



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:29 pm BST

PDB ID : 6MSO  
Title : Crystal structure of mitochondrial fumarate hydratase from Leishmania major in a complex with inhibitor thiomalate  
Authors : Feliciano, P.R.; Drennan, C.L.; Nonato, M.C.  
Deposited on : 2018-10-17  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

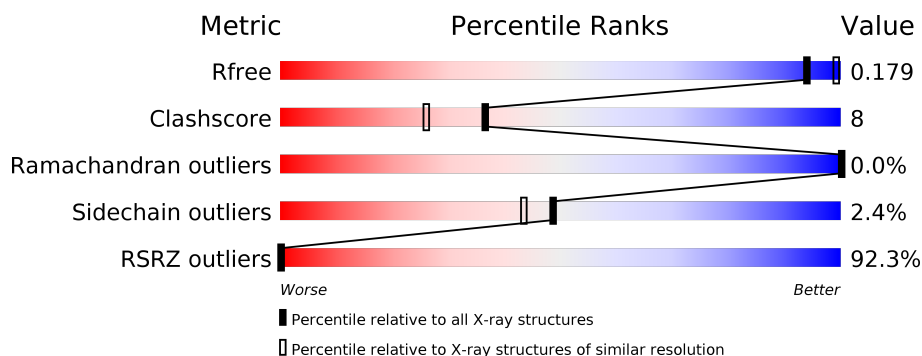
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	585	<div> <div>82%</div> <div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	B	585	<div> <div>82%</div> <div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
1	C	585	<div> <div>88%</div> <div> <div>69%</div> <div>20%</div> <div>10%</div> </div> </div>
1	D	585	<div> <div>86%</div> <div> <div>75%</div> <div>16%</div> <div>9%</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
3	GOL	A	604	-	-	-	X
3	GOL	A	605	-	-	-	X
3	GOL	A	606	-	-	-	X
3	GOL	C	602	-	-	-	X
4	1PE	A	607	-	-	-	X
4	1PE	B	605	-	-	-	X
4	1PE	B	606	-	-	-	X
5	JYD	C	604	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17547 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 fumarate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	3	0
			4169	2644	715	780	30			
1	B	540	Total	C	N	O	S	0	4	0
			4174	2649	712	780	33			
1	C	528	Total	C	N	O	S	0	3	0
			4055	2573	698	755	29			
1	D	531	Total	C	N	O	S	0	2	0
			4039	2562	693	755	29			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q4QAU9
A	-34	GLY	-	expression tag	UNP Q4QAU9
A	-33	SER	-	expression tag	UNP Q4QAU9
A	-32	SER	-	expression tag	UNP Q4QAU9
A	-31	HIS	-	expression tag	UNP Q4QAU9
A	-30	HIS	-	expression tag	UNP Q4QAU9
A	-29	HIS	-	expression tag	UNP Q4QAU9
A	-28	HIS	-	expression tag	UNP Q4QAU9
A	-27	HIS	-	expression tag	UNP Q4QAU9
A	-26	HIS	-	expression tag	UNP Q4QAU9
A	-25	SER	-	expression tag	UNP Q4QAU9
A	-24	SER	-	expression tag	UNP Q4QAU9
A	-23	GLY	-	expression tag	UNP Q4QAU9
A	-22	LEU	-	expression tag	UNP Q4QAU9
A	-21	VAL	-	expression tag	UNP Q4QAU9
A	-20	PRO	-	expression tag	UNP Q4QAU9
A	-19	ARG	-	expression tag	UNP Q4QAU9
A	-18	GLY	-	expression tag	UNP Q4QAU9
A	-17	SER	-	expression tag	UNP Q4QAU9
A	-16	HIS	-	expression tag	UNP Q4QAU9
A	-15	MET	-	expression tag	UNP Q4QAU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP Q4QAU9
A	-13	SER	-	expression tag	UNP Q4QAU9
A	-12	MET	-	expression tag	UNP Q4QAU9
A	-11	THR	-	expression tag	UNP Q4QAU9
A	-10	GLY	-	expression tag	UNP Q4QAU9
A	-9	GLY	-	expression tag	UNP Q4QAU9
A	-8	GLN	-	expression tag	UNP Q4QAU9
A	-7	GLN	-	expression tag	UNP Q4QAU9
A	-6	MET	-	expression tag	UNP Q4QAU9
A	-5	GLY	-	expression tag	UNP Q4QAU9
A	-4	ARG	-	expression tag	UNP Q4QAU9
A	-3	GLY	-	expression tag	UNP Q4QAU9
A	-2	SER	-	expression tag	UNP Q4QAU9
A	-1	GLU	-	expression tag	UNP Q4QAU9
A	0	PHE	-	expression tag	UNP Q4QAU9
B	-35	MET	-	initiating methionine	UNP Q4QAU9
B	-34	GLY	-	expression tag	UNP Q4QAU9
B	-33	SER	-	expression tag	UNP Q4QAU9
B	-32	SER	-	expression tag	UNP Q4QAU9
B	-31	HIS	-	expression tag	UNP Q4QAU9
B	-30	HIS	-	expression tag	UNP Q4QAU9
B	-29	HIS	-	expression tag	UNP Q4QAU9
B	-28	HIS	-	expression tag	UNP Q4QAU9
B	-27	HIS	-	expression tag	UNP Q4QAU9
B	-26	HIS	-	expression tag	UNP Q4QAU9
B	-25	SER	-	expression tag	UNP Q4QAU9
B	-24	SER	-	expression tag	UNP Q4QAU9
B	-23	GLY	-	expression tag	UNP Q4QAU9
B	-22	LEU	-	expression tag	UNP Q4QAU9
B	-21	VAL	-	expression tag	UNP Q4QAU9
B	-20	PRO	-	expression tag	UNP Q4QAU9
B	-19	ARG	-	expression tag	UNP Q4QAU9
B	-18	GLY	-	expression tag	UNP Q4QAU9
B	-17	SER	-	expression tag	UNP Q4QAU9
B	-16	HIS	-	expression tag	UNP Q4QAU9
B	-15	MET	-	expression tag	UNP Q4QAU9
B	-14	ALA	-	expression tag	UNP Q4QAU9
B	-13	SER	-	expression tag	UNP Q4QAU9
B	-12	MET	-	expression tag	UNP Q4QAU9
B	-11	THR	-	expression tag	UNP Q4QAU9
B	-10	GLY	-	expression tag	UNP Q4QAU9
B	-9	GLY	-	expression tag	UNP Q4QAU9

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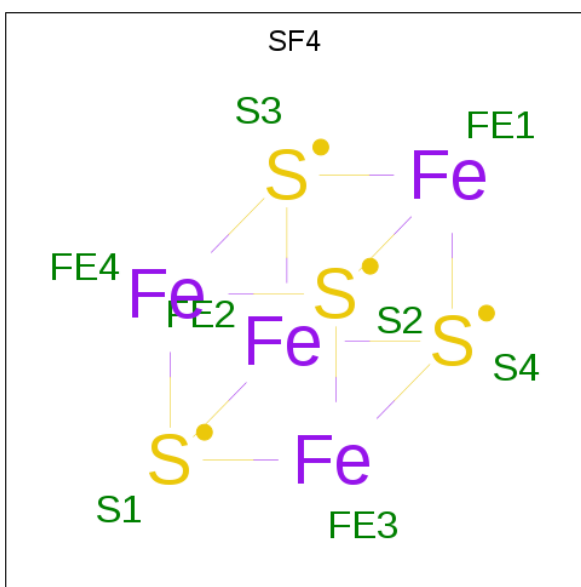
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLN	-	expression tag	UNP Q4QAU9
B	-7	GLN	-	expression tag	UNP Q4QAU9
B	-6	MET	-	expression tag	UNP Q4QAU9
B	-5	GLY	-	expression tag	UNP Q4QAU9
B	-4	ARG	-	expression tag	UNP Q4QAU9
B	-3	GLY	-	expression tag	UNP Q4QAU9
B	-2	SER	-	expression tag	UNP Q4QAU9
B	-1	GLU	-	expression tag	UNP Q4QAU9
B	0	PHE	-	expression tag	UNP Q4QAU9
C	-35	MET	-	initiating methionine	UNP Q4QAU9
C	-34	GLY	-	expression tag	UNP Q4QAU9
C	-33	SER	-	expression tag	UNP Q4QAU9
C	-32	SER	-	expression tag	UNP Q4QAU9
C	-31	HIS	-	expression tag	UNP Q4QAU9
C	-30	HIS	-	expression tag	UNP Q4QAU9
C	-29	HIS	-	expression tag	UNP Q4QAU9
C	-28	HIS	-	expression tag	UNP Q4QAU9
C	-27	HIS	-	expression tag	UNP Q4QAU9
C	-26	HIS	-	expression tag	UNP Q4QAU9
C	-25	SER	-	expression tag	UNP Q4QAU9
C	-24	SER	-	expression tag	UNP Q4QAU9
C	-23	GLY	-	expression tag	UNP Q4QAU9
C	-22	LEU	-	expression tag	UNP Q4QAU9
C	-21	VAL	-	expression tag	UNP Q4QAU9
C	-20	PRO	-	expression tag	UNP Q4QAU9
C	-19	ARG	-	expression tag	UNP Q4QAU9
C	-18	GLY	-	expression tag	UNP Q4QAU9
C	-17	SER	-	expression tag	UNP Q4QAU9
C	-16	HIS	-	expression tag	UNP Q4QAU9
C	-15	MET	-	expression tag	UNP Q4QAU9
C	-14	ALA	-	expression tag	UNP Q4QAU9
C	-13	SER	-	expression tag	UNP Q4QAU9
C	-12	MET	-	expression tag	UNP Q4QAU9
C	-11	THR	-	expression tag	UNP Q4QAU9
C	-10	GLY	-	expression tag	UNP Q4QAU9
C	-9	GLY	-	expression tag	UNP Q4QAU9
C	-8	GLN	-	expression tag	UNP Q4QAU9
C	-7	GLN	-	expression tag	UNP Q4QAU9
C	-6	MET	-	expression tag	UNP Q4QAU9
C	-5	GLY	-	expression tag	UNP Q4QAU9
C	-4	ARG	-	expression tag	UNP Q4QAU9
C	-3	GLY	-	expression tag	UNP Q4QAU9

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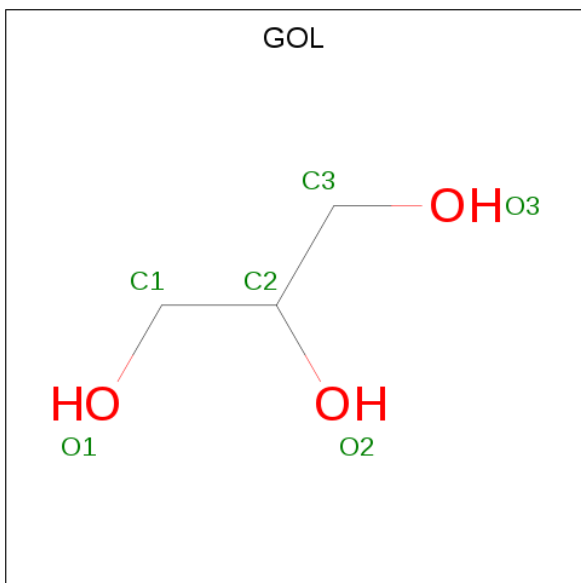
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q4QAU9
C	-1	GLU	-	expression tag	UNP Q4QAU9
C	0	PHE	-	expression tag	UNP Q4QAU9
D	-35	MET	-	initiating methionine	UNP Q4QAU9
D	-34	GLY	-	expression tag	UNP Q4QAU9
D	-33	SER	-	expression tag	UNP Q4QAU9
D	-32	SER	-	expression tag	UNP Q4QAU9
D	-31	HIS	-	expression tag	UNP Q4QAU9
D	-30	HIS	-	expression tag	UNP Q4QAU9
D	-29	HIS	-	expression tag	UNP Q4QAU9
D	-28	HIS	-	expression tag	UNP Q4QAU9
D	-27	HIS	-	expression tag	UNP Q4QAU9
D	-26	HIS	-	expression tag	UNP Q4QAU9
D	-25	SER	-	expression tag	UNP Q4QAU9
D	-24	SER	-	expression tag	UNP Q4QAU9
D	-23	GLY	-	expression tag	UNP Q4QAU9
D	-22	LEU	-	expression tag	UNP Q4QAU9
D	-21	VAL	-	expression tag	UNP Q4QAU9
D	-20	PRO	-	expression tag	UNP Q4QAU9
D	-19	ARG	-	expression tag	UNP Q4QAU9
D	-18	GLY	-	expression tag	UNP Q4QAU9
D	-17	SER	-	expression tag	UNP Q4QAU9
D	-16	HIS	-	expression tag	UNP Q4QAU9
D	-15	MET	-	expression tag	UNP Q4QAU9
D	-14	ALA	-	expression tag	UNP Q4QAU9
D	-13	SER	-	expression tag	UNP Q4QAU9
D	-12	MET	-	expression tag	UNP Q4QAU9
D	-11	THR	-	expression tag	UNP Q4QAU9
D	-10	GLY	-	expression tag	UNP Q4QAU9
D	-9	GLY	-	expression tag	UNP Q4QAU9
D	-8	GLN	-	expression tag	UNP Q4QAU9
D	-7	GLN	-	expression tag	UNP Q4QAU9
D	-6	MET	-	expression tag	UNP Q4QAU9
D	-5	GLY	-	expression tag	UNP Q4QAU9
D	-4	ARG	-	expression tag	UNP Q4QAU9
D	-3	GLY	-	expression tag	UNP Q4QAU9
D	-2	SER	-	expression tag	UNP Q4QAU9
D	-1	GLU	-	expression tag	UNP Q4QAU9
D	0	PHE	-	expression tag	UNP Q4QAU9

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



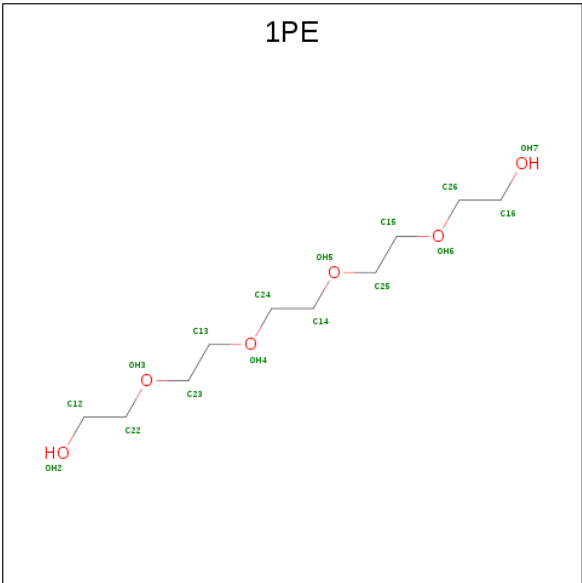
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



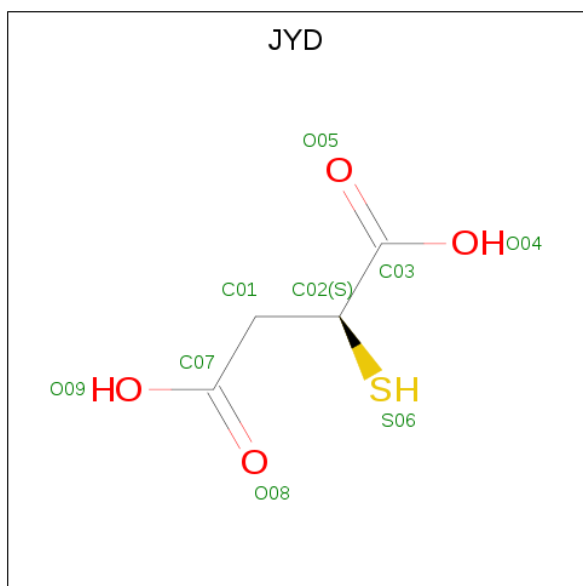
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is (2S)-2-sulfanylbutanedioic acid (three-letter code: JYD) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	1
			18	8	8	2		
5	B	1	Total	C	O	S	0	1
			18	8	8	2		
5	C	1	Total	C	O	S	0	0
			9	4	4	1		
5	D	1	Total	C	O	S	0	0
			9	4	4	1		

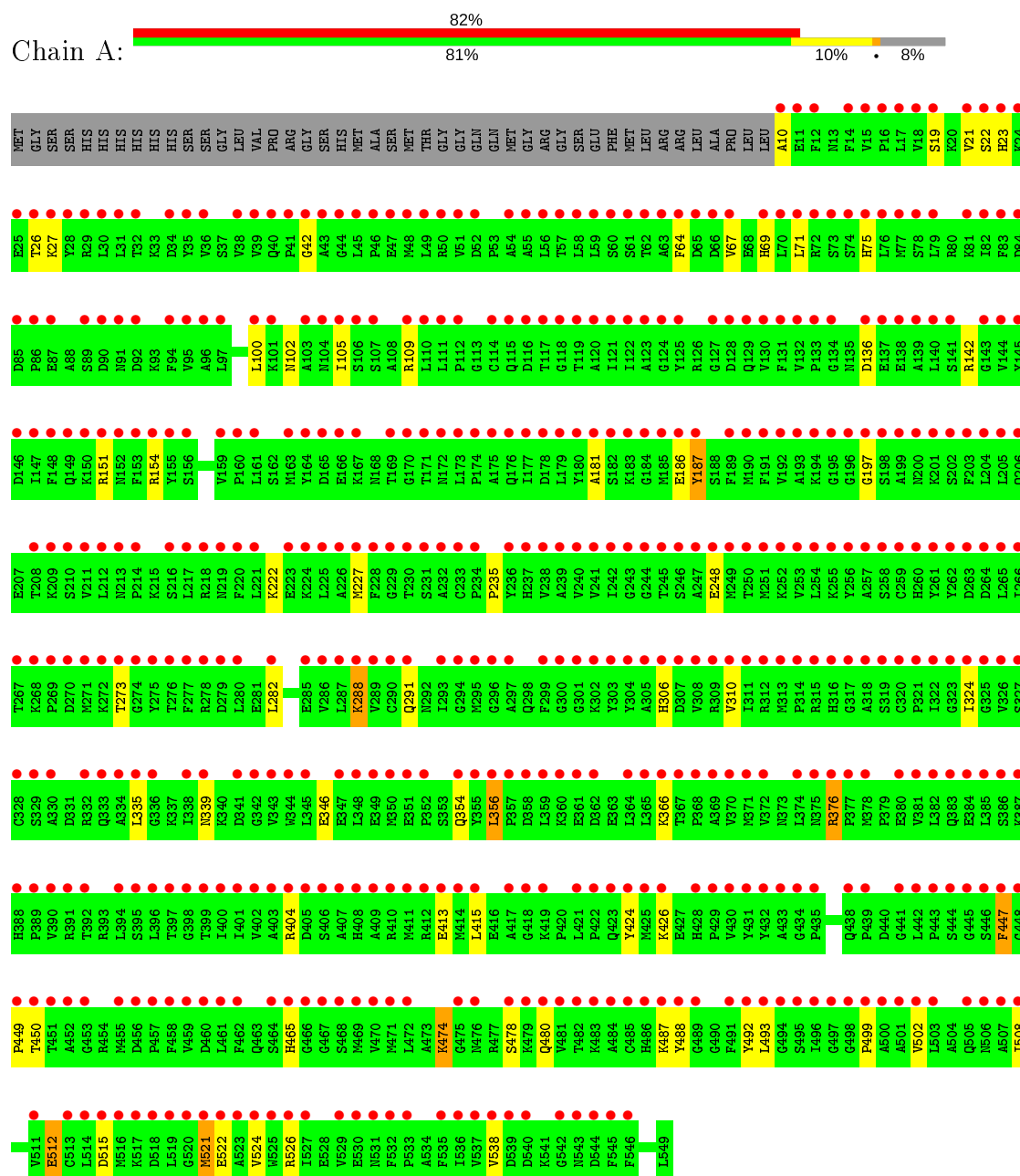
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total 252	O 252	0	1
6	B	282	Total 282	O 282	0	0
6	C	166	Total 167	O 167	0	1
6	D	168	Total 169	O 169	0	1

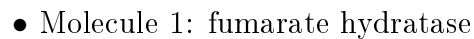
### 3 Residue-property plots

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.

