LEU:HD22	1:B:225:VAL:HG23	1.75	0.67
1:B:149:LEU:HD11	3:B:354:EST:H121	1.76	0.67
1:D:142:SER:HB2	4:D:362:NAP:C6N	2.25	0.67
1:D:13:GLY:O	1:D:17:HIS:HD2	1.78	0.66
1:A:240:PHE:O	1:A:244:LEU:HD23	1.95	0.66
1:D:143:VAL:HB	3:D:352:EST:C12	2.25	0.66
1:C:266:ARG:NH2	1:D:167:GLU:OE2	2.23	0.65
1:A:150:PRO:HD3	1:B:171:VAL:HG11	1.78	0.65
1:A:266:ARG:HH21	1:B:167:GLU:CD	2.00	0.65
1:D:50:ARG:NH1	5:D:594:HOH:O	2.29	0.65
1:C:190:THR:O	1:C:191:ALA:CB	2.43	0.65
1:C:239:VAL:HG21	1:C:255:THR:HG22	1.78	0.65
1:A:260:LEU:N	1:A:261:PRO:CD	2.60	0.64
1:C:116:VAL:HG12	1:C:120:ARG:NH1	2.12	0.64
1:B:27:SER:O	1:B:28:GLN:HB2	1.97	0.64
1:B:191:ALA:O	1:B:194:GLU:HG2	1.96	0.64
1:C:42:GLN:NE2	1:C:46:TRP:HE1	1.95	0.64
1:C:260:LEU:HA	1:C:263:LEU:HB2	1.80	0.64
1:C:119:VAL:O	1:C:123:GLN:HG2	1.98	0.63
1:A:142:SER:HB2	4:A:361:NAP:H6N	1.80	0.63
1:C:240:PHE:O	1:C:244:LEU:HD23	1.98	0.63
1:D:260:LEU:HB3	1:D:264:ARG:NH2	2.13	0.63
1:A:31:LYS:HE2	1:A:33:TYR:CE1	2.35	0.62
1:B:174:LEU:N	1:B:175:PRO:HD2	2.15	0.62
1:D:66:VAL:HG22	4:D:362:NAP:N1A	2.14	0.61
1:A:262:LEU:CD1	1:A:265:MET:HG2	2.29	0.61
1:A:189:HIS:CE1	1:A:230:ALA:HB3	2.35	0.61
1:B:187:PRO:HB3	1:B:226:PHE:CD2	2.35	0.60
1:B:31:LYS:HZ1	1:B:60:GLU:HG3	1.65	0.60
1:A:244:LEU:HA	5:A:556:HOH:O	2.02	0.59
1:D:189:HIS:CE1	1:D:230:ALA:HB3	2.37	0.59
1:C:260:LEU:N	1:C:261:PRO:CD	2.65	0.59
1:C:42:GLN:HE21	1:C:46:TRP:HE1	1.50	0.59
1:C:191:ALA:O	1:C:195:LYS:HG3	2.03	0.59
1:A:82:GLY:O	1:A:83:ARG:HB3	2.03	0.58
1:A:175:PRO:HG3	1:B:280:HIS:CE1	2.38	0.58
1:A:232:ASN:HB3	1:A:234:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:NH2	1:B:167:GLU:OE2	2.35	0.58
1:C:222:SER:HB3	3:C:353:EST:H61	1.84	0.58
1:C:202:GLU:HB3	1:C:206:ARG:HH21	1.68	0.58
1:C:116:VAL:HG12	1:C:120:ARG:CZ	2.33	0.58
1:C:232:ASN:HB3	1:C:234:GLU:HG2	1.84	0.58
1:D:279:MET:O	1:D:283:VAL:HG23	2.04	0.58
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.68	0.58
1:B:141:GLY:HA3	1:B:184:GLU:HA	1.86	0.58
1:C:257:GLU:HA	1:C:260:LEU:HD13	1.86	0.58
1:B:13:GLY:HA3	4:B:364:NAP:O2N	2.03	0.58
1:D:83:ARG:HH11	1:D:83:ARG:HG2	1.69	0.58
1:B:131:ARG:HH12	1:B:132:ARG:NH2	2.02	0.57
1:A:174:LEU:HD12	1:A:174:LEU:C	2.25	0.57
1:C:137:VAL:O	1:C:180:LEU:HA	2.05	0.57
1:D:149:LEU:CD1	3:D:352:EST:H182	2.35	0.57
1:B:65:ASP:OD2	1:B:67:ARG:NH1	2.38	0.57
1:D:207:THR:OG1	1:D:211:THR:HB	2.05	0.56
1:B:172:LEU:HD12	1:B:172:LEU:O	2.05	0.56
1:C:35:THR:HA	1:C:62:LEU:O	2.05	0.56
1:B:233:PRO:HD2	1:B:234:GLU:OE2	2.06	0.56
1:C:188:VAL:HG21	1:C:236:VAL:HG21	1.86	0.56
1:D:73:ALA:O	1:D:77:GLU:HG2	2.05	0.56
1:D:98:PRO:HG2	1:D:203:VAL:HG13	1.87	0.56
1:C:96:LEU:HB2	1:C:196:VAL:HG12	1.87	0.56
1:D:257:GLU:HG2	1:D:260:LEU:HD22	1.87	0.56
1:D:27:SER:O	1:D:28:GLN:HB2	2.04	0.56
1:A:52:LEU:HD11	5:A:696:HOH:O	2.04	0.56
1:C:13:GLY:O	1:C:17:HIS:HD2	1.89	0.56
1:D:154:VAL:N	5:D:603:HOH:O	2.38	0.56
1:D:8:THR:HA	1:D:35:THR:CG2	2.36	0.56
1:B:13:GLY:O	1:B:17:HIS:HD2	1.87	0.56
1:C:160:PHE:HB3	1:D:160:PHE:HB3	1.86	0.56
1:D:8:THR:HA	1:D:35:THR:HG22	1.88	0.56
1:D:203:VAL:HG21	1:D:215:PHE:HE2	1.72	0.55
1:A:9:GLY:O	1:A:15:GLY:HA3	2.06	0.55
1:A:8:THR:HA	1:A:35:THR:OG1	2.06	0.55
1:D:31:LYS:NZ	1:D:60:GLU:HG3	2.21	0.55
1:D:34:ALA:HB3	1:D:61:THR:HG22	1.88	0.55
1:B:52:LEU:O	1:B:53:ALA:HB3	2.05	0.55
1:C:221:LEU:C	1:C:221:LEU:HD13	2.26	0.55
1:C:81:GLU:H	1:C:81:GLU:CD	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASP:OD1	1:D:67:ARG:HG2	2.06	0.55
1:A:187:PRO:HG3	3:A:351:EST:H9	1.88	0.54
1:A:31:LYS:HE2	1:A:33:TYR:CZ	2.42	0.54
1:B:96:LEU:HD23	1:B:196:VAL:HG11	1.89	0.54
1:B:136:ARG:NH1	1:B:249:PRO:HG3	2.22	0.54
1:D:232:ASN:HB2	1:D:235:GLU:HG3	1.89	0.54
1:B:31:LYS:HZ2	1:B:60:GLU:HG3	1.71	0.54
1:D:233:PRO:HD2	1:D:234:GLU:OE2	2.06	0.54
1:B:166:CYS:HB3	1:B:180:LEU:HD21	1.87	0.54
1:B:224:GLN:O	1:B:228:GLU:HG3	2.06	0.54
1:C:42:GLN:HE21	1:C:61:THR:HG21	1.72	0.54
1:B:104:GLU:HG3	5:B:679:HOH:O	2.06	0.54
1:B:187:PRO:HB3	1:B:226:PHE:CE2	2.43	0.54
1:B:203:VAL:HG12	1:B:204:LEU:N	2.22	0.54
1:A:231:GLN:NE2	5:A:571:HOH:O	2.28	0.54
1:B:138:LEU:CD2	1:B:181:SER:HB2	2.37	0.54
1:B:263:LEU:O	1:B:266:ARG:HB3	2.07	0.54
1:A:13:GLY:HA2	1:A:190:THR:HG22	1.90	0.54
1:B:1:ALA:HB1	1:B:2:ARG:NH2	2.23	0.53
1:C:14:ILE:HG12	1:C:236:VAL:HG11	1.91	0.53
1:C:96:LEU:HB2	1:C:196:VAL:CG1	2.39	0.53
1:C:221:LEU:O	1:C:225:VAL:HG23	2.09	0.53
1:C:114:ASN:O	1:C:162:LEU:HD21	2.08	0.53
1:D:193:MET:HA	1:D:196:VAL:HG23	1.91	0.53
1:D:38:ASP:OD1	1:D:38:ASP:C	2.46	0.53
1:C:119:VAL:HG22	1:C:165:LEU:HD11	1.91	0.53
1:D:187:PRO:HB3	1:D:226:PHE:CE1	2.43	0.53
1:C:196:VAL:O	1:C:197:LEU:CB	2.57	0.53
1:D:122:LEU:O	1:D:126:LEU:HB2	2.09	0.53
1:C:216:TYR:CD1	1:C:219:LEU:HD12	2.43	0.53
1:D:212:PHE:O	1:D:215:PHE:HB3	2.09	0.53
1:A:64:LEU:HD21	1:A:72:VAL:HG22	1.91	0.52
1:A:163:GLU:OE2	1:A:184:GLU:OE2	2.27	0.52
1:C:281:ARG:NH1	1:C:282:GLU:OE2	2.42	0.52
1:D:10:CYS:HA	1:D:15:GLY:HA3	1.90	0.52
1:B:89:CYS:HB3	1:B:118:THR:HG23	1.91	0.52
1:D:204:LEU:HD23	1:D:212:PHE:CE1	2.44	0.52
1:D:76:ARG:NH1	1:D:76:ARG:HG2	2.25	0.52
1:D:187:PRO:HB3	1:D:226:PHE:CD1	2.44	0.52
1:C:136:ARG:NH2	1:C:246:ALA:O	2.40	0.52
1:B:37:ARG:HH21	4:B:364:NAP:P2B	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:VAL:O	1:D:157:ALA:HB3	2.10	0.52
1:D:174:LEU:CB	1:D:175:PRO:CD	2.72	0.52
1:C:142:SER:HB2	4:C:363:NAP:H6N	1.90	0.52
1:B:221:LEU:HD22	1:B:225:VAL:CG2	2.37	0.52
1:B:37:ARG:NH2	4:B:364:NAP:O2X	2.43	0.52
1:D:143:VAL:CB	3:D:352:EST:H121	2.40	0.52
1:A:11:SER:O	1:A:12:SER:HB3	2.10	0.52
1:D:141:GLY:N	1:D:183:ILE:O	2.42	0.52
1:C:39:LEU:HB2	5:C:591:HOH:O	2.10	0.51
1:D:173:LEU:O	1:D:174:LEU:C	2.48	0.51
1:C:44:ARG:NH2	2:C:403:SO4:S	2.83	0.51
1:C:45:LEU:C	1:C:45:LEU:HD13	2.30	0.51
1:B:128:ASP:OD2	1:B:131:ARG:NH1	2.43	0.51
1:C:96:LEU:CB	1:C:196:VAL:HG12	2.40	0.51
1:D:236:VAL:HG12	1:D:240:PHE:HE1	1.75	0.51
1:D:34:ALA:CB	1:D:45:LEU:HD11	2.41	0.51
1:A:65:ASP:CG	1:A:67:ARG:HH21	2.14	0.51
1:B:204:LEU:O	1:B:204:LEU:HD22	2.11	0.51
1:D:262:LEU:O	1:D:265:MET:HB3	2.11	0.51
1:C:11:SER:CB	1:C:36:LEU:HD23	2.40	0.51
1:D:231:GLN:NE2	5:D:541:HOH:O	2.43	0.51
1:D:204:LEU:HD23	1:D:212:PHE:CZ	2.46	0.51
1:C:184:GLU:HA	1:C:184:GLU:OE1	2.10	0.51
1:D:31:LYS:HZ2	1:D:60:GLU:HG3	1.74	0.51
1:C:183:ILE:HG13	1:C:240:PHE:CD2	2.46	0.51
5:C:569:HOH:O	1:D:104:GLU:HG3	2.10	0.51
1:C:271:SER:HB2	1:D:250:THR:CG2	2.41	0.50
1:D:126:LEU:N	1:D:127:PRO:HD2	2.27	0.50
1:A:257:GLU:HA	1:A:260:LEU:HD13	1.93	0.50
1:B:189:HIS:O	1:B:233:PRO:HG3	2.11	0.50
1:A:174:LEU:CB	1:A:175:PRO:CD	2.90	0.50
1:B:17:HIS:O	1:B:21:ARG:HB2	2.11	0.50
1:D:73:ALA:O	1:D:76:ARG:HB3	2.11	0.50
1:A:264:ARG:CA	1:A:267:LEU:HD12	2.34	0.50
1:B:221:LEU:O	1:B:225:VAL:HG23	2.11	0.50
1:C:16:LEU:O	1:C:19:ALA:HB3	2.12	0.50
1:C:225:VAL:O	1:C:229:ALA:HB3	2.11	0.50
1:A:26:PRO:O	1:A:27:SER:C	2.49	0.50
1:B:21:ARG:HD2	1:B:21:ARG:O	2.11	0.50
1:B:279:MET:HG3	1:B:279:MET:O	2.12	0.50
1:B:232:ASN:CB	1:B:235:GLU:HG3	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:N	1:B:261:PRO:HD2	2.27	0.50
1:C:2:ARG:HH21	1:C:83:ARG:NH2	2.10	0.50
1:D:126:LEU:N	1:D:127:PRO:CD	2.74	0.50
1:C:140:THR:HG21	4:C:363:NAP:O4D	2.11	0.50
1:D:203:VAL:HG11	1:D:215:PHE:CD2	2.47	0.50
1:A:136:ARG:HD3	5:A:556:HOH:O	2.11	0.49
1:C:2:ARG:HH21	1:C:83:ARG:HH22	1.59	0.49
1:A:241:LEU:N	1:A:241:LEU:HD12	2.27	0.49