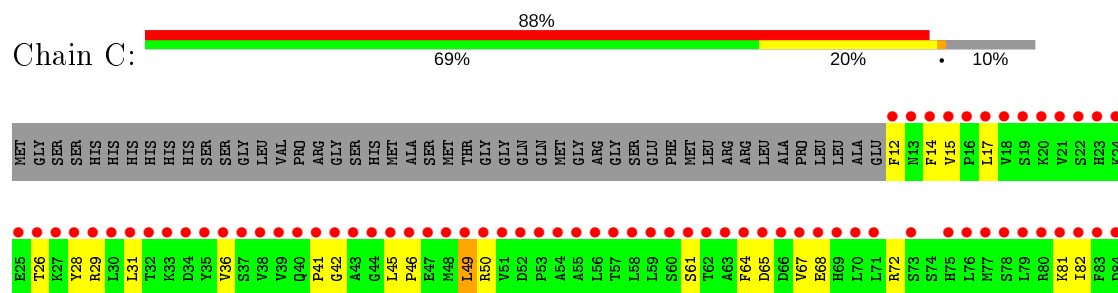
- Molecule 1: fumarate hydratase

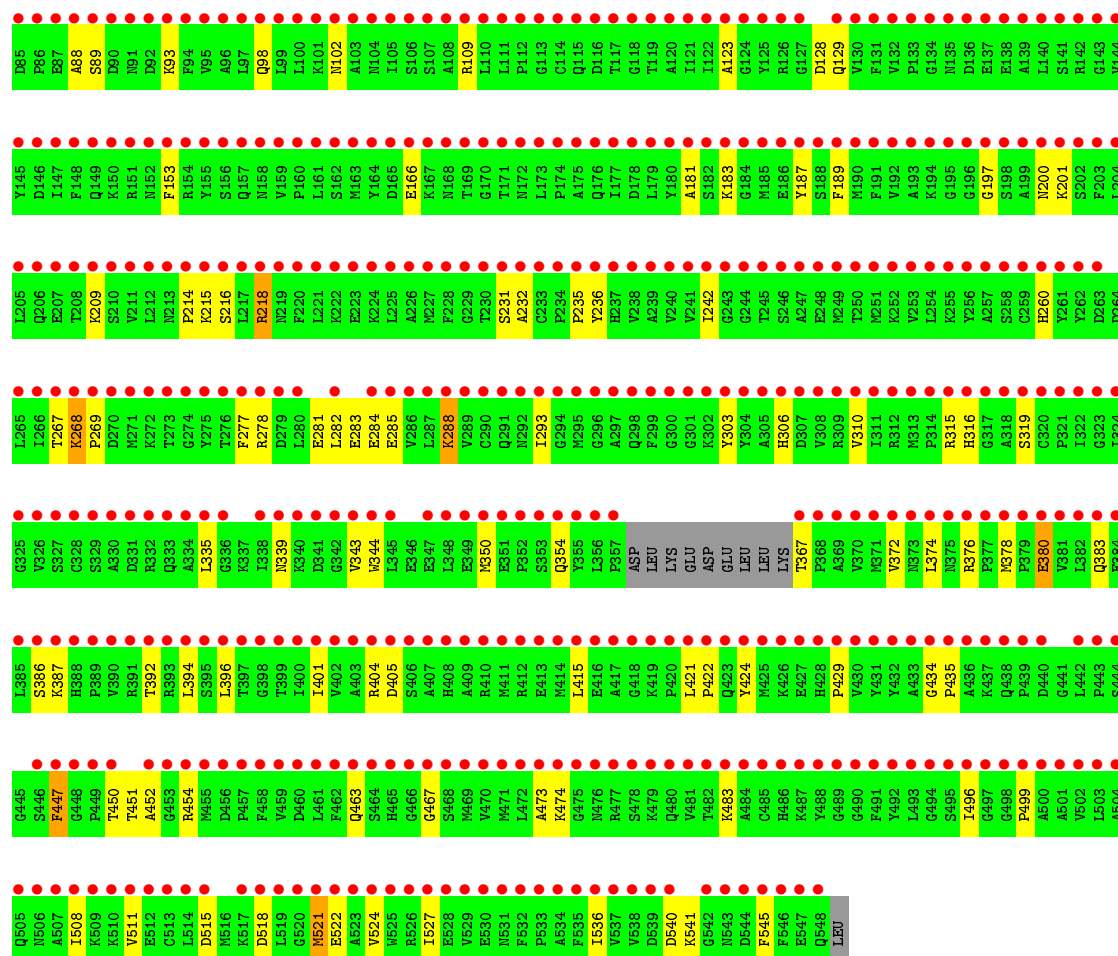


Chain B:

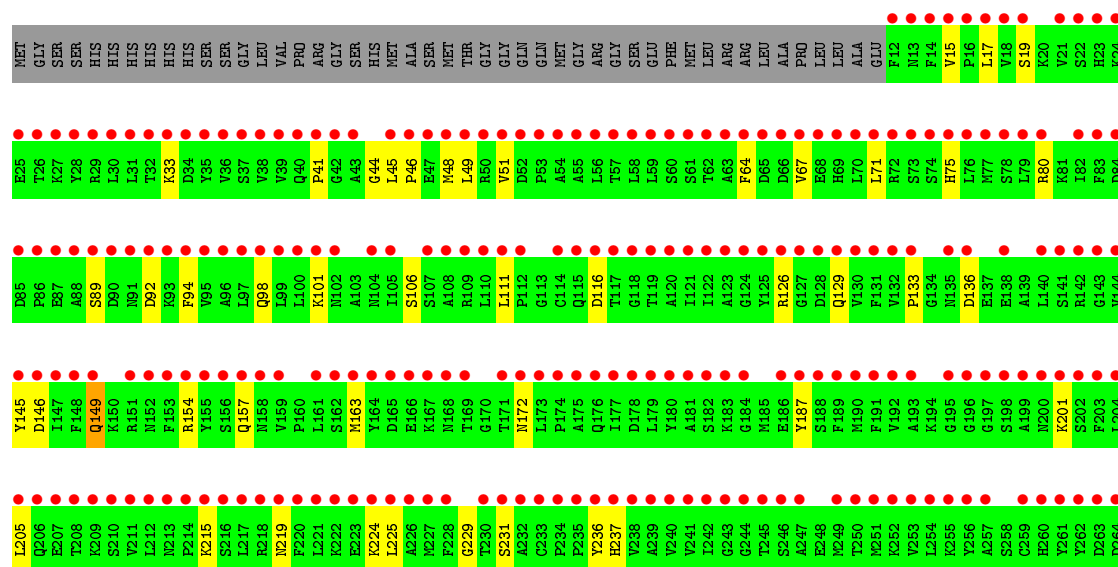
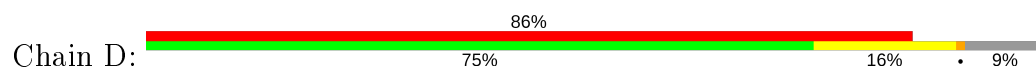


Chain C:





• Molecule 1: fumarate hydratase



Q505	N506	A507	I508	K509	K510	V511	E512	G513	L514	D515	M516	K517	D518	L519	G520	M521	E522	A523	V524	M525	R526	I527	E528	V529	E530	N531	F532	P533	A534	F535	I536	V537	V538	D539	D540	K541	G542	N543	D544	F545	F546	E547	Q548	LEU															
G445	S386	F447	G448	P449	T450	T451	A452	G453	R454	M455	D456	P457	F458	V459	D460	L461	F462	Q463	S464	H465	G466	G467	S468	M469	V470	M471	L472	A473	K474	G475	N476	R477	S478	K479	Q480	V481	T482	K483	A484	C485	H486	K487	Y488	G489	G490	F491	Y492	L493	G494	S495	I496	G497	G498	P499	A500	A501	V502	L503	A504
L385	S386	K387	E388	P389	V390	R391	T392	R393	L394	S395	L396	T397	G398	T399	L400	L401	V402	A403	R404	D405	S406	A407	H408	A409	R410	M411	R412	E413	M414	L415	E416	A417	G418	K419	P420	L421	P422	Q423	Y424	M425	K426	E427	H428	P429	V430	Y431	Y432	A433	G434	P435	A436	K437	Q438	P439	D440	G441	L442	P443	S444
G325	V326	S327	C328	S329	A330	D331	R332	Q333	A334	L335	G336	K337	I338	N339	K340	D341	G342	V343	V344	L345	E346	E347	L348	E349	K350	E351	P352	S353	Q354	Y355	L356	F357	D358	L359	K360	GLU	ASP	GLU	LEU	LEU	LYS	T367	P368	A369	V370	N371	Y372	Y373	L374	R375	R376	F377	N378	P379	E380	V381	L382	Q383	E384
L285	I286	T287	K288	P289	D270	K271	K272	T273	G274	Y275	T276	F277	R278	D279	L280	E281	L282	E283	E284	E285	V286	L287	K288	V289	C290	Q291	N292	I293	G294	K295	G296	A297	Q298	F299	G300	G301	K302	Y303	Y304	A305	H306	D307	V308	K309	V310	I311	R312	K313	P314	R315	R316	G317	A318	S319	C320	P321	I322	G323	I324

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.74Å 138.44Å 138.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 2.05 48.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.88-2.05) 98.1 (48.88-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	341.80 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.159 , 0.204 0.145 , 0.179	Depositor DCC
$R_{free}$ test set	9057 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.418 for -h,-l,-k 0.409 for -h,l,k 0.448 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SF4, JYD, 1PE

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	0.45	0/4259	0.63	0/5761
1	B	0.44	0/4264	0.62	0/5768
1	C	0.41	0/4144	0.63	1/5609 (0.0%)
1	D	0.40	0/4128	0.60	0/5595
All	All	0.43	0/16795	0.62	1/22733 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	LEU	CB-CG-CD1	-5.24	102.09	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4169	0	4113	46	0
1	B	4174	0	4120	62	0
1	C	4055	0	3975	88	0
1	D	4039	0	3915	71	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	0	0	0
2	D	8	0	0	0	0
3	A	30	0	37	3	0
3	B	12	0	15	1	0
3	C	6	0	8	3	0
4	A	40	0	50	4	0
4	B	23	0	29	3	0
4	C	27	0	33	4	0
4	D	16	0	22	4	0
5	A	18	0	0	4	0
5	B	18	0	0	2	0
5	C	9	0	0	2	0
5	D	9	0	0	1	0
6	A	252	0	0	3	0
6	B	282	0	0	8	0
6	C	167	0	0	5	0
6	D	169	0	0	5	0
All	All	17547	0	16317	259	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 8.