1:B:38:ASP:OD1	1:B:40:LYS:HG2	2.12	0.49
1:A:33:TYR:HD2	1:A:62:LEU:HD11	1.77	0.49
1:A:90:ASN:O	1:A:91:ALA:C	2.51	0.49
1:B:10:CYS:HA	1:B:15:GLY:HA3	1.94	0.49
1:D:137:VAL:O	1:D:180:LEU:HA	2.13	0.49
1:D:66:VAL:HG22	4:D:362:NAP:C6A	2.43	0.49
1:A:4:VAL:HG21	1:A:81:GLU:HG2	1.94	0.49
1:C:202:GLU:HB3	1:C:206:ARG:HE	1.77	0.49
1:C:203:VAL:O	1:C:207:THR:HG22	2.13	0.49
3:A:351:EST:H17	4:A:361:NAP:C4N	2.43	0.49
3:A:351:EST:H17	4:A:361:NAP:H4N	1.94	0.49
1:A:37:ARG:HG3	4:A:361:NAP:N1A	2.28	0.49
1:B:231:GLN:HG3	5:B:649:HOH:O	2.12	0.49
1:B:143:VAL:CG1	3:B:354:EST:H122	2.44	0.48
1:C:37:ARG:NH1	4:C:363:NAP:O3X	2.46	0.48
1:B:126:LEU:N	1:B:127:PRO:HD2	2.28	0.48
1:C:37:ARG:HG3	4:C:363:NAP:N1A	2.28	0.48
1:C:148:GLY:HA3	1:D:167:GLU:HB3	1.95	0.48
1:A:5:VAL:HG13	1:A:86:VAL:HG12	1.94	0.48
1:C:245:ARG:O	1:C:246:ALA:C	2.51	0.48
1:C:38:ASP:OD1	1:C:40:LYS:HB2	2.13	0.48
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.78	0.48
1:A:37:ARG:NH1	4:A:361:NAP:O3X	2.46	0.48
1:A:281:ARG:HA	1:A:285:GLY:O	2.14	0.48
1:A:45:LEU:CD1	1:A:59:LEU:HD21	2.40	0.48
1:B:1:ALA:O	1:B:2:ARG:HB2	2.14	0.48
1:C:200:PRO:O	1:C:204:LEU:HB2	2.13	0.48
1:C:174:LEU:CB	1:C:175:PRO:CD	2.87	0.48
1:C:31:LYS:HD3	1:C:81:GLU:OE2	2.14	0.48
1:D:37:ARG:NH1	4:D:362:NAP:O3X	2.46	0.48
1:C:126:LEU:HB2	1:C:127:PRO:HD3	1.96	0.48
3:C:353:EST:H17	4:C:363:NAP:H4N	1.95	0.47
1:A:183:ILE:HG13	1:A:240:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:SER:HB2	4:B:364:NAP:O3B	2.14	0.47
1:C:216:TYR:CE1	1:C:219:LEU:HD12	2.49	0.47
1:C:95:LEU:HD11	1:C:102:LEU:HD22	1.96	0.47
1:A:155:TYR:CE1	1:A:192:PHE:HZ	2.32	0.47
1:D:189:HIS:O	1:D:233:PRO:HG3	2.13	0.47
1:B:25:ASP:OD1	1:B:26:PRO:HD2	2.14	0.47
1:B:226:PHE:HE2	3:B:354:EST:H151	1.79	0.47
1:D:20:VAL:HG12	1:D:49:ALA:HB2	1.96	0.47
1:D:52:LEU:O	1:D:53:ALA:HB3	2.14	0.47
1:C:11:SER:HB2	1:C:36:LEU:HD23	1.97	0.47
1:C:45:LEU:O	1:C:45:LEU:HD13	2.14	0.47
1:D:209:ILE:HG23	1:D:210:HIS:N	2.29	0.47
1:D:34:ALA:HB1	1:D:45:LEU:HD11	1.96	0.47
1:A:78:ARG:HB3	1:A:78:ARG:HE	1.52	0.47
1:D:76:ARG:HH11	1:D:76:ARG:HG2	1.79	0.47
4:A:361:NAP:O1N	4:A:361:NAP:H2N	2.13	0.47
1:C:78:ARG:HB3	1:C:78:ARG:HH11	1.80	0.47
1:D:31:LYS:HE2	1:D:33:TYR:CE1	2.50	0.47
1:B:185:CYS:HA	1:B:255:THR:OG1	2.15	0.47
1:B:18:LEU:HD11	1:B:22:LEU:HD11	1.96	0.47
1:D:269:ASP:HA	1:D:270:PRO:HD2	1.69	0.47
1:D:13:GLY:N	2:D:402:SO4:O2	2.41	0.47
1:B:17:HIS:CD2	1:B:233:PRO:HB2	2.50	0.47
1:C:187:PRO:HB3	1:C:226:PHE:CE1	2.50	0.47
1:A:174:LEU:HB3	1:A:175:PRO:CD	2.45	0.47
1:B:129:MET:HB3	1:B:134:SER:O	2.15	0.47
1:C:269:ASP:HA	1:C:270:PRO:HD2	1.54	0.47
1:D:187:PRO:HB2	1:D:230:ALA:HA	1.97	0.46
1:D:281:ARG:O	1:D:282:GLU:C	2.53	0.46
1:B:138:LEU:HD13	1:B:183:ILE:HD11	1.97	0.46
1:A:149:LEU:CD1	3:A:351:EST:H182	2.46	0.46
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.80	0.46
1:A:5:VAL:HG13	1:A:86:VAL:CG1	2.46	0.46
1:D:215:PHE:O	1:D:218:TYR:HB3	2.15	0.46
1:A:279:MET:O	1:A:283:VAL:HG23	2.16	0.46
1:C:271:SER:HB2	1:D:250:THR:HG21	1.98	0.46
1:A:219:LEU:O	1:A:223:LYS:HG3	2.16	0.46
1:A:241:LEU:HA	1:A:244:LEU:CD2	2.45	0.46
1:A:144:GLY:H	3:A:351:EST:H183	1.81	0.46
1:B:94:GLY:HA2	1:B:155:TYR:CD1	2.51	0.46
1:C:199:SER:OG	1:C:199:SER:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HG	1:A:175:PRO:HD3	1.96	0.46
1:B:189:HIS:CE1	1:B:230:ALA:HB3	2.51	0.46
1:B:64:LEU:HD21	1:B:72:VAL:HG22	1.98	0.46
1:D:122:LEU:HD21	1:D:137:VAL:HG11	1.97	0.46
1:A:144:GLY:N	3:A:351:EST:H183	2.30	0.46
1:D:14:ILE:HD13	1:D:236:VAL:HG11	1.97	0.46
1:B:226:PHE:CE2	3:B:354:EST:H151	2.51	0.46
1:C:172:LEU:O	1:C:175:PRO:HD2	2.16	0.46
1:C:221:LEU:O	1:C:221:LEU:HD13	2.17	0.45
1:D:123:GLN:HE21	1:D:123:GLN:HB2	1.50	0.45
1:D:31:LYS:HE2	1:D:33:TYR:CZ	2.51	0.45
1:D:35:THR:HG23	1:D:64:LEU:CB	2.41	0.45
1:B:143:VAL:HG12	3:B:354:EST:H122	1.99	0.45
1:A:174:LEU:HB3	1:A:175:PRO:HD3	1.99	0.45
1:D:193:MET:HA	1:D:196:VAL:CG2	2.47	0.45
1:C:214:ARG:HB3	1:C:284:PHE:CE1	2.51	0.45
1:A:167:GLU:OE1	1:B:266:ARG:NH2	2.45	0.45
1:B:4:VAL:HG11	1:B:83:ARG:O	2.17	0.45
1:C:122:LEU:O	1:C:123:GLN:C	2.55	0.45
1:D:149:LEU:HD13	3:D:352:EST:H182	1.98	0.45
1:D:191:ALA:O	1:D:194:GLU:HB2	2.16	0.45
1:D:246:ALA:HA	1:D:247:PRO:HD2	1.86	0.45
1:C:131:ARG:HA	1:C:131:ARG:HD3	1.74	0.45
1:D:203:VAL:HG12	1:D:207:THR:HG21	1.98	0.45
1:B:3:THR:HG21	1:B:30:PHE:CE1	2.52	0.45
1:C:129:MET:HG2	1:C:135:GLY:HA3	1.98	0.45
1:A:34:ALA:O	1:A:61:THR:HA	2.16	0.45
1:C:239:VAL:O	1:C:240:PHE:C	2.54	0.45
1:D:65:ASP:CG	1:D:67:ARG:HH11	2.20	0.44
1:A:163:GLU:OE2	1:A:182:LEU:HD13	2.18	0.44
1:B:269:ASP:OD2	1:B:274:ASN:HB2	2.17	0.44
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.32	0.44
1:B:231:GLN:HB3	1:B:235:GLU:OE2	2.18	0.44
1:A:14:ILE:H	1:A:14:ILE:HD12	1.81	0.44
1:B:21:ARG:HD2	1:B:21:ARG:C	2.38	0.44
1:C:115:VAL:HG22	1:C:161:ALA:HB3	2.00	0.44
1:C:25:ASP:OD1	1:C:27:SER:OG	2.36	0.44
1:D:49:ALA:HB1	1:D:54:CYS:SG	2.57	0.44
1:B:263:LEU:O	1:B:267:LEU:HG	2.17	0.44
1:A:219:LEU:HB3	1:A:223:LYS:HE3	1.99	0.44
1:D:192:PHE:O	1:D:196:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:OD1	1:B:65:ASP:C	2.55	0.44
1:C:95:LEU:CD1	1:C:102:LEU:HD22	2.48	0.44
1:D:166:CYS:HB3	1:D:180:LEU:CD2	2.39	0.44
1:D:239:VAL:O	1:D:240:PHE:C	2.56	0.44
1:A:126:LEU:HD11	1:A:169:LEU:HD11	1.99	0.44
1:A:142:SER:HB3	1:A:159:LYS:HD2	2.00	0.44
1:A:96:LEU:CB	1:A:196:VAL:HG13	2.48	0.44
1:B:31:LYS:HE2	1:B:33:TYR:CE1	2.53	0.44
1:C:75:ALA:O	1:C:76:ARG:C	2.54	0.44
1:A:116:VAL:HG21	5:A:665:HOH:O	2.16	0.43
1:B:275:TYR:O	1:B:276:VAL:C	2.55	0.43
1:C:25:ASP:O	1:C:28:GLN:N	2.51	0.43
1:B:33:TYR:O	1:B:35:THR:HG23	2.18	0.43
1:A:86:VAL:HA	1:A:136:ARG:O	2.18	0.43
1:B:173:LEU:O	1:B:174:LEU:C	2.57	0.43
1:B:2:ARG:HA	1:B:83:ARG:NH2	2.34	0.43
1:A:78:ARG:NH1	5:A:629:HOH:O	2.43	0.43
1:D:261:PRO:HA	1:D:264:ARG:HD2	2.00	0.43
1:A:193:MET:O	1:A:194:GLU:C	2.57	0.43
1:A:203:VAL:HG12	1:A:212:PHE:CE1	2.54	0.43
1:A:45:LEU:C	1:A:45:LEU:HD13	2.38	0.43
1:A:88:VAL:HA	1:A:138:LEU:O	2.19	0.43
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.71	0.43
1:C:174:LEU:HD12	1:C:174:LEU:C	2.39	0.43
1:C:17:HIS:CD2	1:C:233:PRO:HB2	2.53	0.43
1:C:42:GLN:NE2	1:C:61:THR:HG21	2.34	0.43
1:D:159:LYS:HD3	1:D:159:LYS:HA	1.81	0.43
1:A:38:ASP:OD1	1:A:40:LYS:N	2.50	0.43
1:C:199:SER:O	1:C:202:GLU:N	2.52	0.43
1:B:239:VAL:O	1:B:242:THR:HB	2.19	0.43
1:C:175:PRO:HG3	1:D:280:HIS:CE1	2.54	0.43
1:C:193:MET:CA	1:C:196:VAL:HG23	2.27	0.43
1:A:25:ASP:HA	1:A:26:PRO:HD3	1.85	0.42
1:A:5:VAL:HG11	1:A:22:LEU:CD1	2.49	0.42
1:A:264:ARG:O	1:A:265:MET:C	2.57	0.42
1:A:33:TYR:HA	1:A:60:GLU:O	2.19	0.42
1:B:263:LEU:HD13	1:B:267:LEU:HD11	2.00	0.42
1:A:224:GLN:HG2	1:A:227:ARG:NH2	2.35	0.42
1:B:136:ARG:NH2	1:B:246:ALA:O	2.52	0.42
1:C:132:ARG:HG3	1:C:132:ARG:NH1	2.33	0.42
1:C:4:VAL:HG21	1:C:81:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ARG:HA	1:D:120:ARG:NH1	2.35	0.42
1:A:116:VAL:HG11	5:A:665:HOH:O	2.18	0.42
1:A:52:LEU:N	1:A:52:LEU:HD12	2.35	0.42
1:A:157:ALA:HB1	1:B:161:ALA:HB1	2.01	0.42
1:C:2:ARG:HH22	1:C:81:GLU:CG	2.33	0.42
1:C:38:ASP:O	1:C:41:THR:OG1	2.38	0.42
1:B:132:ARG:HD2	5:B:506:HOH:O	2.19	0.42
1:B:16:LEU:O	1:B:19:ALA:HB3	2.19	0.42
1:B:39:LEU:HD22	1:B:42:GLN:NE2	2.34	0.42
1:C:145:GLY:O	1:C:163:GLU:HG3	2.20	0.42
1:A:122:LEU:O	1:A:123:GLN:C	2.58	0.42
1:A:122:LEU:HD21	1:A:137:VAL:HG11	2.02	0.42