All (259) 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:A:413:GLU:HG2	4:A:610:1PE:H152	1.39	1.02
1:C:267:THR:O	1:C:268:LYS:HD2	1.62	1.00
1:B:391:ARG:NH2	6:B:701:HOH:O	2.00	0.91
1:C:521:MET:HE2	1:C:522:GLU:HG2	1.58	0.85
1:A:42:GLY:H	1:B:42:GLY:H	1.23	0.84
1:D:434:GLY:HA3	1:D:521:MET:CE	2.07	0.83
1:C:41:PRO:HB2	1:D:41:PRO:HB2	1.61	0.83
1:D:33:LYS:HD2	4:D:603:1PE:H222	1.64	0.79
1:D:410:ARG:NH1	1:D:518[A]:ASP:OD2	2.16	0.79
1:C:267:THR:O	1:C:268:LYS:CD	2.31	0.77
1:B:509:LYS:HG3	1:B:530:GLU:HG3	1.67	0.74
1:C:166:GLU:OE1	1:D:315:ARG:NE	2.21	0.74
4:D:603:1PE:H241	4:D:603:1PE:H161	1.69	0.73
1:D:477:ARG:HD3	1:D:481:VAL:HG11	1.70	0.73
1:B:399:THR:OG1	1:B:528:GLU:OE2	2.05	0.71
1:C:278:ARG:NE	1:C:283:GLU:OE2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HG2	1:B:339:ASN:HB3	1.74	0.70
1:C:235:PRO:HB2	1:C:306:HIS:CE1	2.28	0.69
1:C:404:ARG:NH1	5:C:604:JYD:O09	2.26	0.68
1:D:404:ARG:HD3	1:D:521:MET:CE	2.23	0.68
3:B:602:GOL:O1	3:B:602:GOL:O3	1.96	0.68
1:A:354:GLN:HG3	4:A:609:1PE:H151	1.77	0.67
1:D:434:GLY:HA3	1:D:521:MET:HE1	1.77	0.66
1:B:198:SER:HB3	1:B:328:CYS:HB3	1.80	0.64
1:D:237:HIS:HB2	1:D:327:SER:HB3	1.80	0.63
1:C:181:ALA:HB1	1:D:126:ARG:CZ	2.28	0.63
1:D:19:SER:HB3	1:D:273:THR:O	1.99	0.62
1:A:186:GLU:HG2	1:A:339:ASN:HB3	1.80	0.62
1:C:31:LEU:HD13	1:C:343:VAL:HG12	1.82	0.62
1:C:109:ARG:NH2	1:C:350:MET:SD	2.73	0.62
1:C:26:THR:HG21	1:C:335:LEU:HD12	1.81	0.61
1:D:410:ARG:HD2	1:D:516:MET:SD	2.40	0.61
1:D:516:MET:HG3	1:D:524:VAL:HG23	1.82	0.61
1:A:424:TYR:OH	1:A:515:ASP:OD2	2.15	0.60
1:D:80:ARG:HD3	1:D:355:TYR:O	2.01	0.60
1:B:499:PRO:HB2	1:B:502:VAL:HG22	1.86	0.58
1:D:145:TYR:O	1:D:149[A]:GLN:HG2	2.03	0.58
1:A:10:ALA:O	1:B:145:TYR:OH	2.12	0.58
1:C:36:VAL:CG1	1:C:49:LEU:HD11	2.33	0.58
1:A:521:MET:SD	1:A:522:GLU:HG2	2.44	0.58
1:D:229:GLY:O	1:D:236:TYR:OH	2.18	0.58
1:C:50:ARG:NH1	1:D:44:GLY:HA3	2.19	0.57
1:D:489:GLY:HA2	1:D:540:ASP:HB2	1.86	0.57
1:D:378:MET:HE1	1:D:429:PRO:HD3	1.85	0.57
1:D:404:ARG:HD3	1:D:521:MET:HE1	1.87	0.57
1:C:61:SER:O	1:C:65:ASP:HB2	2.04	0.57
1:D:374:LEU:HD11	1:D:396:LEU:HB3	1.85	0.57
1:D:452:ALA:HB2	1:D:473:ALA:HB3	1.86	0.57
1:A:288:LYS:HD3	6:A:709:HOH:O	2.05	0.57
1:A:282:LEU:HD23	1:A:310:VAL:HG11	1.87	0.57
1:A:26:THR:HG21	1:A:335:LEU:HD12	1.86	0.56
1:C:515:ASP:HB3	1:C:524:VAL:HB	1.87	0.56
1:B:11:GLU:OE2	1:B:12:PHE:N	2.33	0.56
1:D:402:VAL:HB	1:D:525:TRP:HB2	1.88	0.56
1:D:215:LYS:NZ	1:D:219:ASN:OD1	2.25	0.56
1:D:94:PHE:O	1:D:98:GLN:HG2	2.06	0.56
1:C:434:GLY:HA3	1:C:521:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:TYR:HB3	1:D:538:VAL:HB	1.88	0.55
1:D:434:GLY:HA3	1:D:521:MET:HE3	1.87	0.55
1:C:421:LEU:HD12	1:C:422:PRO:HD2	1.89	0.55
1:B:452:ALA:HB2	1:B:473:ALA:HB3	1.88	0.55
1:C:36:VAL:HG11	1:C:339:ASN:O	2.07	0.55
1:A:105:ILE:HD12	1:A:502:VAL:HG12	1.89	0.55
1:C:282:LEU:HD12	1:C:310:VAL:HG21	1.89	0.54
1:D:154:ARG:HD2	1:D:521:MET:SD	2.47	0.54
1:B:48:MET:CE	6:B:910:HOH:O	2.56	0.54
1:D:518[A]:ASP:OD1	1:D:518[A]:ASP:N	2.40	0.54
1:C:452:ALA:HB2	1:C:473:ALA:HB3	1.90	0.54
1:B:90:ASP:OD1	6:B:702:HOH:O	2.19	0.53
1:B:402:VAL:HB	1:B:525:TRP:HB2	1.91	0.53
1:A:136:ASP:OD2	1:A:187:TYR:OH	2.20	0.53
1:D:205:LEU:HD22	1:D:224:LYS:HE3	1.91	0.53
1:C:129:GLN:NE2	6:C:722:HOH:O	2.41	0.52
1:C:269:PRO:HG3	1:C:277:PHE:CD1	2.44	0.52
1:B:315:ARG:HD2	1:B:319:SER:O	2.09	0.52
1:B:478:SER:OG	1:B:480:GLN:HG2	2.10	0.52
1:C:483:LYS:O	1:C:483:LYS:HD3	2.09	0.52
1:A:19:SER:HB3	1:A:273:THR:O	2.10	0.52
1:D:373:ASN:O	1:D:376:ARG:HD3	2.09	0.52
1:C:315:ARG:HD2	1:C:319:SER:O	2.10	0.52
1:D:537:VAL:HA	1:D:545:PHE:HB2	1.91	0.52
1:C:64:PHE:HA	1:C:67:VAL:HG22	1.92	0.51
1:B:94:PHE:O	1:B:98:GLN:HG2	2.10	0.51
1:C:209:LYS:HD3	1:C:315:ARG:NH2	2.26	0.51
1:C:242:ILE:HG13	1:D:163:MET:CE	2.41	0.51
1:C:450:THR:HG23	1:C:454:ARG:NH1	2.26	0.51
1:D:146:ASP:OD2	6:D:701:HOH:O	2.19	0.51
1:B:512:GLU:OE2	1:B:526:ARG:HB3	2.11	0.50
1:A:71:LEU:HD13	1:A:75:HIS:CD2	2.47	0.50
1:D:404:ARG:NH1	1:D:521:MET:HE1	2.27	0.50
1:A:69:HIS:CD2	1:A:109:ARG:HA	2.47	0.50
1:C:405:ASP:OD2	6:C:701:HOH:O	2.19	0.50
1:C:72:ARG:HD2	6:C:705:HOH:O	2.11	0.50
1:D:390:VAL:HG12	1:D:536:ILE:HG22	1.92	0.50
1:A:478:SER:OG	1:A:480:GLN:HG2	2.13	0.49
1:C:214:PRO:O	1:C:218[B]:ARG:HG2	2.12	0.49
1:C:36:VAL:HG12	1:C:49:LEU:HD11	1.93	0.49
1:C:197:GLY:O	1:C:201[B]:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:PRO:O	1:B:502:VAL:HG22	2.13	0.49
1:C:394:LEU:HD11	1:C:536:ILE:HG13	1.93	0.49
1:D:33:LYS:CD	4:D:603:1PE:H222	2.40	0.49
1:D:89:SER:O	1:D:92:ASP:HB2	2.13	0.49
1:D:352:PRO:HG3	6:D:823:HOH:O	2.13	0.49
1:C:201[A]:LYS:HE2	1:C:231:SER:HB2	1.94	0.49
1:C:374:LEU:HD11	1:C:396:LEU:HB3	1.94	0.49
1:B:104:ASN:OD1	1:B:353:SER:HB3	2.13	0.48
1:C:376:ARG:HB2	1:C:380[A]:GLU:HG2	1.95	0.48
1:B:400:ILE:HG21	1:B:431:TYR:HB2	1.94	0.48
1:B:11:GLU:CD	1:B:12:PHE:H	2.15	0.48
1:C:451:THR:OG1	5:C:604:JYD:O05	2.28	0.48
1:B:48:MET:HE1	6:B:910:HOH:O	2.11	0.48
1:B:391:ARG:HG2	1:B:545:PHE:CE2	2.48	0.48
1:D:154:ARG:CZ	1:D:521:MET:SD	3.01	0.48
1:A:181:ALA:HB1	1:B:126:ARG:NH2	2.28	0.48
1:C:378:MET:HE1	1:C:429:PRO:HD3	1.96	0.48
1:A:248:GLU:OE2	1:B:255:LYS:NZ	2.42	0.48
1:B:509:LYS:NZ	6:B:722:HOH:O	2.40	0.48
1:A:154:ARG:NH1	5:A:608[B]:JYD:O09	2.26	0.48
1:B:11:GLU:CD	1:B:12:PHE:N	2.67	0.48
1:B:250:THR:HG22	1:B:251:MET:HE1	1.96	0.48
1:B:80:ARG:HD3	1:B:355:TYR:O	2.12	0.48
1:A:447:PHE:HB3	1:A:508:ILE:HD13	1.95	0.48
1:D:41:PRO:HG2	1:D:45:LEU:HB2	1.95	0.47
1:B:69:HIS:CD2	1:B:109:ARG:HA	2.49	0.47
1:A:492:TYR:HB3	1:A:538:VAL:HB	1.97	0.47
1:C:281:GLU:O	1:C:285:GLU:HG2	2.14	0.47
1:A:487:LYS:HD2	1:A:488:TYR:CE2	2.50	0.47
1:C:269:PRO:HG3	1:C:277:PHE:CE1	2.49	0.47
1:B:128:ASP:HB2	1:B:183:LYS:HA	1.97	0.47
1:C:447:PHE:HB3	1:C:508:ILE:HD13	1.96	0.47
4:A:609:1PE:H222	4:A:609:1PE:H132	1.60	0.47
1:D:64:PHE:HA	1:D:67:VAL:HG22	1.96	0.47
1:C:284:GLU:O	1:C:288:LYS:HD3	2.15	0.47
1:D:201:LYS:HE3	1:D:231:SER:HB2	1.96	0.47
1:A:515:ASP:HB3	1:A:524:VAL:HB	1.97	0.47
1:B:169:THR:O	6:B:703:HOH:O	2.21	0.47
1:C:278:ARG:NH2	1:C:283:GLU:OE1	2.48	0.47
1:A:499:PRO:O	1:A:502:VAL:HG22	2.15	0.46
1:C:28:TYR:HB3	1:C:344:TRP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:N	1:D:129:GLN:O	2.38	0.46
1:C:12:PHE:CZ	1:C:14:PHE:HB2	2.50	0.46
1:C:293:ILE:HG22	6:C:763:HOH:O	2.15	0.46
1:C:415:LEU:HD21	1:C:421:LEU:HB2	1.96	0.46
1:C:288:LYS:HD2	1:C:288:LYS:N	2.30	0.46
1:B:415:LEU:HD13	1:B:465:HIS:CD2	2.50	0.46
1:C:98:GLN:HG3	1:C:496:ILE:HD13	1.96	0.46
1:A:21:VAL:HG12	1:A:22:SER:O	2.16	0.46
1:C:88:ALA:HB2	1:C:303:TYR:HE2	1.81	0.46
1:A:512:GLU:HG2	1:A:526:ARG:O	2.16	0.46
1:D:471:MET:SD	1:D:477:ARG:NH1	2.84	0.46
1:B:197:GLY:N	5:B:604[B]:JYD:S06	2.87	0.46
1:C:383:GLN:O	1:C:387:LYS:HG3	2.16	0.46
1:A:227:MET:HE3	1:A:324:ILE:HD11	1.98	0.45
1:C:463:GLN:HA	1:C:467:GLY:O	2.16	0.45
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.62	0.45
1:A:447:PHE:HB3	1:A:508:ILE:CD1	2.47	0.45
4:A:611:1PE:H131	4:A:611:1PE:H141	1.60	0.45
1:C:540:ASP:OD2	1:C:541:LYS:NZ	2.37	0.45
1:A:404:ARG:NH1	5:A:608[B]:JYD:O08	2.48	0.45
1:D:101:LYS:HE3	1:D:101:LYS:HB2	1.79	0.45
1:C:386:SER:OG	1:C:540:ASP:OD1	2.18	0.45
1:A:142:ARG:NH1	6:A:719:HOH:O	2.39	0.45
1:C:102:ASN:CG	1:C:499:PRO:HA	2.37	0.45
1:C:232:ALA:HB3	1:C:236:TYR:CE1	2.51	0.45
1:D:515:ASP:HB3	1:D:524:VAL:HB	1.97	0.45
1:C:29:ARG:NH1	6:C:713:HOH:O	2.33	0.45
1:A:450:THR:HG23	5:A:608[B]:JYD:O04	2.17	0.45
1:A:291:GLN:HE22	3:A:603:GOL:H2	1.82	0.45
1:D:116:ASP:HB2	5:D:602:JYD:C07	2.47	0.45
1:C:200:ASN:ND2	1:D:318:ALA:O	2.50	0.45
4:B:606:1PE:H131	6:B:774:HOH:O	2.16	0.45
1:C:372:VAL:HG21	1:C:394:LEU:HD23	1.98	0.45
1:C:401:ILE:HA	1:C:401:ILE:HD13	1.72	0.45
1:C:42:GLY:N	1:D:41:PRO:O	2.36	0.44
1:A:23:HIS:HB2	3:A:602:GOL:O2	2.17	0.44
1:D:33:LYS:HD2	4:D:603:1PE:H232	1.99	0.44
1:B:415:LEU:HD23	1:B:419:LYS:O	2.17	0.44
1:B:237:HIS:HB2	1:B:327:SER:HB3	1.98	0.44
1:B:410:ARG:O	1:B:414:MET:HG3	2.18	0.44
1:C:435:PRO:HB3	1:C:447:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LYS:NZ	6:D:705:HOH:O	2.27	0.44
1:B:218:ARG:HE	1:B:222:LYS:HZ1	1.64	0.44
1:B:275:TYR:HB3	1:B:314:PRO:HG3	2.00	0.44
1:B:499:PRO:HB2	1:B:502:VAL:CG2	2.48	0.44
1:D:51:VAL:O	1:D:133:PRO:HD2	2.18	0.44
1:B:404:ARG:HH12	5:B:604[A]:JYD:C07	2.30	0.44
1:C:45:LEU:HD11	1:D:48:MET:HG3	2.00	0.44
1:B:447:PHE:HB3	1:B:508:ILE:CD1	2.47	0.44
1:C:434:GLY:HA3	1:C:521:MET:CE	2.48	0.44
1:C:242:ILE:HG13	1:D:163:MET:HE1	2.00	0.44
1:C:447:PHE:HB3	1:C:508:ILE:CD1	2.48	0.43
1:D:315:ARG:HD2	1:D:319:SER:O	2.18	0.43
1:B:351:GLU:O	1:B:354:GLN:HG2	2.19	0.43
1:D:71:LEU:HD23	1:D:75:HIS:CD2	2.54	0.43
1:B:268:LYS:HA	1:B:268:LYS:HD3	1.44	0.43
1:C:282:LEU:HD12	1:C:310:VAL:CG2	2.49	0.43
1:C:392:THR:HB	1:C:536:ILE:HD12	2.00	0.43
1:D:483:LYS:O	1:D:487:LYS:HB2	2.18	0.43
1:A:235:PRO:HB2	1:A:306:HIS:CE1	2.53	0.43
4:C:605:1PE:H152	4:C:605:1PE:H142	1.85	0.43
1:B:209:LYS:HD3	1:B:315:ARG:NH2	2.33	0.43
1:A:100:LEU:HB3	1:A:356:LEU:HD13	2.01	0.43
1:A:64:PHE:HA	1:A:67:VAL:HG22	1.99	0.43
1:C:81:LYS:HD2	4:C:606:1PE:H231	2.00	0.43
1:D:289:VAL:O	6:D:703:HOH:O	2.22	0.43
1:D:451:THR:N	1:D:474:LYS:HE3	2.34	0.43
1:B:472:LEU:HA	1:B:493:LEU:O	2.19	0.43
1:C:123:ALA:O	1:C:189:PHE:HA	2.19	0.42
1:C:215:LYS:HG3	3:C:602:GOL:H11	2.00	0.42
1:D:500:ALA:HB2	6:D:782:HOH:O	2.18	0.42
1:B:16:PRO:HG2	1:B:273:THR:O	2.19	0.42
1:C:316:HIS:HE2	1:D:116:ASP:CG	2.22	0.42
1:A:71:LEU:HD13	1:A:75:HIS:HD2	1.84	0.42
1:A:415:LEU:HD13	1:A:465:HIS:CD2	2.55	0.42
1:B:218:ARG:NE	1:B:222:LYS:HZ1	2.17	0.42
1:C:45:LEU:HA	1:C:46:PRO:HD3	1.93	0.42
1:B:33:LYS:HE3	4:B:605:1PE:H142	2.02	0.42
1:C:82:ILE:HG12	1:C:303:TYR:CZ	2.54	0.42
1:B:129:GLN:CB	1:B:185:MET:HG3	2.50	0.42
1:B:208:THR:O	1:B:211:VAL:HG12	2.19	0.42
1:C:376:ARG:CB	1:C:380[A]:GLU:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LEU:HD11	1:D:286:VAL:HG13	2.01	0.42
1:C:68:GLU:HG3	1:C:153:PHE:CZ	2.55	0.42
1:D:521:MET:HG3	1:D:522:GLU:N	2.33	0.42
1:A:346:GLU:O	6:A:702:HOH:O	2.21	0.42
1:B:447:PHE:HB3	1:B:508:ILE:HD13	2.02	0.42
1:C:128:ASP:OD1	1:C:183:LYS:HA	2.19	0.42
1:C:284:GLU:OE1	4:C:605:1PE:OH6	2.38	0.41
1:D:106:SER:HB2	1:D:111:LEU:O	2.20	0.41
1:B:234:PRO:HD2	1:B:298:GLN:HG2	2.01	0.41
1:B:391:ARG:HH11	1:B:391:ARG:HB3	1.86	0.41
1:B:33:LYS:CE	4:B:605:1PE:H131	2.50	0.41
1:A:197:GLY:HA3	5:A:608[A]:JYD:O05	2.21	0.41
1:C:216:SER:HA	3:C:602:GOL:O1	2.20	0.41
1:C:89:SER:O	1:C:93:LYS:HG3	2.21	0.41
1:B:373:ASN:O	1:B:376:ARG:NE	2.51	0.41
1:B:400:ILE:HG12	1:B:429:PRO:HB2	2.03	0.41
1:A:449:PRO:HG2	1:A:474:LYS:HG2	2.03	0.41
3:C:602:GOL:O3	3:C:602:GOL:O1	2.23	0.41
1:A:102:ASN:CG	1:A:499:PRO:HA	2.41	0.41
1:B:270:ASP:OD2	1:B:273:THR:HG23	2.20	0.41
1:C:521:MET:HB2	1:C:521:MET:HE3	1.91	0.41
1:C:511:VAL:HG13	1:C:527:ILE:HG22	2.03	0.41
1:C:354:GLN:OE1	4:C:603:1PE:OH4	2.39	0.41
1:D:45:LEU:HA	1:D:46:PRO:HD3	1.95	0.41
1:B:477:ARG:HD3	1:B:481:VAL:HG11	2.03	0.41
1:C:82:ILE:HG12	1:C:303:TYR:CE2	2.56	0.41
1:D:402:VAL:O	1:D:524:VAL:HA	2.21	0.41
1:D:390:VAL:HA	1:D:536:ILE:HB	2.03	0.40
1:A:151:ARG:HH12	3:A:604:GOL:H32	1.85	0.40
1:A:376:ARG:HD2	1:A:376:ARG:HA	1.89	0.40
1:B:128:ASP:OD2	6:B:704:HOH:O	2.22	0.40
1:D:157:GLN:HG2	1:D:172:ASN:OD1	2.20	0.40
1:D:389:PRO:O	1:D:392:THR:OG1	2.28	0.40
1:B:251:MET:HE1	1:B:323:GLY:HA3	2.03	0.40
1:A:426:LYS:HE2	1:A:465:HIS:O	2.21	0.40
1:B:64:PHE:O	1:B:68:GLU:HG2	2.22	0.40
1:C:242:ILE:HG13	1:D:163:MET:HE3	2.04	0.40
1:C:424:TYR:CE1	1:C:524:VAL:HG11	2.55	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	541/585 (92%)	523 (97%)	17 (3%)	1 (0%)	47	39
1	B	542/585 (93%)	525 (97%)	17 (3%)	0	100	100
1	C	527/585 (90%)	506 (96%)	21 (4%)	0	100	100
1	D	529/585 (90%)	509 (96%)	20 (4%)	0	100	100
All	All	2139/2340 (91%)	2063 (96%)	75 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	LYS

### 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	445/491 (91%)	435 (98%)	10 (2%)	52	46
1	B	446/491 (91%)	437 (98%)	9 (2%)	55	51
1	C	428/491 (87%)	412 (96%)	16 (4%)	34	27
1	D	421/491 (86%)	410 (97%)	11 (3%)	46	40
All	All	1740/1964 (89%)	1694 (97%)	46 (3%)	49	40

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	187	TYR
1	A	288	LYS
1	A	356	LEU
1	A	376	ARG
1	A	447	PHE
1	A	474	LYS
1	A	493	LEU
1	A	512	GLU
1	A	521	MET
1	B	11	GLU
1	B	16	PRO
1	B	21	VAL
1	B	187	TYR
1	B	282	LEU
1	B	447	PHE
1	B	474	LYS
1	B	521[A]	MET
1	B	521[B]	MET
1	C	15	VAL
1	C	17	LEU
1	C	187	TYR
1	C	218[A]	ARG
1	C	218[B]	ARG
1	C	260	HIS
1	C	268	LYS
1	C	288	LYS
1	C	367	THR
1	C	380[A]	GLU
1	C	380[B]	GLU
1	C	447	PHE
1	C	474	LYS
1	C	518	ASP
1	C	521	MET
1	C	545	PHE
1	D	15	VAL
1	D	17	LEU
1	D	136	ASP
1	D	149[A]	GLN
1	D	149[B]	GLN
1	D	187	TYR
1	D	282	LEU
1	D	447	PHE

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Mol	Chain	Res	Type
1	D	474	LYS
1	D	518[A]	ASP
1	D	518[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

28 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	$\# Z  > 2$
2	SF4	A	601	1,5	0,12,12	0.00	-	-		
2	SF4	D	601	1,5	0,12,12	0.00	-	-		
4	1PE	B	605	-	12,12,15	0.55	0	11,11,14	0.67	0
4	1PE	C	605	-	9,9,15	0.27	0	8,8,14	0.50	0
3	GOL	C	602	-	5,5,5	0.90	0	5,5,5	1.05	0
4	1PE	C	603	-	6,6,15	0.50	0	5,5,14	0.37	0
3	GOL	A	604	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1PE	C	606	-	9,9,15	0.26	0	8,8,14	0.50	0
3	GOL	B	603	-	5,5,5	1.19	1 (20%)	5,5,5	1.09	0
4	1PE	D	603	-	15,15,15	0.55	0	14,14,14	0.39	0
3	GOL	A	606	-	5,5,5	1.15	1 (20%)	5,5,5	1.00	0
2	SF4	B	601	1,5	0,12,12	0.00	-	-		
4	1PE	A	611	-	9,9,15	0.28	0	8,8,14	0.39	0
5	JYD	B	604[A]	2	1,8,8	0.28	0	0,10,10	0.00	-
5	JYD	B	604[B]	2	1,8,8	0.12	0	0,10,10	0.00	-
4	1PE	B	606	-	9,9,15	0.29	0	8,8,14	0.41	0
4	1PE	A	609	-	12,12,15	0.51	0	11,11,14	0.60	0
5	JYD	A	608[B]	2	1,8,8	0.03	0	0,10,10	0.00	-
3	GOL	A	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.93	0
3	GOL	A	605	-	5,5,5	1.30	1 (20%)	5,5,5	0.80	0
5	JYD	A	608[A]	2	1,8,8	0.31	0	0,10,10	0.00	-
3	GOL	B	602	-	5,5,5	0.84	0	5,5,5	1.56	1 (20%)
4	1PE	A	607	-	6,6,15	0.50	0	5,5,14	0.38	0
5	JYD	C	604	2	1,8,8	0.07	0	0,10,10	0.00	-
5	JYD	D	602	2	1,8,8	0.17	0	0,10,10	0.00	-
3	GOL	A	602	-	5,5,5	1.72	1 (20%)	5,5,5	1.08	1 (20%)
4	1PE	A	610	-	9,9,15	0.36	0	8,8,14	0.35	0
2	SF4	C	601	1,5	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	601	1,5	-	-	0/6/5/5
2	SF4	D	601	1,5	-	-	0/6/5/5
4	1PE	B	605	-	-	3/10/10/13	-
4	1PE	C	605	-	-	4/7/7/13	-
3	GOL	C	602	-	-	2/4/4/4	-
4	1PE	C	603	-	-	4/4/4/13	-
3	GOL	A	604	-	-	4/4/4/4	-
4	1PE	C	606	-	-	3/7/7/13	-
3	GOL	B	603	-	-	0/4/4/4	-
4	1PE	D	603	-	-	11/13/13/13	-
3	GOL	A	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	601	1,5	-	-	0/6/5/5
4	1PE	A	611	-	-	5/7/7/13	-
5	JYD	B	604[A]	2	-	1/2/8/8	-
5	JYD	B	604[B]	2	-	2/2/8/8	-
4	1PE	B	606	-	-	4/7/7/13	-
4	1PE	A	609	-	-	7/10/10/13	-
5	JYD	A	608[B]	2	-	1/2/8/8	-
3	GOL	A	603	-	-	2/4/4/4	-
3	GOL	A	605	-	-	2/4/4/4	-
5	JYD	A	608[A]	2	-	1/2/8/8	-
3	GOL	B	602	-	-	4/4/4/4	-
4	1PE	A	607	-	-	1/4/4/13	-
5	JYD	C	604	2	-	2/2/8/8	-
5	JYD	D	602	2	-	2/2/8/8	-
3	GOL	A	602	-	-	0/4/4/4	-
4	1PE	A	610	-	-	5/7/7/13	-
2	SF4	C	601	1,5	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GOL	O2-C2	-3.33	1.33	1.43
3	A	605	GOL	O2-C2	-2.77	1.35	1.43
3	A	603	GOL	O2-C2	-2.70	1.35	1.43
3	B	603	GOL	O2-C2	-2.32	1.36	1.43
3	A	606	GOL	O2-C2	-2.10	1.37	1.43
3	A	604	GOL	O2-C2	-2.06	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	GOL	C3-C2-C1	-2.63	101.50	111.70
3	A	602	GOL	C3-C2-C1	-2.04	103.76	111.70

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	606	GOL	C1-C2-C3-O3
5	B	604[A]	JYD	C07-C01-C02-S06
5	B	604[B]	JYD	C07-C01-C02-C03
5	B	604[B]	JYD	C07-C01-C02-S06
3	A	603	GOL	O1-C1-C2-C3
5	A	608[A]	JYD	C07-C01-C02-S06
5	C	604	JYD	C07-C01-C02-S06
5	D	602	JYD	C07-C01-C02-S06
4	A	609	1PE	C13-C23-OH3-C22
4	A	611	1PE	C14-C24-OH4-C13
4	C	606	1PE	OH5-C14-C24-OH4
4	B	605	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH5-C14-C24-OH4
4	D	603	1PE	OH4-C13-C23-OH3
4	A	609	1PE	OH4-C13-C23-OH3
4	A	610	1PE	OH5-C14-C24-OH4
4	B	606	1PE	OH5-C14-C24-OH4
3	C	602	GOL	O1-C1-C2-O2
4	A	607	1PE	OH4-C13-C23-OH3
4	C	603	1PE	OH4-C13-C23-OH3
4	D	603	1PE	OH2-C12-C22-OH3
4	D	603	1PE	OH7-C16-C26-OH6
3	A	604	GOL	C1-C2-C3-O3
3	A	605	GOL	O1-C1-C2-C3
3	B	602	GOL	O1-C1-C2-C3
3	B	602	GOL	C1-C2-C3-O3
4	A	610	1PE	OH6-C15-C25-OH5
4	D	603	1PE	OH5-C14-C24-OH4
3	A	604	GOL	O1-C1-C2-O2
3	A	606	GOL	O2-C2-C3-O3
3	A	603	GOL	O1-C1-C2-O2
3	B	602	GOL	O2-C2-C3-O3
4	A	611	1PE	OH4-C13-C23-OH3
4	B	606	1PE	OH4-C13-C23-OH3
4	C	606	1PE	C24-C14-OH5-C25
5	C	604	JYD	C07-C01-C02-C03
4	D	603	1PE	OH6-C15-C25-OH5
4	C	605	1PE	C15-C25-OH5-C14
4	C	603	1PE	OH2-C12-C22-OH3
4	C	606	1PE	OH4-C13-C23-OH3
4	B	605	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
4	A	609	1PE	OH2-C12-C22-OH3
4	A	609	1PE	C24-C14-OH5-C25
4	A	610	1PE	C23-C13-OH4-C24
4	A	610	1PE	C24-C14-OH5-C25
4	C	603	1PE	C13-C23-OH3-C22
4	C	605	1PE	C23-C13-OH4-C24
4	B	606	1PE	C14-C24-OH4-C13
3	A	604	GOL	O2-C2-C3-O3
4	B	606	1PE	C24-C14-OH5-C25
4	A	609	1PE	C14-C24-OH4-C13
4	A	611	1PE	OH6-C15-C25-OH5
4	A	610	1PE	C14-C24-OH4-C13
4	C	603	1PE	C12-C22-OH3-C23
4	D	603	1PE	C25-C15-OH6-C26
4	D	603	1PE	C24-C14-OH5-C25
4	D	603	1PE	C12-C22-OH3-C23
5	A	608[B]	JYD	C07-C01-C02-C03
5	D	602	JYD	C07-C01-C02-C03
4	D	603	1PE	C23-C13-OH4-C24
4	D	603	1PE	C13-C23-OH3-C22
4	A	611	1PE	OH5-C14-C24-OH4
4	A	609	1PE	OH6-C15-C25-OH5
4	C	605	1PE	OH6-C15-C25-OH5
3	A	605	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-O2
4	D	603	1PE	C16-C26-OH6-C15
4	C	605	1PE	OH5-C14-C24-OH4
4	A	611	1PE	C15-C25-OH5-C14
4	B	605	1PE	OH5-C14-C24-OH4

There are no ring outliers.

20 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	1PE	2	0
4	C	605	1PE	2	0
3	C	602	GOL	3	0
4	C	603	1PE	1	0
3	A	604	GOL	1	0
4	C	606	1PE	1	0
4	D	603	1PE	4	0
4	A	611	1PE	1	0

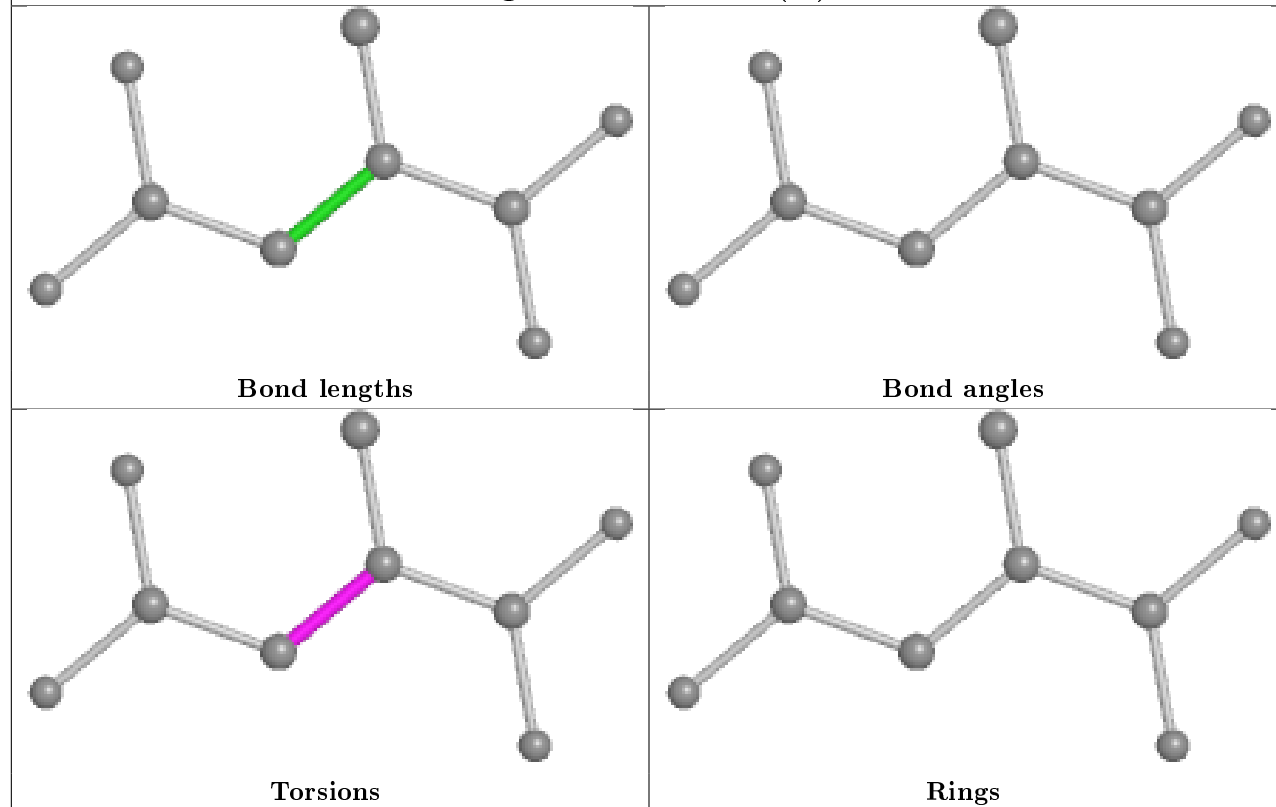
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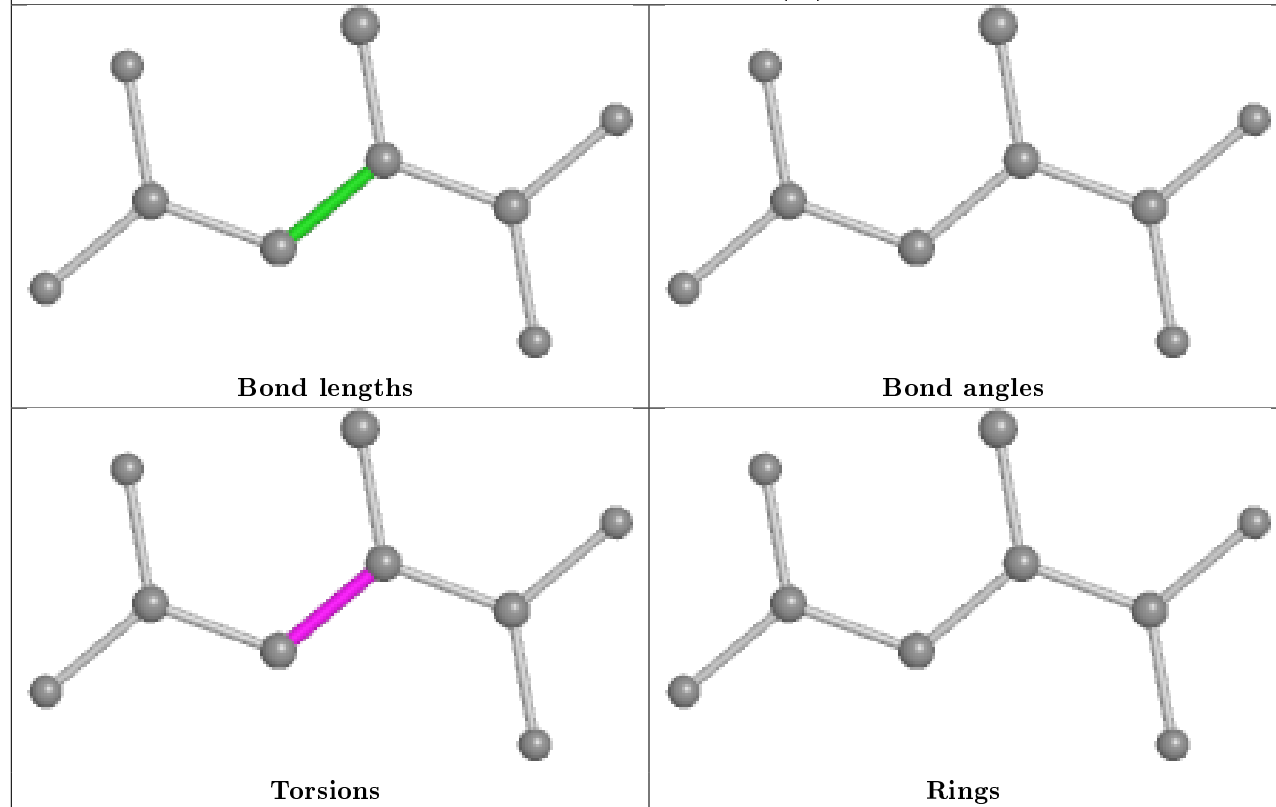
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604[A]	JYD	1	0
5	B	604[B]	JYD	1	0
4	B	606	1PE	1	0
4	A	609	1PE	2	0
5	A	608[B]	JYD	3	0
3	A	603	GOL	1	0
5	A	608[A]	JYD	1	0
3	B	602	GOL	1	0
5	C	604	JYD	2	0
5	D	602	JYD	1	0
3	A	602	GOL	1	0
4	A	610	1PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

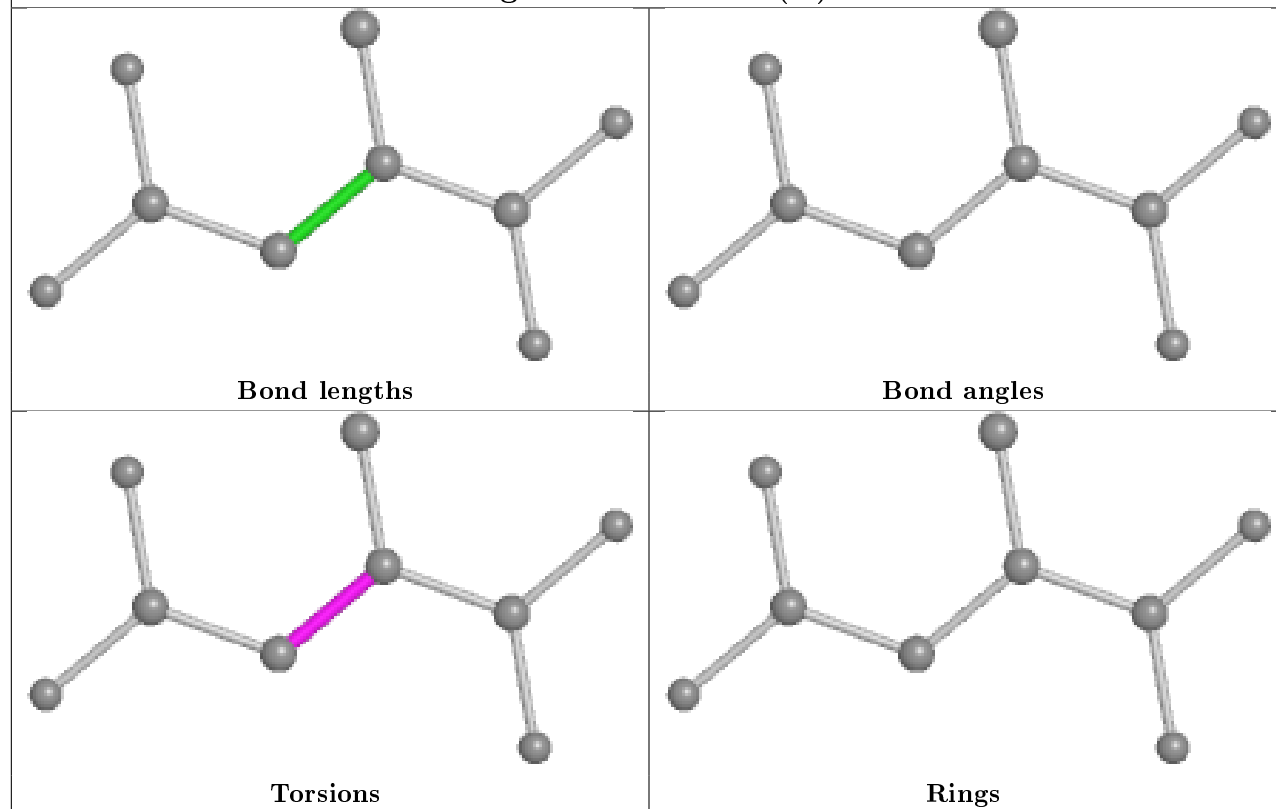
## Ligand JYD B 604 (A)



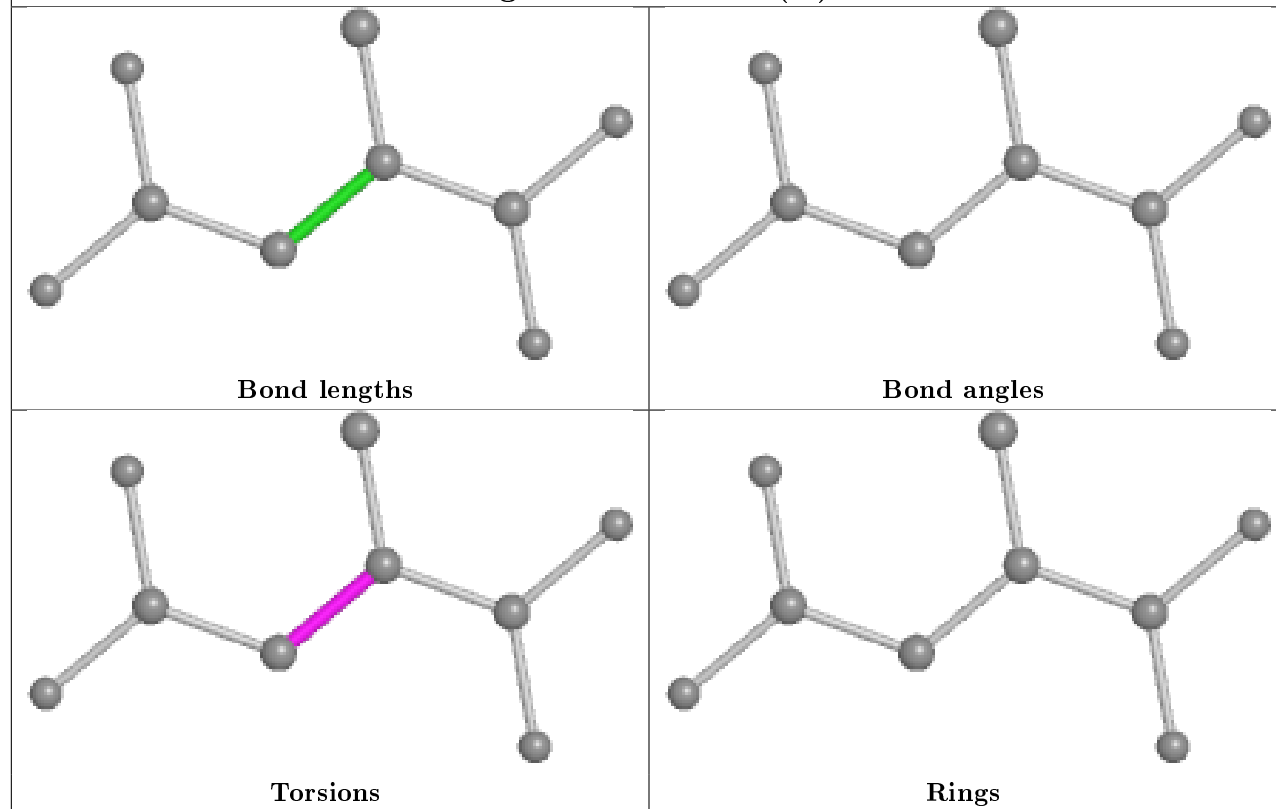
## Ligand JYD B 604 (B)