1:A:231:GLN:HG3	5:A:571:HOH:O	2.20	0.42
1:C:202:GLU:O	1:C:205:ASP:HB3	2.19	0.42
1:C:22:LEU:CD2	1:C:241:LEU:HD11	2.49	0.42
1:D:149:LEU:HD11	3:D:352:EST:H111	2.02	0.42
1:D:138:LEU:CD2	1:D:181:SER:HB2	2.49	0.42
1:D:248:LYS:HG2	1:D:248:LYS:O	2.18	0.42
1:A:221:LEU:HD13	1:A:225:VAL:HG23	2.02	0.42
1:A:218:TYR:OH	3:A:351:EST:H62	2.20	0.42
1:B:100:GLU:HG3	1:B:206:ARG:O	2.20	0.42
1:A:174:LEU:CB	1:A:175:PRO:HD3	2.50	0.42
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.85	0.42
1:C:52:LEU:HD12	1:C:52:LEU:N	2.35	0.42
1:D:37:ARG:HH11	1:D:37:ARG:HD3	1.39	0.42
1:A:132:ARG:HD2	5:A:635:HOH:O	2.20	0.41
1:A:156:CYS:O	1:A:157:ALA:C	2.57	0.41
1:A:236:VAL:O	1:A:237:ALA:C	2.54	0.41
1:A:149:LEU:HD11	3:A:351:EST:H182	2.01	0.41
1:C:136:ARG:NH1	1:C:244:LEU:HA	2.35	0.41
1:A:17:HIS:CD2	1:A:233:PRO:HB2	2.55	0.41
1:A:81:GLU:CD	1:A:81:GLU:H	2.23	0.41
1:B:143:VAL:HG12	3:B:354:EST:C12	2.50	0.41
1:B:204:LEU:HD23	1:B:212:PHE:CE2	2.55	0.41
1:D:138:LEU:HD22	1:D:181:SER:HB2	2.02	0.41
1:A:167:GLU:CD	1:B:266:ARG:HH21	2.23	0.41
1:C:262:LEU:HA	1:C:262:LEU:HD12	1.92	0.41
1:C:2:ARG:HH22	1:C:81:GLU:HG2	1.85	0.41
1:A:136:ARG:HA	1:A:179:HIS:O	2.21	0.41
1:A:245:ARG:O	1:A:246:ALA:C	2.58	0.41
1:A:33:TYR:CD2	1:A:62:LEU:HD11	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HB2	1:A:67:ARG:HE	1.55	0.41
1:B:204:LEU:HA	1:B:212:PHE:CE2	2.55	0.41
1:B:34:ALA:O	1:B:61:THR:HA	2.19	0.41
1:D:275:TYR:O	1:D:276:VAL:C	2.58	0.41
1:A:173:LEU:O	1:A:174:LEU:C	2.59	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD12	1.84	0.41
1:A:155:TYR:CE2	3:A:351:EST:H162	2.56	0.41
1:B:39:LEU:O	1:B:42:GLN:HG2	2.20	0.41
1:D:106:ALA:O	1:D:110:VAL:HG23	2.20	0.41
1:D:232:ASN:HB2	1:D:235:GLU:CG	2.50	0.41
1:B:129:MET:O	1:B:133:GLY:N	2.54	0.41
1:A:153:ASP:OD1	1:B:169:LEU:HG	2.21	0.41
1:C:256:THR:OG1	1:C:257:GLU:N	2.53	0.41
1:C:74:ALA:O	1:C:75:ALA:C	2.57	0.41
1:D:42:GLN:NE2	1:D:46:TRP:NE1	2.65	0.41
1:A:5:VAL:HG11	1:A:22:LEU:HD13	2.03	0.41
1:B:239:VAL:HG21	1:B:255:THR:HA	2.03	0.41
1:B:3:THR:HG21	1:B:30:PHE:HE1	1.85	0.41
1:B:126:LEU:HD13	1:B:173:LEU:HD21	2.03	0.41
1:C:188:VAL:CG2	1:C:236:VAL:HG21	2.49	0.41
1:D:166:CYS:CB	1:D:180:LEU:HD21	2.44	0.41
1:D:77:GLU:HG2	1:D:77:GLU:H	1.71	0.41
1:A:111:LEU:HD23	1:A:158:SER:CB	2.45	0.41
1:A:275:TYR:C	1:A:275:TYR:CD1	2.94	0.41
1:A:280:HIS:CD2	1:A:280:HIS:C	2.93	0.41
1:C:155:TYR:CE1	1:C:192:PHE:HZ	2.39	0.41
1:C:2:ARG:NH2	1:C:83:ARG:HH22	2.18	0.41
1:B:239:VAL:HG21	1:B:255:THR:HG22	2.03	0.41
1:A:187:PRO:HB3	1:A:226:PHE:CE1	2.56	0.40
1:A:208:ASP:OD1	1:A:211:THR:HB	2.21	0.40
1:A:96:LEU:HB3	1:A:196:VAL:HG13	2.03	0.40
1:B:115:VAL:O	1:B:116:VAL:C	2.58	0.40
1:D:218:TYR:HD1	1:D:283:VAL:CG1	2.34	0.40
1:D:44:ARG:NH2	2:D:402:SO4:O1	2.54	0.40
1:D:35:THR:CG2	1:D:64:LEU:HB3	2.42	0.40
1:B:144:GLY:O	1:B:156:CYS:HA	2.22	0.40
1:C:239:VAL:HG21	1:C:255:THR:CG2	2.49	0.40
1:C:252:ARG:HG3	1:C:252:ARG:NH1	2.36	0.40
1:C:25:ASP:HA	1:C:26:PRO:HD3	1.93	0.40
1:C:7:ILE:HG23	1:C:88:VAL:HB	2.02	0.40
1:D:136:ARG:NH1	1:D:249:PRO:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LEU:O	1:D:175:PRO:HD2	2.21	0.40
1:B:106:ALA:O	1:B:110:VAL:HG23	2.21	0.40
1:C:188:VAL:HG12	1:C:190:THR:HG23	2.03	0.40
1:C:239:VAL:CG2	1:C:255:THR:HG22	2.50	0.40
1:D:35:THR:HG21	1:D:64:LEU:HD13	2.03	0.40
1:A:137:VAL:O	1:A:180:LEU:HA	2.20	0.40
1:B:204:LEU:HD23	1:B:212:PHE:CD2	2.57	0.40
1:B:244:LEU:C	1:B:244:LEU:HD12	2.41	0.40
1:C:16:LEU:HD21	1:C:48:ALA:CB	2.51	0.40
1:D:246:ALA:O	1:D:249:PRO:HD3	2.21	0.40
1:A:192:PHE:CE2	3:A:351:EST:H161	2.56	0.40
1:A:269:ASP:OD2	1:A:274:ASN:HB2	2.21	0.40
1:B:166:CYS:HB3	1:B:180:LEU:CD2	2.51	0.40
1:B:141:GLY:N	1:B:183:ILE:O	2.51	0.40
1:B:218:TYR:O	1:B:219:LEU:C	2.58	0.40
1:C:87:LEU:HD22	1:C:125:PHE:HB2	2.02	0.40
1:D:180:LEU:O	1:D:180:LEU:HD23	2.21	0.40
1:C:271:SER:HA	1:D:252:ARG:HB2	2.04	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	277/327 (85%)	245 (88%)	31 (11%)	1 (0%)	38	66
1	B	276/327 (84%)	246 (89%)	25 (9%)	5 (2%)	10	25
1	C	283/327 (86%)	253 (89%)	25 (9%)	5 (2%)	10	25
1	D	277/327 (85%)	250 (90%)	26 (9%)	1 (0%)	38	66
All	All	1113/1308 (85%)	994 (89%)	107 (10%)	12 (1%)	17	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	197	LEU
1	C	199	SER
1	C	271	SER
1	D	174	LEU
1	C	270	PRO
1	B	34	ALA
1	B	127	PRO
1	B	258	ARG
1	C	151	PHE
1	A	174	LEU
1	B	2	ARG
1	B	151	PHE

### 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	231/258 (90%)	205 (89%)	26 (11%)	7	16
1	B	231/258 (90%)	196 (85%)	35 (15%)	3	8
1	C	235/258 (91%)	199 (85%)	36 (15%)	3	8
1	D	232/258 (90%)	205 (88%)	27 (12%)	6	15
All	All	929/1032 (90%)	805 (87%)	124 (13%)	4	11

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	63	GLN
1	A	78	ARG
1	A	81	GLU
1	A	83	ARG
1	A	105	ASP
1	A	143	VAL
1	A	153	ASP
1	A	169	LEU
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	181	SER
1	A	195	LYS
1	A	196	VAL
1	A	204	LEU
1	A	206	ARG
1	A	210	HIS
1	A	221	LEU
1	A	222	SER
1	A	224	GLN
1	A	238	GLU
1	A	244	LEU
1	A	263	LEU
1	A	265	MET
1	A	271	SER
1	A	279	MET
1	A	284	PHE
1	B	2	ARG
1	B	18	LEU
1	B	20	VAL
1	B	21	ARG
1	B	40	LYS
1	B	45	LEU
1	B	50	ARG
1	B	67	ARG
1	B	69	SER
1	B	71	SER
1	B	78	ARG
1	B	96	LEU
1	B	104	GLU
1	B	109	SER
1	B	114	ASN
1	B	120	ARG
1	B	129	MET
1	B	131	ARG
1	B	134	SER
1	B	136	ARG
1	B	153	ASP
1	B	176	PHE
1	B	203	VAL
1	B	204	LEU
1	B	207	THR
1	B	221	LEU

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Mol	Chain	Res	Type
1	B	222	SER
1	B	238	GLU
1	B	241	LEU
1	B	244	LEU
1	B	248	LYS
1	B	257	GLU
1	B	263	LEU
1	B	269	ASP
1	B	271	SER
1	C	2	ARG
1	C	28	GLN
1	C	29	SER
1	C	31	LYS
1	C	39	LEU
1	C	63	GLN
1	C	69	SER
1	C	81	GLU
1	C	83	ARG
1	C	109	SER
1	C	123	GLN
1	C	131	ARG
1	C	132	ARG
1	C	153	ASP
1	C	173	LEU
1	C	174	LEU
1	C	182	LEU
1	C	195	LYS
1	C	197	LEU
1	C	199	SER
1	C	204	LEU
1	C	206	ARG
1	C	222	SER
1	C	224	GLN
1	C	226	PHE
1	C	227	ARG
1	C	234	GLU
1	C	238	GLU
1	C	241	LEU
1	C	244	LEU
1	C	256	THR
1	C	257	GLU
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	265	MET
1	C	266	ARG
1	C	269	ASP
1	D	2	ARG
1	D	35	THR
1	D	45	LEU
1	D	67	ARG
1	D	76	ARG
1	D	83	ARG
1	D	104	GLU
1	D	109	SER
1	D	126	LEU
1	D	127	PRO
1	D	134	SER
1	D	142	SER
1	D	153	ASP
1	D	174	LEU
1	D	197	LEU
1	D	204	LEU
1	D	206	ARG
1	D	209	ILE
1	D	221	LEU
1	D	250	THR
1	D	256	THR
1	D	260	LEU
1	D	262	LEU
1	D	263	LEU
1	D	268	ASP
1	D	269	ASP
1	D	281	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	123	GLN
1	A	179	HIS
1	A	189	HIS
1	A	274	ASN
1	A	280	HIS
1	B	17	HIS
1	B	42	GLN

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	189	HIS
1	B	210	HIS
1	B	274	ASN
1	B	280	HIS
1	C	17	HIS
1	C	42	GLN
1	C	123	GLN
1	C	152	ASN
1	C	179	HIS
1	C	189	HIS
1	C	224	GLN
1	C	231	GLN
1	C	274	ASN
1	D	17	HIS
1	D	42	GLN
1	D	123	GLN
1	D	152	ASN
1	D	189	HIS
1	D	213	HIS
1	D	224	GLN
1	D	231	GLN
1	D	274	ASN
1	D	280	HIS

### 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 ⓘ

12 ligands are modelled in this entry.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	EST	A	351	-	23,23,23	0.80	1 (4%)	36,36,36	2.41	16 (44%)
4	NAP	A	361	-	44,52,52	1.95	8 (18%)	51,80,80	2.00	8 (15%)
2	SO4	A	401	-	4,4,4	0.81	0	6,6,6	0.87	0
3	EST	B	354	-	23,23,23	1.08	1 (4%)	36,36,36	2.65	11 (30%)
4	NAP	B	364	-	44,52,52	1.67	5 (11%)	51,80,80	2.00	10 (19%)
2	SO4	B	400	-	4,4,4	0.79	0	6,6,6	0.62	0