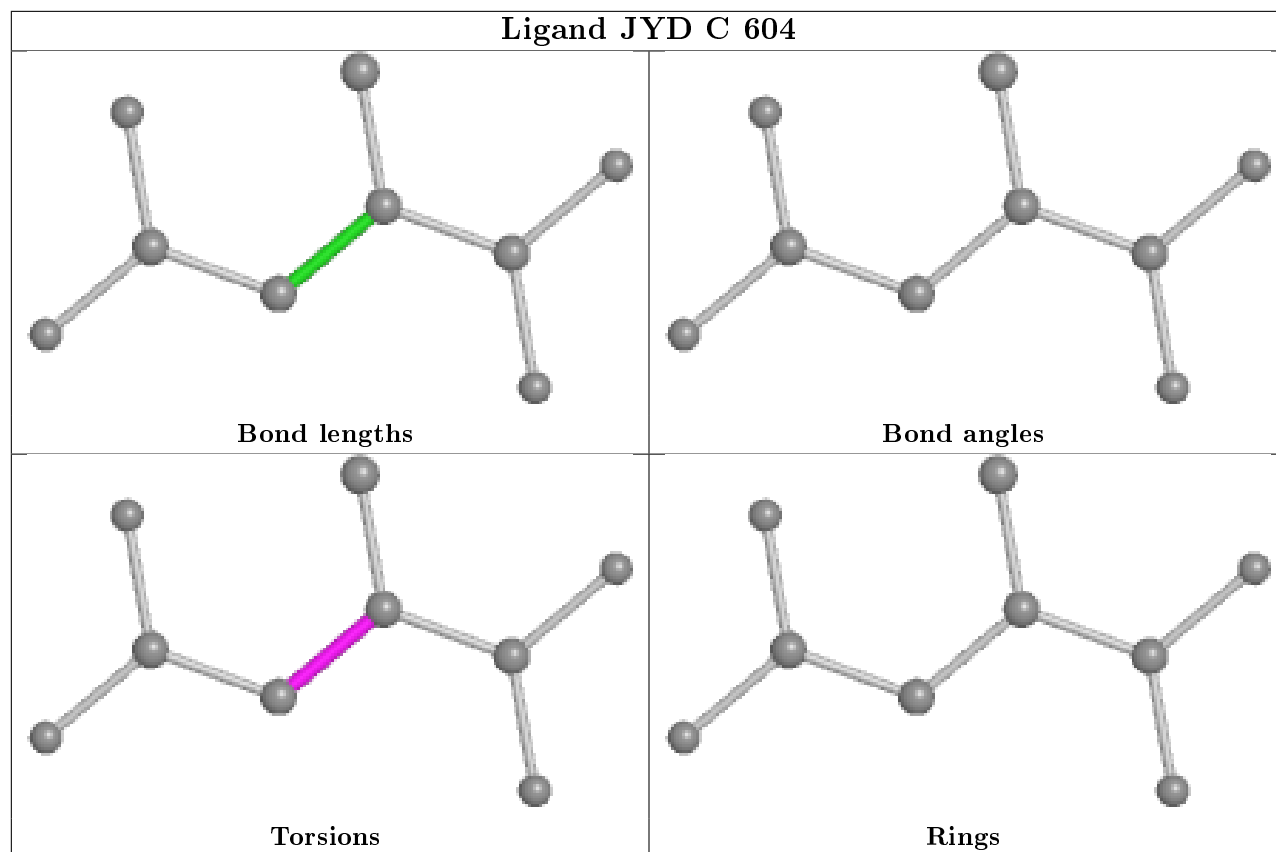
## Ligand JYD A 608 (B)



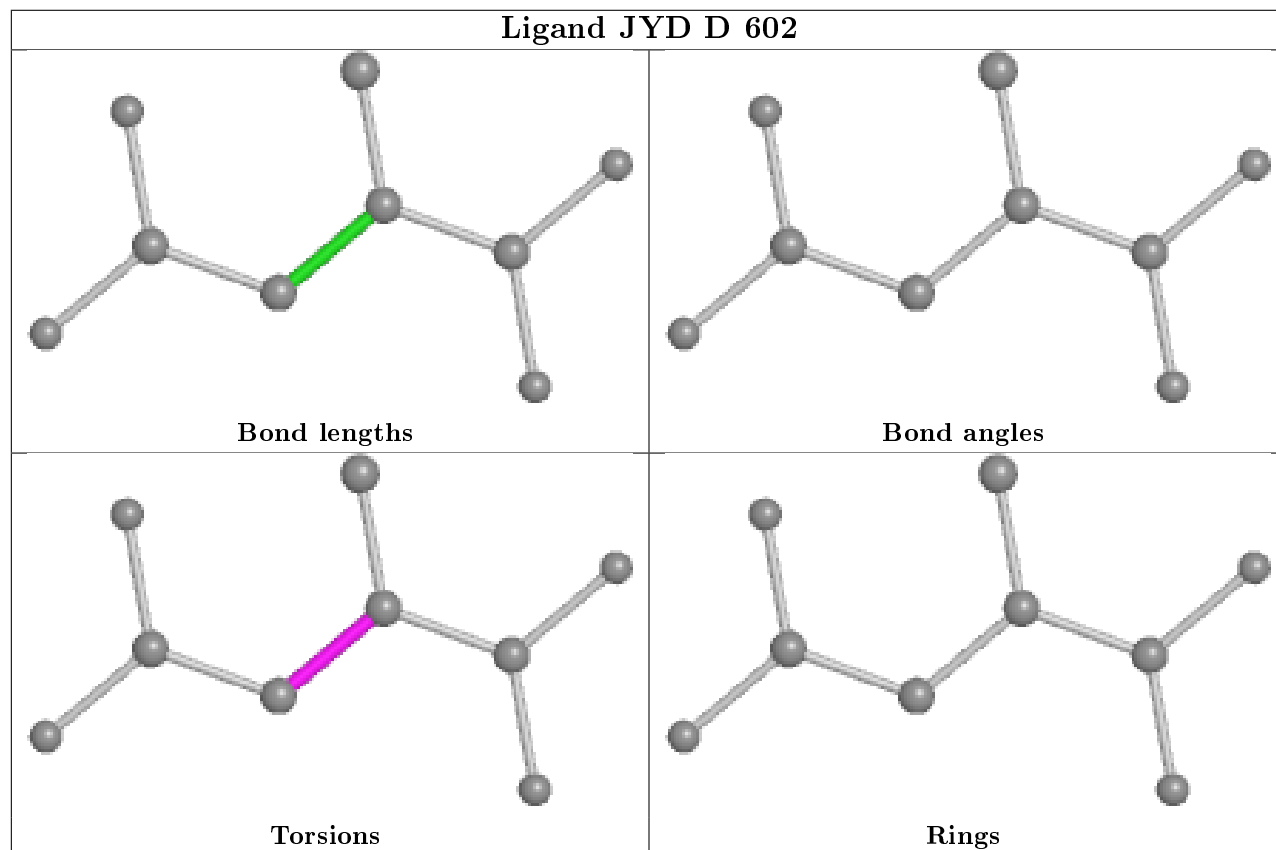
## Ligand JYD A 608 (A)



## Ligand JYD C 604



## Ligand JYD D 602



## 5.7 Other polymers

There are no such residues in this entry.











## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	540/585 (92%)	3.64	478 (88%)  	12, 20, 34, 51	0
1	B	540/585 (92%)	3.76	480 (88%)  	12, 20, 37, 49	0
1	C	528/585 (90%)	5.40	515 (97%)  	20, 33, 48, 64	0
1	D	531/585 (90%)	5.01	501 (94%)  	20, 34, 55, 69	0
All	All	2139/2340 (91%)	4.44	1974 (92%)  	12, 28, 48, 69	0

All (1974) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	SER	21.5
1	C	183	LYS	15.4
1	C	545	PHE	14.2
1	D	88	ALA	14.1
1	D	38	VAL	14.1
1	C	303	TYR	14.0
1	C	155	TYR	14.0
1	C	394	LEU	13.9
1	D	83	PHE	13.7
1	D	509	LYS	13.7
1	C	234	PRO	13.6
1	C	467	GLY	13.3
1	C	43	ALA	13.2
1	C	282	LEU	13.2
1	C	131	PHE	13.1
1	C	100	LEU	12.9
1	C	225	LEU	12.5
1	C	31	LEU	12.5
1	C	132	VAL	12.5
1	D	529	VAL	12.1
1	D	482	THR	12.0

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Mol	Chain	Res	Type	RSRZ
1	D	191	PHE	12.0
1	D	441	GLY	12.0
1	C	397	THR	11.9
1	A	301	GLY	11.9
1	D	417	ALA	11.9
1	C	30	LEU	11.8
1	D	156	SER	11.7
1	C	351	GLU	11.7
1	C	398	GLY	11.7
1	D	424	TYR	11.6
1	D	400	ILE	11.6
1	C	432	TYR	11.6
1	D	502	VAL	11.5
1	D	367	THR	11.5
1	D	398	GLY	11.4
1	D	262	TYR	11.1
1	C	434	GLY	11.0
1	C	371	MET	11.0
1	D	41	PRO	11.0
1	C	259	CYS	10.9
1	C	507	ALA	10.9
1	D	226	ALA	10.9
1	D	130	VAL	10.9
1	C	379	PRO	10.9
1	C	114	CYS	10.8
1	D	189	PHE	10.8
1	D	330	ALA	10.8
1	D	360	LYS	10.7
1	C	420	PRO	10.7
1	C	245	THR	10.7
1	C	187	TYR	10.7
1	C	454	ARG	10.6
1	B	498	GLY	10.5
1	A	444	SER	10.5
1	C	162	SER	10.5
1	C	62	THR	10.4
1	C	529	VAL	10.3
1	C	274	GLY	10.3
1	C	367	THR	10.3
1	C	97	LEU	10.3
1	D	192	VAL	10.2
1	D	54	ALA	10.1

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Mol	Chain	Res	Type	RSRZ
1	C	357	PRO	10.1
1	D	443	PRO	10.1
1	C	191	PHE	10.1
1	D	228	PHE	10.0
1	D	303	TYR	10.0
1	C	435	PRO	10.0
1	C	184	GLY	10.0
1	D	491	PHE	10.0
1	D	45	LEU	9.9
1	C	519	LEU	9.8
1	D	143	GLY	9.8
1	B	118	GLY	9.7
1	C	399	THR	9.7
1	B	54	ALA	9.6
1	C	55	ALA	9.6
1	C	79	LEU	9.6
1	C	370	VAL	9.6
1	B	549	LEU	9.6
1	D	69	HIS	9.5
1	D	261	TYR	9.5
1	D	181	ALA	9.5
1	C	520	GLY	9.5
1	A	537	VAL	9.4
1	A	314	PRO	9.4
1	B	508	ILE	9.4
1	B	39	VAL	9.4
1	C	295	MET	9.4
1	B	330	ALA	9.3
1	D	369	ALA	9.3
1	C	470	VAL	9.3
1	D	263	ASP	9.2
1	B	525	TRP	9.1
1	C	129	GLN	9.1
1	D	212	LEU	9.1
1	C	325	GLY	9.1
1	D	523	ALA	9.1
1	D	256	TYR	9.1
1	D	82	ILE	9.1
1	C	119	THR	9.0
1	D	499	PRO	8.9
1	D	140	LEU	8.9
1	C	220	PHE	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	17	LEU	8.9
1	D	299	PHE	8.9
1	D	59	LEU	8.9
1	B	164	TYR	8.9
1	C	400	ILE	8.8
1	D	520	GLY	8.8
1	C	535	PHE	8.8
1	C	216	SER	8.8
1	D	243	GLY	8.8
1	C	297	ALA	8.8
1	B	275	TYR	8.8
1	C	48	MET	8.7
1	C	262	TYR	8.7
1	D	63	ALA	8.7
1	C	386	SER	8.7
1	A	285	GLU	8.7
1	C	503	LEU	8.7
1	B	320	CYS	8.6
1	C	504	ALA	8.6
1	C	70	LEU	8.6
1	C	291	GLN	8.6
1	B	532	PHE	8.6
1	A	247	ALA	8.5
1	C	409	ALA	8.5
1	C	181	ALA	8.5
1	B	537	VAL	8.5
1	C	52	ASP	8.5
1	B	261	TYR	8.5
1	A	36	VAL	8.4
1	C	352	PRO	8.4
1	A	311	ILE	8.4
1	D	343	VAL	8.4
1	D	33	LYS	8.3
1	A	185	MET	8.3
1	C	431	TYR	8.3
1	D	55	ALA	8.3
1	D	528	GLU	8.3
1	D	496	ILE	8.3
1	C	464	SER	8.3
1	A	264	ASP	8.3
1	B	450[A]	THR	8.3
1	D	100	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
1	D	338	ILE	8.2
1	D	374	LEU	8.2
1	C	153	PHE	8.2
1	A	517	LYS	8.2
1	D	379	PRO	8.1
1	B	499	PRO	8.1
1	D	372	VAL	8.1
1	C	497	GLY	8.1
1	C	71	LEU	8.1
1	D	205	LEU	8.1
1	D	91	ASN	8.0
1	D	286	VAL	8.0
1	D	494	GLY	8.0
1	D	222	LYS	8.0
1	D	15	VAL	7.9
1	D	459	VAL	7.9
1	C	232	ALA	7.9
1	C	83	PHE	7.9
1	C	21	VAL	7.8
1	A	10	ALA	7.8
1	B	529	VAL	7.8
1	D	427	GLU	7.8
1	D	351	GLU	7.8
1	A	422	PRO	7.8
1	D	415	LEU	7.8
1	C	417	ALA	7.8
1	C	546	PHE	7.8
1	C	175	ALA	7.7
1	C	433	ALA	7.7
1	B	424	TYR	7.7
1	B	250	THR	7.7
1	D	368	PRO	7.7
1	D	13	ASN	7.7
1	D	136	ASP	7.7
1	D	484	ALA	7.7
1	D	352	PRO	7.6
1	C	145	TYR	7.6
1	C	44	GLY	7.6
1	C	33	LYS	7.6
1	A	216	SER	7.6
1	A	137	GLU	7.6
1	D	86	PRO	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	182	SER	7.6
1	C	51	VAL	7.5
1	C	468	SER	7.5
1	D	153	PHE	7.5
1	B	466	GLY	7.5
1	B	42	GLY	7.5
1	B	128	ASP	7.5
1	B	205	LEU	7.5
1	D	25	GLU	7.5
1	C	107	SER	7.5
1	D	320	CYS	7.5
1	C	161	LEU	7.4
1	D	290	CYS	7.4
1	B	308	VAL	7.4
1	C	439	PRO	7.4
1	C	82	ILE	7.4
1	A	180	TYR	7.4
1	C	316	HIS	7.4
1	D	208	THR	7.4
1	A	325	GLY	7.4
1	C	189	PHE	7.4
1	C	38	VAL	7.4
1	A	141	SER	7.4
1	B	152	ASN	7.4
1	C	178	ASP	7.4
1	A	134	GLY	7.3
1	D	62	THR	7.3
1	D	385	LEU	7.3
1	C	29	ARG	7.3
1	D	174	PRO	7.3
1	C	338	ILE	7.3
1	C	211	VAL	7.3
1	C	236	TYR	7.3
1	B	45	LEU	7.2
1	A	164	TYR	7.2
1	A	174	PRO	7.2
1	D	120	ALA	7.2
1	C	270	ASP	7.2
1	D	95	VAL	7.2
1	D	546	PHE	7.2
1	D	17	LEU	7.2
1	B	239	ALA	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	161[A]	LEU	7.1
1	A	418	GLY	7.1
1	B	322	ILE	7.1
1	D	32	THR	7.1
1	C	289	VAL	7.1
1	C	58	LEU	7.1
1	A	28	TYR	7.1
1	A	495	SER	7.1
1	A	293	ILE	7.0
1	C	492	TYR	7.0
1	A	103	ALA	7.0
1	C	233	CYS	7.0
1	D	220	PHE	7.0
1	B	382	LEU	7.0
1	C	89	SER	7.0
1	C	369	ALA	7.0
1	B	329	SER	7.0
1	C	273	THR	7.0
1	A	545	PHE	7.0
1	C	94	PHE	7.0
1	D	277	PHE	7.0
1	D	397	THR	6.9
1	D	60	SER	6.9
1	D	406	SER	6.9
1	C	76	LEU	6.9
1	C	304	TYR	6.9
1	D	145	TYR	6.9
1	D	135	ASN	6.9
1	C	307	ASP	6.9
1	B	402	VAL	6.9
1	D	511	VAL	6.9
1	A	56	LEU	6.9
1	C	536	ILE	6.9
1	C	459	VAL	6.9
1	D	230	THR	6.9
1	A	345	LEU	6.9
1	B	364	LEU	6.9
1	A	402	VAL	6.9
1	D	94	PHE	6.9
1	C	442	LEU	6.8
1	C	91	ASN	6.8
1	C	127	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	105	ILE	6.8
1	A	289	VAL	6.8
1	C	209	LYS	6.8
1	D	350	MET	6.8
1	C	195	GLY	6.8
1	C	380[A]	GLU	6.8
1	D	178	ASP	6.8
1	D	213	ASN	6.8
1	C	280	LEU	6.8
1	D	49	LEU	6.8
1	C	456	ASP	6.8
1	A	64	PHE	6.8
1	D	458	PHE	6.8
1	D	335	LEU	6.8
1	D	468	SER	6.8
1	C	393	ARG	6.8
1	C	493	LEU	6.8
1	D	313	MET	6.8
1	C	377	PRO	6.8
1	D	245	THR	6.8
1	C	509	LYS	6.7
1	C	188	SER	6.7
1	C	174	PRO	6.7
1	C	513	CYS	6.7
1	C	49	LEU	6.7
1	B	21	VAL	6.7
1	C	530	GLU	6.7
1	C	172	ASN	6.7
1	C	219	ASN	6.7
1	D	211	VAL	6.7
1	C	198	SER	6.7
1	B	536	ILE	6.7
1	C	528	GLU	6.7
1	C	88	ALA	6.7
1	D	396	LEU	6.6
1	C	500	ALA	6.6
1	C	149	GLN	6.6
1	C	80	ARG	6.6
1	D	304	TYR	6.6
1	C	354	GLN	6.6
1	C	23	HIS	6.6
1	D	326	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	209	LYS	6.6
1	C	348	LEU	6.6
1	C	537	VAL	6.6
1	A	542	GLY	6.6
1	C	111	LEU	6.5
1	D	274	GLY	6.5
1	B	12	PHE	6.5
1	A	67	VAL	6.5
1	D	175	ALA	6.5
1	D	126	ARG	6.5
1	D	97	LEU	6.5
1	D	147	ILE	6.5
1	B	485	CYS	6.4
1	D	254	LEU	6.4
1	C	521	MET	6.4
1	D	98	GLN	6.4
1	D	324	ILE	6.4
1	C	495	SER	6.4
1	C	448	GLY	6.4
1	C	314	PRO	6.4
1	A	287	LEU	6.4
1	D	356	LEU	6.4
1	A	344	TRP	6.4
1	D	253	VAL	6.4
1	C	141	SER	6.3
1	A	384	GLU	6.3
1	D	530	GLU	6.3
1	A	278	ARG	6.3
1	D	387	LYS	6.3
1	D	284	GLU	6.3
1	B	97	LEU	6.3
1	D	282	LEU	6.3
1	A	238	VAL	6.3
1	C	26	THR	6.3
1	C	144	VAL	6.3
1	D	159	VAL	6.3
1	C	463	GLN	6.3
1	C	288	LYS	6.3
1	D	30	LEU	6.3
1	D	31	LEU	6.3
1	D	207	GLU	6.3
1	B	95	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	6.3
1	A	380	GLU	6.2
1	A	501	ALA	6.2
1	D	318	ALA	6.2
1	B	514	LEU	6.2
1	D	421	LEU	6.2
1	B	353	SER	6.2
1	B	375	ASN	6.2
1	D	276	THR	6.2
1	B	294	GLY	6.2
1	C	428	HIS	6.2
1	A	110	LEU	6.2
1	C	385	LEU	6.2
1	C	390	VAL	6.2
1	C	293	ILE	6.2
1	B	143	GLY	6.2
1	A	396	LEU	6.2
1	A	237	HIS	6.2
1	B	510	LYS	6.2
1	A	181	ALA	6.2
1	B	493	LEU	6.2
1	D	381	VAL	6.2
1	B	481	VAL	6.2
1	C	18	VAL	6.2
1	D	485	CYS	6.1
1	C	510	LYS	6.1
1	D	109	ARG	6.1
1	B	238	VAL	6.1
1	D	308	VAL	6.1
1	B	305	ALA	6.1
1	B	276	THR	6.1
1	C	204	LEU	6.1
1	C	542	GLY	6.1
1	C	343	VAL	6.1
1	D	440	ASP	6.1
1	D	169	THR	6.1
1	A	322	ILE	6.1
1	A	11	GLU	6.1
1	C	47	GLU	6.1
1	D	418	GLY	6.1
1	D	526	ARG	6.1
1	C	193	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	6.1
1	B	277	PHE	6.1
1	D	176	GLN	6.1
1	D	371	MET	6.1
1	B	358	ASP	6.1
1	D	215	LYS	6.0
1	C	110	LEU	6.0
1	C	64	PHE	6.0
1	D	447	PHE	6.0
1	B	369	ALA	6.0
1	C	46	PRO	6.0
1	D	423	GLN	6.0
1	C	96	ALA	6.0
1	D	96	ALA	6.0
1	D	334	ALA	6.0
1	D	514	LEU	6.0
1	D	310	VAL	6.0
1	A	318	ALA	6.0
1	A	536	ILE	6.0
1	B	383	GLN	6.0
1	C	205	LEU	6.0
1	C	77	MET	6.0
1	A	131	PHE	6.0
1	D	322	ILE	6.0
1	D	408	HIS	6.0
1	D	22	SER	5.9
1	D	355	TYR	5.9
1	A	232	ALA	5.9
1	D	43	ALA	5.9
1	C	356	LEU	5.9
1	C	511	VAL	5.9
1	C	99	LEU	5.9
1	A	43	ALA	5.9
1	D	125	TYR	5.9
1	A	221	LEU	5.9
1	C	396	LEU	5.9
1	D	225	LEU	5.9
1	C	19	SER	5.9
1	B	362	ASP	5.9
1	D	131	PHE	5.9
1	A	265	LEU	5.9
1	B	59	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	287	LEU	5.9
1	B	541	LYS	5.9
1	A	117	THR	5.8
1	B	171	THR	5.8
1	C	315	ARG	5.8
1	B	271	MET	5.8
1	B	44	GLY	5.8
1	B	108	ALA	5.8
1	D	164	TYR	5.8
1	B	539	ASP	5.8
1	C	444	SER	5.8
1	D	110	LEU	5.8
1	D	420	PRO	5.8
1	B	350[A]	MET	5.8
1	B	64	PHE	5.8
1	C	443	PRO	5.8
1	C	150	LYS	5.8
1	D	168	ASN	5.7
1	B	218	ARG	5.7
1	A	546	PHE	5.7
1	A	275	TYR	5.7
1	A	280	LEU	5.7
1	C	421	LEU	5.7
1	C	488	TYR	5.7
1	C	84	ASP	5.7
1	D	34	ASP	5.7
1	A	124	GLY	5.7
1	D	218	ARG	5.7
1	B	389	PRO	5.7
1	D	46	PRO	5.7
1	A	111	LEU	5.7
1	A	122	ILE	5.7
1	C	515	ASP	5.7
1	D	527	ILE	5.7
1	B	513	CYS	5.7
1	C	336	GLY	5.7
1	A	16	PRO	5.7
1	B	429	PRO	5.7
1	A	239	ALA	5.7
1	B	403	ALA	5.7
1	B	56	LEU	5.7
1	C	134	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	125	TYR	5.7
1	D	344	TRP	5.7
1	D	370	VAL	5.7
1	C	534	ALA	5.7
1	C	485	CYS	5.7
1	A	326	VAL	5.7
1	C	28	TYR	5.7
1	A	78	SER	5.6
1	D	107	SER	5.6
1	B	368	PRO	5.6
1	C	173	LEU	5.6
1	D	280	LEU	5.6
1	D	518[A]	ASP	5.6
1	C	151	ARG	5.6
1	B	314	PRO	5.6
1	D	58	LEU	5.6
1	C	103	ALA	5.6
1	A	315	ARG	5.6
1	C	471	MET	5.6
1	D	210	SER	5.6
1	D	513	CYS	5.6
1	D	242	ILE	5.6
1	D	293	ILE	5.6
1	D	535	PHE	5.6
1	D	93	LYS	5.6
1	B	420	PRO	5.6
1	C	331	ASP	5.6
1	D	358	ASP	5.6
1	A	212	LEU	5.6
1	A	324	ILE	5.6
1	D	231	SER	5.6
1	D	390	VAL	5.6
1	B	371	MET	5.6
1	D	378	MET	5.6
1	C	203	PHE	5.6
1	D	144	VAL	5.6
1	C	483	LYS	5.5
1	A	269	PRO	5.5
1	C	341	ASP	5.5
1	A	304	TYR	5.5
1	D	187	TYR	5.5
1	D	111	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	359	LEU	5.5
1	A	130	VAL	5.5
1	C	148	PHE	5.5
1	A	466	GLY	5.5
1	C	414	MET	5.5
1	C	300	GLY	5.5
1	C	22	SER	5.5
1	C	321	PRO	5.5
1	C	426	LYS	5.5
1	D	543	ASN	5.5
1	C	130	VAL	5.5
1	C	223	GLU	5.5
1	D	233	CYS	5.5
1	B	120	ALA	5.5
1	C	123	ALA	5.5
1	B	427	GLU	5.5
1	A	21	VAL	5.5
1	C	419	LYS	5.5
1	C	514	LEU	5.5
1	B	511	VAL	5.4
1	C	192	VAL	5.4
1	C	266	ILE	5.4
1	D	462	PHE	5.4
1	D	40	GLN	5.4
1	D	373	ASN	5.4
1	D	66	ASP	5.4
1	C	218[A]	ARG	5.4
1	B	496	ILE	5.4
1	D	121	ILE	5.4
1	D	16	PRO	5.4
1	C	45	LEU	5.4
1	C	508	ILE	5.4
1	D	77	MET	5.4
1	A	205	LEU	5.4
1	A	199	ALA	5.4
1	D	395	SER	5.4
1	D	146	ASP	5.4
1	C	382	LEU	5.4
1	A	516	MET	5.4
1	C	122	ILE	5.4
1	C	544	ASP	5.4
1	A	377	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	5.4
1	D	234	PRO	5.4
1	C	95	VAL	5.3
1	C	329	SER	5.3
1	C	372	VAL	5.3
1	D	238	VAL	5.3
1	B	336	GLY	5.3
1	D	376	ARG	5.3
1	C	242	ILE	5.3
1	C	322	ILE	5.3
1	C	496	ILE	5.3
1	D	35	TYR	5.3
1	B	41	PRO	5.3
1	C	27	LYS	5.3
1	C	328	CYS	5.3
1	D	179	LEU	5.3
1	B	381	VAL	5.3
1	C	332	ARG	5.3
1	D	12	PHE	5.3
1	B	103	ALA	5.3
1	A	24	LYS	5.3
1	C	243	GLY	5.3
1	C	453	GLY	5.3
1	C	526	ARG	5.3
1	C	501	ALA	5.3
1	D	23	HIS	5.3
1	B	365	LEU	5.3
1	A	240	VAL	5.2
1	C	75	HIS	5.2
1	C	531	ASN	5.2
1	B	512	GLU	5.2
1	C	124	GLY	5.2
1	D	108	ALA	5.2
1	B	425	MET	5.2
1	B	282	LEU	5.2
1	A	224	LYS	5.2
1	A	26	THR	5.2
1	A	471	MET	5.2
1	D	414	MET	5.2
1	C	133	PRO	5.2
1	D	540	ASP	5.2
1	C	258	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	441	GLY	5.2
1	C	241	VAL	5.2
1	B	355	TYR	5.2
1	C	171	THR	5.2
1	D	532	PHE	5.2
1	B	197	GLY	5.2
1	B	370	VAL	5.2
1	C	276	THR	5.2
1	D	402	VAL	5.2
1	B	14	PHE	5.2
1	B	373	ASN	5.2
1	C	460	ASP	5.2
1	D	488	TYR	5.1
1	C	224	LYS	5.1
1	C	53	PRO	5.1
1	C	402	VAL	5.1
1	C	478	SER	5.1
1	C	165	ASP	5.1
1	D	90	ASP	5.1
1	B	98	GLN	5.1
1	D	463	GLN	5.1
1	A	251	MET	5.1
1	B	367	THR	5.1
1	B	521[A]	MET	5.1
1	D	471	MET	5.1
1	B	527	ILE	5.1
1	A	183	LYS	5.1
1	A	32	THR	5.1
1	A	156	SER	5.1
1	A	271	MET	5.1
1	B	10	ALA	5.1
1	C	227	MET	5.1
1	D	465	HIS	5.1
1	B	286	VAL	5.1
1	D	236	TYR	5.1
1	D	68	GLU	5.1
1	D	104	ASN	5.1
1	A	403	ALA	5.1
1	B	407	ALA	5.1
1	A	170	GLY	5.1
1	A	493	LEU	5.1
1	D	506	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	401	ILE	5.1
1	D	275	TYR	5.1
1	D	288	LYS	5.1
1	B	287	LEU	5.1
1	D	71	LEU	5.1
1	A	343	VAL	5.0
1	D	92	ASP	5.0
1	D	132	VAL	5.0
1	A	414	MET	5.0
1	D	425	MET	5.0
1	C	430	VAL	5.0
1	D	114	CYS	5.0
1	C	104	ASN	5.0
1	D	177	ILE	5.0
1	A	364	LEU	5.0
1	C	106	SER	5.0
1	C	406	SER	5.0
1	D	173	LEU	5.0
1	A	357	PRO	5.0
1	A	193	ALA	5.0
1	D	508	ILE	5.0
1	D	167	LYS	5.0
1	B	422	PRO	5.0
1	C	139	ALA	5.0
1	D	541	LYS	5.0
1	C	296	GLY	5.0
1	A	241	VAL	4.9
1	D	48	MET	4.9
1	D	227	MET	4.9
1	D	403	ALA	4.9
1	D	115	GLN	4.9
1	A	338	ILE	4.9
1	D	124	GLY	4.9
1	A	447	PHE	4.9
1	B	256	TYR	4.9
1	C	512	GLU	4.9
1	D	76	LEU	4.9
1	B	414	MET	4.9
1	B	240	VAL	4.9
1	D	250	THR	4.9
1	D	172	ASN	4.9
1	D	353	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	512	GLU	4.9
1	B	343	VAL	4.9
1	C	237	HIS	4.9
1	D	409	ALA	4.9
1	A	508	ILE	4.9