3	EST	C	353	-	23,23,23	0.78	0	36,36,36	1.85	9 (25%)
4	NAP	C	363	-	44,52,52	1.89	7 (15%)	51,80,80	2.00	6 (11%)
2	SO4	C	403	-	4,4,4	0.69	0	6,6,6	0.64	0
3	EST	D	352	-	23,23,23	1.11	1 (4%)	36,36,36	2.37	15 (41%)
4	NAP	D	362	-	44,52,52	1.70	5 (11%)	51,80,80	1.98	6 (11%)
2	SO4	D	402	-	4,4,4	0.68	0	6,6,6	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EST	A	351	-	-	0/0/40/40	0/4/4/4
4	NAP	A	361	-	-	0/27/67/67	0/5/5/5
2	SO4	A	401	-	-	0/0/0/0	0/0/0/0
3	EST	B	354	-	-	0/0/40/40	0/4/4/4
4	NAP	B	364	-	-	0/27/67/67	0/5/5/5
2	SO4	B	400	-	-	0/0/0/0	0/0/0/0
3	EST	C	353	-	-	0/0/40/40	0/4/4/4
4	NAP	C	363	-	-	0/27/67/67	0/5/5/5
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
3	EST	D	352	-	-	0/0/40/40	0/4/4/4
4	NAP	D	362	-	-	0/27/67/67	0/5/5/5
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	361	NAP	P2B-O2B	-10.27	1.41	1.59
4	C	363	NAP	P2B-O2B	-9.78	1.42	1.59
4	D	362	NAP	P2B-O2B	-8.34	1.45	1.59
4	B	364	NAP	P2B-O2B	-8.08	1.45	1.59
4	D	362	NAP	P2B-O3X	-3.11	1.42	1.54
4	C	363	NAP	P2B-O1X	-3.10	1.40	1.50
4	B	364	NAP	P2B-O3X	-3.07	1.42	1.54
4	C	363	NAP	P2B-O3X	-2.99	1.42	1.54
4	D	362	NAP	P2B-O1X	-2.96	1.40	1.50
4	C	363	NAP	P2B-O2X	-2.67	1.43	1.54
4	A	361	NAP	P2B-O3X	-2.62	1.44	1.54
4	D	362	NAP	P2B-O2X	-2.51	1.44	1.54
4	B	364	NAP	P2B-O2X	-2.47	1.44	1.54
4	A	361	NAP	P2B-O2X	-2.30	1.45	1.54
4	D	362	NAP	C5A-N7A	-2.28	1.31	1.39
4	A	361	NAP	PA-O2A	-2.28	1.43	1.55
4	B	364	NAP	P2B-O1X	-2.26	1.43	1.50
4	C	363	NAP	PA-O2A	-2.22	1.43	1.55
4	A	361	NAP	O4B-C1B	-2.17	1.38	1.41
4	A	361	NAP	C5A-N7A	-2.16	1.32	1.39
4	A	361	NAP	P2B-O1X	-2.10	1.43	1.50
3	A	351	EST	C12-C11	2.00	1.57	1.53
4	C	363	NAP	O4D-C1D	2.03	1.44	1.41
3	B	354	EST	C9-C8	2.04	1.56	1.54
4	C	363	NAP	C6N-N1N	2.04	1.40	1.35
4	B	364	NAP	C3N-C7N	2.15	1.53	1.50
4	A	361	NAP	C6N-N1N	2.27	1.41	1.35
3	D	352	EST	C4-C3	2.36	1.42	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	364	NAP	N3A-C2A-N1A	-10.28	119.91	128.86
4	C	363	NAP	N3A-C2A-N1A	-9.87	120.26	128.86
4	A	361	NAP	N3A-C2A-N1A	-9.62	120.48	128.86
4	D	362	NAP	N3A-C2A-N1A	-9.61	120.49	128.86
4	C	363	NAP	O4B-C1B-C2B	-4.62	98.51	106.59
4	D	362	NAP	C3N-C7N-N7N	-4.24	112.94	117.77
3	A	351	EST	C18-C13-C17	-3.97	103.38	109.53
3	D	352	EST	C18-C13-C17	-3.93	103.44	109.53
4	C	363	NAP	C3B-C2B-C1B	-3.75	95.41	102.75
4	C	363	NAP	O7N-C7N-N7N	-3.73	117.28	122.58
4	B	364	NAP	C2D-C3D-C4D	-3.70	95.41	102.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	353	EST	C18-C13-C17	-3.52	104.08	109.53
4	D	362	NAP	O3D-C3D-C4D	-3.36	101.28	111.09
4	A	361	NAP	O7N-C7N-N7N	-3.25	117.96	122.58
3	A	351	EST	C18-C13-C12	-3.22	105.33	110.59
3	D	352	EST	C16-C17-C13	-3.18	101.97	104.53
4	B	364	NAP	O3D-C3D-C4D	-3.02	102.26	111.09
3	A	351	EST	C1-C10-C5	-2.90	115.18	118.74
3	B	354	EST	C16-C17-C13	-2.75	102.31	104.53
3	B	354	EST	C3-C4-C5	-2.70	118.01	120.79
3	B	354	EST	C13-C14-C8	-2.65	110.34	114.39
3	D	352	EST	C11-C9-C10	-2.49	110.91	113.77
4	B	364	NAP	O4D-C4D-C3D	-2.48	100.24	105.17
3	A	351	EST	C11-C12-C13	-2.44	108.55	112.80
3	B	354	EST	C18-C13-C17	-2.43	105.76	109.53
4	B	364	NAP	O7N-C7N-N7N	-2.42	119.13	122.58
4	B	364	NAP	C5D-C4D-C3D	-2.41	106.12	115.29
3	D	352	EST	C12-C13-C17	-2.29	111.87	115.24
4	A	361	NAP	O4B-C1B-C2B	-2.28	102.61	106.59
4	B	364	NAP	C1B-N9A-C4A	-2.12	122.97	126.64
4	C	363	NAP	C5N-C6N-N1N	-2.12	117.14	120.40
3	A	351	EST	C6-C5-C10	-2.11	118.15	121.14
3	C	353	EST	C11-C12-C13	-2.08	109.18	112.80
3	D	352	EST	C3-C4-C5	-2.05	118.68	120.79
3	D	352	EST	C18-C13-C12	2.00	113.86	110.59
4	A	361	NAP	O3X-P2B-O1X	2.04	118.49	110.50
4	B	364	NAP	O3X-P2B-O2B	2.06	115.36	106.00
3	A	351	EST	C15-C14-C8	2.06	122.34	119.07
3	C	353	EST	C7-C6-C5	2.08	116.73	112.86
3	D	352	EST	C12-C13-C14	2.13	110.61	107.27
4	B	364	NAP	O2A-PA-O1A	2.24	123.89	112.28
3	A	351	EST	C9-C8-C14	2.40	112.32	108.81
4	B	364	NAP	C3N-C2N-N1N	2.41	122.86	120.43
3	D	352	EST	O17-C17-C16	2.42	117.12	111.56
3	A	351	EST	C7-C6-C5	2.58	117.65	112.86
3	D	352	EST	C18-C13-C14	2.66	116.76	111.73
4	D	362	NAP	C3N-C2N-N1N	2.69	123.14	120.43
4	A	361	NAP	O2N-PN-O1N	2.77	126.62	112.28
3	C	353	EST	C10-C9-C8	2.78	114.85	111.53
4	D	362	NAP	O2A-PA-O1A	2.86	127.08	112.28
3	B	354	EST	O17-C17-C13	2.86	120.49	114.79
4	C	363	NAP	O7N-C7N-C3N	2.87	122.97	119.62
3	D	352	EST	C9-C8-C14	2.92	113.08	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	361	NAP	C3N-C7N-N7N	2.95	121.14	117.77
3	A	351	EST	C15-C14-C13	2.96	107.48	103.83
3	C	353	EST	C15-C14-C8	3.05	123.92	119.07
3	B	354	EST	C10-C9-C8	3.08	115.21	111.53
3	C	353	EST	C14-C13-C17	3.15	102.49	99.24
3	B	354	EST	C6-C7-C8	3.18	115.13	110.64
3	D	352	EST	C7-C6-C5	3.23	118.86	112.86
3	C	353	EST	C11-C9-C8	3.29	115.85	111.33
3	A	351	EST	C7-C8-C14	3.33	117.64	112.05
3	A	351	EST	C14-C13-C17	3.45	102.79	99.24
3	A	351	EST	C12-C13-C17	3.47	120.36	115.24
3	C	353	EST	C9-C8-C14	3.59	114.05	108.81
4	A	361	NAP	C4B-O4B-C1B	3.64	113.65	109.77
3	A	351	EST	C18-C13-C14	3.68	118.70	111.73
4	A	361	NAP	C4D-O4D-C1D	3.89	113.91	109.77
3	D	352	EST	C10-C9-C8	4.04	116.35	111.53
3	A	351	EST	C7-C8-C9	4.25	113.43	109.28
3	D	352	EST	C7-C8-C14	4.52	119.64	112.05
3	C	353	EST	C7-C8-C14	4.62	119.81	112.05
3	A	351	EST	C16-C17-C13	5.11	108.63	104.53
3	A	351	EST	C6-C7-C8	5.34	118.16	110.64
3	B	354	EST	C15-C14-C8	5.55	127.90	119.07
3	B	354	EST	C11-C12-C13	5.61	122.57	112.80
3	D	352	EST	C15-C14-C8	5.63	128.03	119.07
3	D	352	EST	C6-C7-C8	5.65	118.60	110.64
3	B	354	EST	C12-C11-C9	5.79	118.83	112.23
4	D	362	NAP	O7N-C7N-C3N	5.80	126.41	119.62
3	B	354	EST	C7-C8-C14	8.47	126.28	112.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	EST	10	0
4	A	361	NAP	6	0
3	B	354	EST	6	0
4	B	364	NAP	5	0
3	C	353	EST	3	0
4	C	363	NAP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	SO4	2	0
3	D	352	EST	6	0
4	D	362	NAP	5	0
2	D	402	SO4	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	281/327 (85%)	-0.27	7 (2%) 58 58	8, 23, 48, 55	10 (3%)
1	B	280/327 (85%)	-0.35	4 (1%) 75 76	8, 22, 44, 52	13 (4%)
1	C	285/327 (87%)	-0.15	4 (1%) 75 76	8, 23, 49, 56	11 (3%)
1	D	281/327 (85%)	-0.36	6 (2%) 64 65	10, 23, 45, 50	10 (3%)
All	All	1127/1308 (86%)	-0.28	21 (1%) 67 68	8, 23, 47, 56	44 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	LEU	5.8
1	A	285	GLY	4.2
1	D	2	ARG	3.7
1	D	1	ALA	3.7
1	D	197	LEU	3.4
1	B	1	ALA	3.4
1	D	202	GLU	3.2
1	B	203	VAL	2.6
1	A	265	MET	2.6
1	C	285	GLY	2.5
1	A	2	ARG	2.4
1	A	248	LYS	2.3
1	C	1	ALA	2.3
1	A	246	ALA	2.2
1	B	2	ARG	2.2
1	D	268	ASP	2.2
1	A	1	ALA	2.2
1	D	245	ARG	2.2
1	A	227	ARG	2.1
1	B	264	ARG	2.0
1	C	264	ARG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EST	B	354	20/20	0.73	0.31	6.78	56,58,59,59	0
3	EST	D	352	20/20	0.79	0.30	6.52	47,50,51,51	0
3	EST	A	351	20/20	0.81	0.30	3.62	48,50,51,52	0
2	SO4	A	401	5/5	0.95	0.19	3.54	42,43,43,43	0
3	EST	C	353	20/20	0.83	0.29	2.85	61,63,64,64	1
2	SO4	D	402	5/5	0.98	0.17	0.70	42,43,43,43	0
2	SO4	C	403	5/5	0.95	0.17	0.13	43,43,44,44	0
2	SO4	B	400	5/5	0.97	0.13	-0.32	46,47,47,47	0
4	NAP	A	361	48/48	0.97	0.12	-0.51	13,16,19,21	0
4	NAP	D	362	48/48	0.97	0.12	-0.54	12,17,21,22	0
4	NAP	C	363	48/48	0.97	0.12	-0.68	13,17,21,23	0
4	NAP	B	364	48/48	0.97	0.12	-0.89	10,17,21,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.