1	D	311	ILE	4.9
1	B	461	LEU	4.9
1	C	450	THR	4.9
1	D	36	VAL	4.9
1	D	269	PRO	4.9
1	C	69	HIS	4.9
1	A	227	MET	4.9
1	D	182	SER	4.9
1	C	461	LEU	4.9
1	D	79	LEU	4.9
1	D	542	GLY	4.9
1	B	211	VAL	4.9
1	C	381	VAL	4.9
1	D	341	ASP	4.9
1	B	119	THR	4.9
1	D	466	GLY	4.9
1	C	247	ALA	4.8
1	C	491	PHE	4.8
1	C	117	THR	4.8
1	B	76	LEU	4.8
1	A	432	TYR	4.8
1	A	395	SER	4.8
1	C	163	MET	4.8
1	B	436	ALA	4.8
1	D	507	ALA	4.8
1	B	222	LYS	4.8
1	A	442	LEU	4.8
1	B	111	LEU	4.8
1	C	126	ARG	4.8
1	C	326	VAL	4.8
1	C	324	ILE	4.8
1	D	531	ASN	4.8
1	A	225	LEU	4.8
1	B	472	LEU	4.8
1	D	61	SER	4.8
1	B	278	ARG	4.8
1	C	449	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	401	ILE	4.8
1	C	217	LEU	4.8
1	C	277	PHE	4.8
1	C	353	SER	4.8
1	D	340	LYS	4.8
1	A	153	PHE	4.8
1	C	384	GLU	4.8
1	D	244	GLY	4.8
1	A	531	ASN	4.8
1	B	476	ASN	4.8
1	B	377	PRO	4.8
1	D	264	ASP	4.8
1	C	391	ARG	4.8
1	C	221	LEU	4.7
1	C	415	LEU	4.7
1	A	375	ASN	4.7
1	C	447	PHE	4.7
1	D	457	PRO	4.7
1	A	518	ASP	4.7
1	D	273	THR	4.7
1	A	218	ARG	4.7
1	C	490	GLY	4.7
1	A	177	ILE	4.7
1	B	415	LEU	4.7
1	B	94	PHE	4.7
1	C	405	ASP	4.7
1	C	202	SER	4.7
1	C	292	ASN	4.7
1	D	510	LYS	4.7
1	B	207	GLU	4.7
1	B	385	LEU	4.7
1	D	519	LEU	4.7
1	A	371	MET	4.7
1	D	436	ALA	4.7
1	A	472	LEU	4.7
1	B	306	HIS	4.7
1	A	276	THR	4.7
1	C	73	SER	4.7
1	C	102	ASN	4.7
1	A	348	LEU	4.7
1	D	319	SER	4.7
1	A	524	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	193	ALA	4.7
1	C	32	THR	4.6
1	D	493	LEU	4.6
1	C	257	ALA	4.6
1	A	14	PHE	4.6
1	C	299	PHE	4.6
1	B	35	TYR	4.6
1	A	307	ASP	4.6
1	D	456	ASP	4.6
1	D	42	GLY	4.6
1	D	497	GLY	4.6
1	B	254	LEU	4.6
1	D	70	LEU	4.6
1	C	90	ASP	4.6
1	A	522	GLU	4.6
1	A	35	TYR	4.6
1	A	187	TYR	4.6
1	C	256	TYR	4.6
1	C	383	GLN	4.6
1	B	394	LEU	4.6
1	D	265	LEU	4.6
1	C	39	VAL	4.6
1	C	138	GLU	4.6
1	A	277	PHE	4.6
1	B	220	PHE	4.6
1	D	64	PHE	4.6
1	B	469	MET	4.6
1	A	233	CYS	4.6
1	B	366	LYS	4.6
1	B	380	GLU	4.6
1	C	408	HIS	4.6
1	A	71	LEU	4.6
1	A	394	LEU	4.6
1	B	396	LEU	4.6
1	C	179	LEU	4.6
1	B	321	PRO	4.6
1	A	300	GLY	4.6
1	B	196	GLY	4.6
1	B	459	VAL	4.6
1	B	153	PHE	4.6
1	C	532	PHE	4.6
1	D	14	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	190	MET	4.6
1	D	128	ASP	4.6
1	B	175	ALA	4.6
1	D	158	ASN	4.6
1	A	439	PRO	4.6
1	C	105	ILE	4.6
1	C	212	LEU	4.6
1	B	203	PHE	4.6
1	B	462	PHE	4.6
1	C	154	ARG	4.6
1	D	165	ASP	4.6
1	D	460	ASP	4.6
1	C	392	THR	4.6
1	C	472	LEU	4.5
1	D	67	VAL	4.5
1	B	116	ASP	4.5
1	C	60	SER	4.5
1	D	39	VAL	4.5
1	A	267	THR	4.5
1	B	26	THR	4.5
1	D	435	PRO	4.5
1	C	424	TYR	4.5
1	D	155	TYR	4.5
1	A	213	ASN	4.5
1	B	346	GLU	4.5
1	B	356	LEU	4.5
1	D	521	MET	4.5
1	A	308	VAL	4.5
1	B	233	CYS	4.5
1	B	544	ASP	4.5
1	A	175	ALA	4.5
1	A	19	SER	4.5
1	C	135	ASN	4.5
1	C	486	HIS	4.5
1	A	97	LEU	4.5
1	B	57	THR	4.5
1	D	539	ASP	4.5
1	B	517	LYS	4.5
1	C	112	PRO	4.5
1	D	445	GLY	4.5
1	D	354	GLN	4.5
1	B	523	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	350	MET	4.5
1	C	56	LEU	4.5
1	B	399	THR	4.5
1	D	26	THR	4.5
1	B	378	MET	4.4
1	A	155	TYR	4.4
1	A	488	TYR	4.4
1	D	399	THR	4.4
1	A	104	ASN	4.4
1	A	310	VAL	4.4
1	A	63	ALA	4.4
1	A	299	PHE	4.4
1	C	475	GLY	4.4
1	A	258	SER	4.4
1	D	534	ALA	4.4
1	B	272	LYS	4.4
1	C	13	ASN	4.4
1	C	213	ASN	4.4
1	D	251	MET	4.4
1	A	41	PRO	4.4
1	A	391	ARG	4.4
1	A	173	LEU	4.4
1	B	311	ILE	4.4
1	B	192	VAL	4.4
1	A	323	GLY	4.4
1	C	301	GLY	4.4
1	D	453	GLY	4.4
1	B	46	PRO	4.4
1	A	388	HIS	4.4
1	C	345	LEU	4.4
1	D	328	CYS	4.4
1	A	48	MET	4.4
1	B	313	MET	4.4
1	A	203	PHE	4.4
1	C	186	GLU	4.4
1	C	465	HIS	4.4
1	A	49	LEU	4.4
1	A	335	LEU	4.4
1	B	543	ASN	4.4
1	C	349	GLU	4.4
1	C	457	PRO	4.4
1	B	267	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	476	ASN	4.3
1	A	415	LEU	4.3
1	C	206	GLN	4.3
1	C	323	GLY	4.3
1	C	494	GLY	4.3
1	C	525	TRP	4.3
1	B	130	VAL	4.3
1	D	481	VAL	4.3
1	C	469	MET	4.3
1	D	65	ASP	4.3
1	B	317	GLY	4.3
1	B	348	LEU	4.3
1	B	516	MET	4.3
1	B	534	ALA	4.3
1	D	478	SER	4.3
1	B	11	GLU	4.3
1	B	30	LEU	4.3
1	C	200	ASN	4.3
1	C	505	GLN	4.3
1	A	84	ASP	4.3
1	D	171	THR	4.3
1	D	431	TYR	4.3
1	D	99	LEU	4.3
1	A	132	VAL	4.3
1	D	517	LYS	4.3
1	B	90	ASP	4.3
1	D	314	PRO	4.3
1	B	163	MET	4.3
1	D	442	LEU	4.3
1	D	437	LYS	4.3
1	D	536	ILE	4.3
1	A	236	TYR	4.3
1	C	355	TYR	4.3
1	C	533	PRO	4.3
1	D	53	PRO	4.3
1	B	25	GLU	4.2
1	A	114	CYS	4.2
1	D	302	LYS	4.2
1	A	100	LEU	4.2
1	A	169	THR	4.2
1	C	240	VAL	4.2
1	D	430	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	123	ALA	4.2
1	D	166	GLU	4.2
1	D	201	LYS	4.2
1	A	58	LEU	4.2
1	D	259	CYS	4.2
1	A	459	VAL	4.2
1	B	74	SER	4.2
1	C	255	LYS	4.2
1	C	524	VAL	4.2
1	C	16	PRO	4.2
1	C	271	MET	4.2
1	C	342	GLY	4.2
1	B	228	PHE	4.2
1	D	416	GLU	4.2
1	A	160	PRO	4.2
1	A	372	VAL	4.2
1	A	401	ILE	4.2
1	B	430	VAL	4.2
1	B	502	VAL	4.2
1	D	214	PRO	4.2
1	B	183	LYS	4.2
1	A	519	LEU	4.2
1	D	51	VAL	4.2
1	D	537	VAL	4.2
1	A	266	ILE	4.2
1	D	294	GLY	4.2
1	D	162	SER	4.2
1	D	148	PHE	4.2
1	B	110	LEU	4.2
1	C	59	LEU	4.2
1	A	15	VAL	4.2
1	A	511	VAL	4.2
1	D	490	GLY	4.2
1	C	476	ASN	4.2
1	B	227	MET	4.2
1	B	290	CYS	4.2
1	B	465	HIS	4.2
1	D	505	GLN	4.2
1	C	35	TYR	4.2
1	B	265	LEU	4.1
1	C	253	VAL	4.1
1	B	89	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	156	SER	4.1
1	D	78	SER	4.1
1	C	235	PRO	4.1
1	D	393	ARG	4.1
1	B	442	LEU	4.1
1	A	405	ASP	4.1
1	C	146	ASP	4.1
1	B	312	ARG	4.1
1	A	250	THR	4.1
1	B	158	ASN	4.1
1	B	531	ASN	4.1
1	C	506	ASN	4.1
1	B	300	GLY	4.1
1	B	432	TYR	4.1
1	B	49	LEU	4.1
1	D	503	LEU	4.1
1	B	50	ARG	4.1
1	B	72	ARG	4.1
1	C	185	MET	4.1
1	A	360	LYS	4.1
1	C	177	ILE	4.1
1	A	42	GLY	4.1
1	A	129	GLN	4.1
1	D	157	GLN	4.1
1	A	461	LEU	4.1
1	B	400	ILE	4.1
1	B	181	ALA	4.1
1	D	249	MET	4.1
1	C	522	GLU	4.1
1	B	266	ILE	4.1
1	B	324	ILE	4.1
1	B	376	ARG	4.1
1	C	285	GLU	4.0
1	D	492	TYR	4.0
1	C	462	PHE	4.0
1	B	204	LEU	4.0
1	C	140	LEU	4.0
1	D	317	GLY	4.0
1	D	472	LEU	4.0
1	D	533	PRO	4.0
1	B	15	VAL	4.0
1	A	75	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	147	ILE	4.0
1	A	350	MET	4.0
1	B	458	PHE	4.0
1	B	360	LYS	4.0
1	A	50[A]	ARG	4.0
1	C	92	ASP	4.0
1	C	244	GLY	4.0
1	C	411	MET	4.0
1	D	357	PRO	4.0
1	D	429	PRO	4.0
1	A	450	THR	4.0
1	B	392	THR	4.0
1	C	208	THR	4.0
1	C	374	LEU	4.0
1	B	38	VAL	4.0
1	D	289	VAL	4.0
1	C	229	GLY	4.0
1	D	271	MET	4.0
1	C	167	LYS	4.0
1	A	12	PHE	4.0
1	A	94	PHE	4.0
1	C	319	SER	4.0
1	D	52	ASP	4.0
1	C	137	GLU	4.0
1	D	473	ALA	4.0
1	C	86	PRO	4.0
1	C	210	SER	4.0
1	B	179	LEU	4.0
1	B	546	PHE	4.0
1	D	266	ILE	4.0
1	C	66	ASP	3.9
1	B	244	GLY	3.9
1	A	72	ARG	3.9
1	A	144	VAL	3.9
1	B	18	VAL	3.9
1	D	332	ARG	3.9
1	B	518	ASP	3.9
1	A	150	LYS	3.9
1	C	311	ILE	3.9
1	B	106	SER	3.9
1	C	246	SER	3.9
1	A	342	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	143	GLY	3.9
1	B	178	ASP	3.9
1	B	390	VAL	3.9
1	A	467	GLY	3.9
1	A	475	GLY	3.9
1	A	112	PRO	3.9
1	B	31	LEU	3.9
1	B	335	LEU	3.9
1	D	237	HIS	3.9
1	D	433	ALA	3.9
1	B	535	PHE	3.9
1	C	251	MET	3.9
1	A	223	GLU	3.9
1	A	481	VAL	3.9
1	B	182	SER	3.9
1	C	275	TYR	3.9
1	B	142	ARG	3.9
1	B	515	ASP	3.9
1	A	533	PRO	3.9
1	B	247	ALA	3.9
1	D	199	ALA	3.9
1	B	83	PHE	3.9
1	B	299	PHE	3.9
1	C	446	SER	3.9
1	A	178	ASP	3.9
1	B	243	GLY	3.9
1	A	367	THR	3.9
1	A	397	THR	3.9
1	C	527	ILE	3.9
1	D	428	HIS	3.9
1	B	193	ALA	3.9
1	C	50	ARG	3.9
1	A	411	MET	3.9
1	C	176	GLN	3.9
1	D	180	TYR	3.9
1	D	267	THR	3.9
1	D	392	THR	3.9
1	B	122	ILE	3.9
1	B	437	LYS	3.9
1	C	309	ARG	3.8
1	B	96	ALA	3.8
1	D	305	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	163	MET	3.8
1	B	503	LEU	3.8
1	D	301	GLY	3.8
1	B	51	VAL	3.8
1	C	310	VAL	3.8
1	B	230	THR	3.8
1	C	320	CYS	3.8
1	D	278	ARG	3.8
1	B	187	TYR	3.8
1	D	223	GLU	3.8
1	D	452	ALA	3.8
1	B	225	LEU	3.8
1	C	267	THR	3.8
1	C	166	GLU	3.8
1	B	438	GLN	3.8
1	B	88	ALA	3.8
1	B	105	ILE	3.8
1	C	436	ALA	3.8
1	C	452	ALA	3.8
1	C	313	MET	3.8
1	D	221	LEU	3.8
1	D	287	LEU	3.8
1	A	85	ASP	3.8
1	D	57	THR	3.8
1	B	470	VAL	3.8
1	C	387	LYS	3.8
1	D	21	VAL	3.8
1	D	446	SER	3.8
1	A	143	GLY	3.8
1	A	452	ALA	3.8
1	B	48	MET	3.8
1	B	484	ALA	3.8
1	A	496	ILE	3.8
1	D	295	MET	3.8
1	B	140	LEU	3.8
1	C	389	PRO	3.8
1	A	538	VAL	3.8
1	C	14	PHE	3.8
1	B	127	GLY	3.8
1	C	170	GLY	3.8
1	B	295	MET	3.8
1	C	306	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	116	ASP	3.8
1	D	331	ASP	3.8
1	B	99	LEU	3.8
1	B	78	SER	3.8
1	A	243	GLY	3.8
1	C	197	GLY	3.8
1	C	238	VAL	3.8
1	B	43	ALA	3.8
1	B	85	ASP	3.8
1	B	500	ALA	3.8
1	A	22	SER	3.7
1	A	60	SER	3.7
1	C	340	LYS	3.7
1	B	173	LEU	3.7
1	A	211	VAL	3.7
1	A	330	ALA	3.7
1	A	438	GLN	3.7
1	A	358	ASP	3.7
1	A	498	GLY	3.7
1	B	490	GLY	3.7
1	C	118	GLY	3.7
1	D	270	ASP	3.7
1	B	212	LEU	3.7
1	D	461	LEU	3.7
1	B	251	MET	3.7
1	C	404	ARG	3.7
1	C	538	VAL	3.7
1	D	516	MET	3.7
1	B	28	TYR	3.7
1	A	526	ARG	3.7
1	D	56	LEU	3.7
1	B	257	ALA	3.7
1	B	259	CYS	3.7
1	B	339	ASN	3.7
1	C	158	ASN	3.7
1	B	501	ALA	3.7
1	C	425	MET	3.7
1	C	523	ALA	3.7
1	D	257	ALA	3.7
1	D	149[A]	GLN	3.7
1	C	269	PRO	3.7
1	C	440	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	3.7
1	C	482	THR	3.7
1	A	503	LEU	3.7
1	B	199	ALA	3.7
1	C	120	ALA	3.7
1	C	248	GLU	3.7
1	C	254	LEU	3.7
1	C	416	GLU	3.7
1	D	382	LEU	3.7
1	B	62	THR	3.7
1	B	237	HIS	3.7
1	B	268	LYS	3.7
1	C	484	ALA	3.7
1	D	394	LEU	3.7
1	C	308	VAL	3.7
1	D	325	GLY	3.7
1	A	400	ILE	3.6
1	D	255	LYS	3.6
1	B	125	TYR	3.6
1	C	180	TYR	3.6
1	A	305	ALA	3.6
1	B	494	GLY	3.6
1	A	286	VAL	3.6
1	A	288	LYS	3.6
1	B	34	ASP	3.6
1	B	248	GLU	3.6
1	B	53	PRO	3.6
1	B	236	TYR	3.6
1	B	505	GLN	3.6
1	C	250	THR	3.6
1	C	376	ARG	3.6
1	A	347	GLU	3.6
1	C	344	TRP	3.6
1	B	198	SER	3.6
1	B	104	ASN	3.6
1	C	40	GLN	3.6
1	D	401	ILE	3.6
1	D	339	ASN	3.6
1	A	356	LEU	3.6
1	B	260	HIS	3.6
1	D	260	HIS	3.6
1	D	477	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	470	VAL	3.6
1	D	202	SER	3.6
1	D	203	PHE	3.6
1	A	295	MET	3.6
1	C	455	MET	3.6
1	C	543	ASN	3.6
1	D	455	MET	3.6
1	B	55	ALA	3.6
1	C	318	ALA	3.6
1	D	247	ALA	3.6
1	A	303	TYR	3.6
1	B	58	LEU	3.6
1	B	519	LEU	3.6
1	C	265	LEU	3.6
1	A	327	SER	3.6
1	A	46	PRO	3.6
1	A	434	GLY	3.6
1	A	453	GLY	3.6
1	D	329	SER	3.6
1	A	500	ALA	3.6
1	A	147	ILE	3.6
1	A	451	THR	3.6
1	A	514	LEU	3.6
1	B	161	LEU	3.6
1	B	423	GLN	3.6
1	C	333	GLN	3.6
1	C	335	LEU	3.6
1	C	438	GLN	3.6
1	D	217	LEU	3.6
1	D	348	LEU	3.6
1	C	502	VAL	3.6
1	A	448	GLY	3.6
1	D	50	ARG	3.6
1	C	160	PRO	3.6
1	A	190	MET	3.6
1	A	469	MET	3.6
1	C	190	MET	3.6
1	C	305	ALA	3.5
1	B	177	ILE	3.5
1	A	34	ASP	3.5
1	A	128	ASP	3.5
1	A	230	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	273	THR	3.5
1	A	73	SER	3.5
1	A	398	GLY	3.5
1	B	145	TYR	3.5
1	B	303	TYR	3.5
1	B	488	TYR	3.5
1	B	144	VAL	3.5
1	C	378	MET	3.5
1	B	413	GLU	3.5
1	C	157	GLN	3.5
1	B	482	THR	3.5
1	C	272	LYS	3.5
1	B	495	SER	3.5
1	A	499	PRO	3.5
1	C	41	PRO	3.5
1	A	328	CYS	3.5
1	C	164	TYR	3.5
1	C	330	ALA	3.5
1	C	334	ALA	3.5
1	B	13	ASN	3.5
1	A	171	THR	3.5
1	A	494	GLY	3.5
1	D	138	GLU	3.5
1	D	388	HIS	3.5
1	B	253	VAL	3.5
1	B	262	TYR	3.5
1	B	411	MET	3.5
1	A	192	VAL	3.5
1	B	431	TYR	3.5
1	A	270	ASP	3.5
1	B	279	ASP	3.5
1	B	524	VAL	3.5
1	A	369	ALA	3.5
1	B	328	CYS	3.5
1	B	334	ALA	3.5
1	A	302	LYS	3.5
1	D	321	PRO	3.5
1	A	374	LEU	3.5
1	A	378	MET	3.5
1	B	463	GLN	3.5
1	A	229	GLY	3.5
1	B	73	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	316	HIS	3.5
1	D	119	THR	3.5
1	B	65	ASP	3.5
1	A	543	ASN	3.5
1	D	152	ASN	3.5
1	A	70	LEU	3.5
1	A	254	LEU	3.5
1	B	241	VAL	3.5
1	C	228	PHE	3.4
1	C	199	ALA	3.4
1	B	113	GLY	3.4
1	C	263	ASP	3.4
1	A	482	THR	3.4
1	A	220	PHE	3.4
1	A	77	MET	3.4
1	D	281	GLU	3.4
1	B	17	LEU	3.4
1	D	84	ASP	3.4
1	C	194	LYS	3.4
1	C	98	GLN	3.4
1	A	74	SER	3.4
1	A	478	SER	3.4
1	A	527	ILE	3.4
1	A	421	LEU	3.4
1	B	206	GLN	3.4
1	C	15	VAL	3.4
1	D	412	ARG	3.4
1	A	196	GLY	3.4
1	C	222	LYS	3.4
1	A	290	CYS	3.4
1	A	167	LYS	3.4
1	C	116	ASP	3.4
1	D	279	ASP	3.4
1	D	196	GLY	3.4
1	A	506	ASN	3.4
1	B	444	SER	3.4
1	D	200	ASN	3.4
1	A	83	PHE	3.4
1	D	500	ALA	3.4
1	A	385	LEU	3.4
1	B	20	LYS	3.4
1	B	310	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	298	GLN	3.4
1	C	418	GLY	3.4
1	B	91	ASN	3.3
1	B	258	SER	3.3
1	B	395	SER	3.3
1	D	469	MET	3.3
1	A	257	ALA	3.3
1	B	504	ALA	3.3
1	C	226	ALA	3.3
1	C	239	ALA	3.3
1	D	47	GLU	3.3
1	B	293	ILE	3.3
1	D	161	LEU	3.3
1	A	91	ASN	3.3
1	B	538	VAL	3.3
1	B	316	HIS	3.3
1	D	72	ARG	3.3
1	D	142	ARG	3.3
1	A	249	MET	3.3
1	A	540	ASP	3.3
1	A	105	ILE	3.3
1	A	245	THR	3.3
1	B	292	ASN	3.3
1	D	391	ARG	3.3
1	B	374	LEU	3.3
1	B	61	SER	3.3
1	D	515	ASP	3.3
1	C	290	CYS	3.3
1	B	426	LYS	3.3
1	C	339	ASN	3.3
1	D	292	ASN	3.3
1	A	62	THR	3.3
1	A	491	PHE	3.3
1	A	106	SER	3.3
1	B	79	LEU	3.3
1	A	430	VAL	3.3
1	B	67	VAL	3.3
1	A	321	PRO	3.3
1	A	483	LYS	3.3
1	A	523	ALA	3.3
1	C	477	ARG	3.3
1	D	235	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	118	GLY	3.3
1	C	147	ILE	3.3
1	D	154	ARG	3.3
1	C	286	VAL	3.3
1	B	434	GLY	3.3
1	D	306	HIS	3.3
1	A	57	THR	3.3
1	A	513	CYS	3.3
1	A	31	LEU	3.3
1	D	439	PRO	3.3
1	A	66	ASP	3.2
1	B	231	SER	3.2
1	C	327	SER	3.2
1	C	547	GLU	3.2
1	D	454	ARG	3.2
1	D	133	PRO	3.2
1	C	215	LYS	3.2
1	A	390	VAL	3.2
1	A	407	ALA	3.2
1	A	408	HIS	3.2
1	C	36	VAL	3.2
1	D	467	GLY	3.2
1	B	32	THR	3.2
1	A	339	ASN	3.2
1	A	525	TRP	3.2
1	A	242	ILE	3.2
1	D	240	VAL	3.2
1	A	234	PRO	3.2
1	A	435	PRO	3.2
1	A	355	TYR	3.2
1	C	489	GLY	3.2
1	B	409	ALA	3.2
1	C	108	ALA	3.2
1	C	201[A]	LYS	3.2
1	B	341	ASP	3.2
1	C	540	ASP	3.2
1	B	77	MET	3.2
1	B	486	HIS	3.2
1	D	75	HIS	3.2
1	C	395	SER	3.2
1	A	365	LEU	3.2
1	B	70	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	52	ASP	3.2
1	A	163	MET	3.2
1	B	471[A]	MET	3.2
1	D	127	GLY	3.2
1	C	37	SER	3.2
1	D	404	ARG	3.2
1	B	82	ILE	3.2
1	A	119	THR	3.2
1	D	524	VAL	3.2
1	D	377	PRO	3.1
1	B	428	HIS	3.1
1	D	141	SER	3.1
1	C	487	LYS	3.1
1	D	272	LYS	3.1
1	A	87	GLU	3.1
1	B	148	PHE	3.1
1	B	398	GLY	3.1
1	C	67	VAL	3.1
1	A	136	ASP	3.1
1	A	107	SER	3.1
1	B	154	ARG	3.1
1	B	210	SER	3.1
1	A	244	GLY	3.1
1	A	399	THR	3.1
1	B	235	PRO	3.1
1	C	42	GLY	3.1
1	C	85	ASP	3.1
1	A	29	ARG	3.1
1	B	249	MET	3.1
1	D	186	GLU	3.1
1	D	285	GLU	3.1
1	B	123	ALA	3.1
1	A	333	GLN	3.1
1	A	44	GLY	3.1
1	A	376	ARG	3.1
1	C	152	ASN	3.1
1	A	189	PHE	3.1
1	B	447	PHE	3.1
1	B	132	VAL	3.1
1	A	120	ALA	3.1
1	A	139	ALA	3.1
1	B	509	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	183	LYS	3.1
1	B	229	GLY	3.1
1	B	457	PRO	3.1
1	A	45	LEU	3.1
1	A	145	TYR	3.1
1	B	492	TYR	3.1
1	D	432	TYR	3.1
1	A	502	VAL	3.1
1	D	470	VAL	3.1
1	C	54	ALA	3.1
1	B	408	HIS	3.1
1	B	174	PRO	3.1
1	D	224	LYS	3.1
1	B	280	LEU	3.1
1	B	349	GLU	3.1
1	A	191	PHE	3.1
1	A	458	PHE	3.1
1	A	492	TYR	3.1
1	A	535	PHE	3.1
1	D	122	ILE	3.1
1	D	118	GLY	3.0
1	D	239	ALA	3.0
1	D	300	GLY	3.0
1	D	486	HIS	3.0
1	B	480	GLN	3.0
1	C	115	GLN	3.0
1	D	246	SER	3.0
1	A	521	MET	3.0
1	A	259	CYS	3.0
1	B	189	PHE	3.0
1	D	448	GLY	3.0
1	C	548	GLN	3.0
1	C	78	SER	3.0
1	A	279	ASP	3.0
1	C	373	ASN	3.0
1	A	282	LEU	3.0
1	A	465	HIS	3.0
1	B	445	GLY	3.0
1	C	87	GLU	3.0
1	C	294	GLY	3.0
1	D	489	GLY	3.0
1	A	51	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	433	ALA	3.0
1	C	159	VAL	3.0
1	D	538	VAL	3.0
1	A	231	SER	3.0
1	A	319	SER	3.0
1	A	386	SER	3.0
1	D	312	ARG	3.0
1	A	392	THR	3.0
1	A	194	LYS	3.0
1	A	166	GLU	3.0
1	B	506	ASN	3.0
1	A	65	ASP	3.0
1	A	210	SER	3.0
1	B	63	ALA	3.0
1	B	139	ALA	3.0
1	D	18	VAL	3.0
1	A	489	GLY	3.0
1	B	388	HIS	3.0
1	B	418	GLY	3.0
1	C	260	HIS	3.0
1	B	146	ASP	3.0
1	A	256	TYR	3.0
1	B	208	THR	3.0
1	C	169	THR	3.0
1	B	87	GLU	3.0
1	B	60	SER	3.0
1	B	291	GLN	3.0
1	D	548	GLN	3.0
1	A	18	VAL	2.9
1	A	228	PHE	2.9
1	C	57	THR	2.9
1	C	121	ILE	2.9
1	D	195	GLY	2.9
1	D	252	LYS	2.9
1	D	525	TRP	2.9
1	A	445	GLY	2.9
1	B	448	GLY	2.9
1	D	73	SER	2.9
1	A	54	ALA	2.9
1	B	473	ALA	2.9
1	A	17	LEU	2.9
1	A	255	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	370	VAL	2.9
1	D	451	THR	2.9
1	A	182	SER	2.9
1	B	478	SER	2.9
1	A	332	ARG	2.9
1	C	68	GLU	2.9
1	C	473	ALA	2.9
1	D	85	ASP	2.9
1	B	150	LYS	2.9
1	D	151	ARG	2.9
1	D	413	GLU	2.9
1	A	59	LEU	2.9
1	A	179	LEU	2.9
1	A	40	GLN	2.9
1	A	186	GLU	2.9
1	A	419	LYS	2.9
1	B	548	GLN	2.9
1	C	24	LYS	2.9
1	D	419	LYS	2.9
1	B	289	VAL	2.9
1	A	362	ASP	2.9
1	B	155	TYR	2.9
1	A	123	ALA	2.9
1	A	291	GLN	2.9
1	A	349	GLU	2.9
1	C	427	GLU	2.9
1	D	380	GLU	2.9
1	D	80	ARG	2.9
1	A	79	LEU	2.9
1	A	382	LEU	2.9
1	C	249	MET	2.9
1	D	188	SER	2.9
1	A	443	PRO	2.9
1	B	36	VAL	2.9
1	B	326	VAL	2.9
1	A	261	TYR	2.9
1	B	226	ALA	2.9
1	B	452	ALA	2.9
1	A	152	ASN	2.9
1	D	476	ASN	2.9
1	A	246	SER	2.9
1	B	217	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	455	MET	2.9
1	B	285	GLU	2.9
1	D	389	PRO	2.9
1	C	34	ASP	2.8
1	A	76	LEU	2.8
1	A	204	LEU	2.8
1	A	359	LEU	2.8
1	B	121	ILE	2.8
1	B	242	ILE	2.8
1	D	219	ASN	2.8
1	A	462	PHE	2.8
1	C	517	LYS	2.8
1	A	89	SER	2.8
1	A	352	PRO	2.8
1	A	457	PRO	2.8
1	A	529	VAL	2.8
1	D	545	PHE	2.8
1	B	40	GLN	2.8
1	A	86	PRO	2.8
1	A	23	HIS	2.8
1	D	204	LEU	2.8
1	A	487	LYS	2.8
1	B	451	THR	2.8
1	C	207	GLU	2.8
1	C	302	LYS	2.8
1	A	294	GLY	2.8
1	A	30	LEU	2.8
1	A	217	LEU	2.8
1	B	232	ALA	2.8
1	B	52	ASP	2.8
1	B	307	ASP	2.8
1	B	491	PHE	2.8
1	D	307	ASP	2.8
1	C	498	GLY	2.8
1	C	142	ARG	2.8
1	B	337	LYS	2.8
1	A	198	SER	2.8
1	B	22	SER	2.8
1	B	135	ASN	2.7
1	C	168	ASN	2.7
1	C	388	HIS	2.7
1	D	316	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	206	GLN	2.7
1	D	342	GLY	2.7
1	D	411	MET	2.7
1	A	532	PHE	2.7
1	B	131	PHE	2.7
1	C	458	PHE	2.7
1	B	406	SER	2.7
1	C	261	TYR	2.7
1	D	74	SER	2.7
1	B	345	LEU	2.7
1	B	200	ASN	2.7
1	A	429	PRO	2.7
1	C	412	ARG	2.7
1	D	450	THR	2.7
1	B	191	PHE	2.7
1	A	361	GLU	2.7
1	A	133	PRO	2.7
1	A	433	ALA	2.7
1	B	352	PRO	2.7
1	C	368	PRO	2.7
1	D	232	ALA	2.7
1	D	184	GLY	2.7
1	A	456	ASP	2.7
1	B	540	ASP	2.7
1	D	268	LYS	2.7
1	A	206	GLN	2.7
1	A	441	GLY	2.7
1	B	301	GLY	2.7
1	B	323	GLY	2.7
1	A	431	TYR	2.7
1	B	304	TYR	2.7
1	D	28	TYR	2.7
1	B	245	THR	2.7
1	C	230	THR	2.7
1	A	38	VAL	2.7
1	A	268	LYS	2.7
1	A	412	ARG	2.7
1	A	184	GLY	2.7
1	C	422	PRO	2.7
1	C	539	ASP	2.7
1	B	114	CYS	2.7
1	B	468	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	216	SER	2.7
1	D	327	SER	2.7
1	A	248	GLU	2.7
1	B	47	GLU	2.7
1	C	429	PRO	2.7
1	D	383	GLN	2.7
1	B	284	GLU	2.6
1	A	428	HIS	2.6
1	D	27	LYS	2.6
1	B	453	GLY	2.6
1	D	197	GLY	2.6
1	B	338	ILE	2.6
1	D	480	GLN	2.6
1	D	29	ARG	2.6
1	D	315	ARG	2.6
1	A	200	ASN	2.6
1	D	102	ASN	2.6
1	B	359	LEU	2.6
1	B	421	LEU	2.6
1	D	345	LEU	2.6
1	D	444	SER	2.6
1	A	116	ASP	2.6
1	B	126	ARG	2.6
1	C	278	ARG	2.6
1	C	375	ASN	2.6
1	C	93	LYS	2.6
1	B	107	SER	2.6
1	A	125	TYR	2.6
1	A	381	VAL	2.6
1	A	389	PRO	2.6
1	C	481	VAL	2.6
1	D	547	GLU	2.6
1	D	337	LYS	2.6
1	A	409	ALA	2.6
1	B	318	ALA	2.6
1	C	407	ALA	2.6
1	C	12	PHE	2.6
1	D	117	THR	2.6
1	C	279	ASP	2.6
1	B	393	ARG	2.6
1	C	499	PRO	2.6
1	B	92	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	332	ARG	2.6
1	C	136	ASP	2.6
1	C	413	GLU	2.6
1	C	474	LYS	2.6
1	A	424	TYR	2.6
1	B	149	GLN	2.6
1	D	405	ASP	2.6
1	A	464	SER	2.6
1	A	484	ALA	2.6
1	A	274	GLY	2.6
1	B	542	GLY	2.6
1	B	86	PRO	2.6
1	A	92	ASP	2.5
1	A	387	LYS	2.5
1	A	329	SER	2.5
1	A	127	GLY	2.5
1	B	344	TRP	2.5
1	A	505	GLN	2.5
1	A	263	ASP	2.5
1	A	530	GLU	2.5
1	B	464	SER	2.5
1	A	297	ALA	2.5
1	B	170	GLY	2.5
1	C	466	GLY	2.5
1	B	169	THR	2.5
1	C	109	ARG	2.5
1	B	264	ASP	2.5
1	B	283	GLU	2.5
1	C	347	GLU	2.5
1	B	81	LYS	2.5
1	A	404	ARG	2.5
1	A	497	GLY	2.5
1	B	404	ARG	2.5
1	D	298	GLN	2.5
1	A	449	PRO	2.5
1	B	37	SER	2.5
1	B	69	HIS	2.5
1	B	213	ASN	2.5
1	B	124	GLY	2.5
1	D	434	GLY	2.5
1	B	117	THR	2.5
1	D	24	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	39	VAL	2.5
1	D	112	PRO	2.5
1	B	115	GLN	2.5
1	D	495	SER	2.5
1	A	165	ASP	2.5
1	A	341	ASP	2.5
1	A	460	ASP	2.5
1	A	515	ASP	2.5
1	A	197	GLY	2.5
1	A	140	LEU	2.4
1	A	273	THR	2.4
1	B	138	GLU	2.4
1	D	87	GLU	2.4
1	D	498	GLY	2.4
1	A	226	ALA	2.4
1	A	115	GLN	2.4
1	D	129	GLN	2.4
1	B	188	SER	2.4
1	B	246	SER	2.4
1	B	467	GLY	2.4
1	A	320	CYS	2.4
1	C	403	ALA	2.4
1	D	407	ALA	2.4
1	B	185	MET	2.4
1	B	357	PRO	2.4
1	B	387	LYS	2.4
1	B	386	SER	2.4
1	C	156	SER	2.4
1	B	296	GLY	2.4
1	B	325	GLY	2.4
1	C	196	GLY	2.4
1	A	95	VAL	2.4
1	A	423	GLN	2.4
1	A	480	GLN	2.4
1	A	82	ILE	2.4
1	B	112	PRO	2.4
1	A	306	HIS	2.4
1	A	486	HIS	2.4
1	B	327	SER	2.4
1	B	416	GLU	2.4
1	A	81	LYS	2.4
1	A	214	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	252	LYS	2.4
1	C	268	LYS	2.4
1	B	166	GLU	2.4
1	A	507	ALA	2.4
1	A	27	LYS	2.4
1	B	19	SER	2.4
1	B	27	LYS	2.4
1	A	219	ASN	2.3
1	D	375	ASN	2.3
1	B	351	GLU	2.3
1	A	201	LYS	2.3
1	A	209	LYS	2.3
1	A	313	MET	2.3
1	D	89	SER	2.3
1	D	464	SER	2.3
1	A	101	LYS	2.3
1	A	176	GLN	2.3
1	A	312	ARG	2.3
1	B	309	ARG	2.3
1	C	480	GLN	2.3
1	B	202	SER	2.3
1	B	136	ASP	2.3
1	C	63	ALA	2.3
1	A	69	HIS	2.3
1	C	214	PRO	2.3
1	A	336	GLY	2.3
1	A	406	SER	2.3
1	A	446	SER	2.3
1	B	263	ASP	2.3
1	A	426	LYS	2.3
1	A	172	ASN	2.3
1	A	96	ALA	2.3
1	A	309	ARG	2.3
1	A	425	MET	2.3
1	A	354	GLN	2.3
1	C	423	GLN	2.3
1	A	485	CYS	2.3
1	C	437	LYS	2.3
1	B	157	GLN	2.3
1	B	159	VAL	2.3
1	D	241	VAL	2.3
1	A	544	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	410	ARG	2.3
1	D	349	GLU	2.3
1	A	417	ALA	2.2
1	B	100	LEU	2.2
1	B	194	LYS	2.2
1	D	297	ALA	2.2
1	A	413	GLU	2.2
1	C	410	ARG	2.2
1	A	61[A]	SER	2.2
1	D	198	SER	2.2
1	D	296	GLY	2.2
1	D	449	PRO	2.2
1	A	252	LYS	2.2
1	A	272	LYS	2.2
1	D	101	LYS	2.2
1	A	55	ALA	2.2
1	B	190	MET	2.2
1	D	544	ASP	2.2
1	D	501	ALA	2.2
1	D	504	ALA	2.2
1	B	172	ASN	2.2
1	B	288	LYS	2.2
1	C	317	GLY	2.2
1	C	479	LYS	2.2
1	D	426	LYS	2.2
1	C	65	ASP	2.2
1	A	47	GLU	2.2
1	B	363	GLU	2.2
1	A	260	HIS	2.2
1	B	75	HIS	2.2
1	D	487	LYS	2.2
1	C	61	SER	2.2
1	A	253	VAL	2.2
1	B	66	ASP	2.2
1	C	101	LYS	2.2
1	D	309	ARG	2.2
1	B	223	GLU	2.2
1	A	121	ILE	2.2
1	A	90	ASP	2.2
1	B	439	PRO	2.2
1	C	81	LYS	2.2
1	A	262	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	342	GLY	2.2
1	A	479	LYS	2.2
1	D	37	SER	2.2
1	B	16	PRO	2.2
1	B	298	GLN	2.1
1	B	412	ARG	2.2
1	A	351	GLU	2.1
1	B	281	GLU	2.1
1	A	146	ASP	2.1
1	C	20	LYS	2.1
1	A	208	THR	2.1
1	A	383	GLN	2.1
1	C	25	GLU	2.1
1	B	419	LYS	2.1
1	A	151	ARG	2.1
1	A	317	GLY	2.1
1	A	334	ALA	2.1
1	D	19	SER	2.1
1	B	528	GLU	2.1
1	B	533	PRO	2.1
1	B	23	HIS	2.1
1	B	440	ASP	2.1
1	A	138	GLU	2.1
1	A	468	SER	2.1
1	A	366	LYS	2.1
1	B	435	PRO	2.1
1	B	331	ASP	2.1
1	C	518	ASP	2.1
1	B	129	GLN	2.1
1	B	221	LEU	2.1
1	D	479	LYS	2.1
1	A	148	PHE	2.1
1	B	160	PRO	2.1
1	B	214	PRO	2.1
1	B	219	ASN	2.1
1	B	84	ASP	2.1
1	B	270	ASP	2.1
1	A	202	SER	2.1
1	A	455	MET	2.1
1	A	154	ARG	2.1
1	B	347	GLU	2.1
1	B	526	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	2.1
1	D	346	GLU	2.0
1	A	539	ASP	2.0
1	A	368	PRO	2.0
1	B	71	LEU	2.0
1	B	133	PRO	2.0
1	D	438	GLN	2.0
1	B	297	ALA	2.0
1	B	302	LYS	2.0
1	A	149	GLN	2.0
1	C	284	GLU	2.0
1	A	109	ARG	2.0
1	B	176	GLN	2.0
1	B	487	LYS	2.0
1	A	25	GLU	2.0
1	B	454	ARG	2.0
1	B	477	ARG	2.0
1	C	312	ARG	2.0
1	A	520	GLY	2.0
1	B	456	ASP	2.0
1	D	333	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	606	6/6	0.16	0.43	26,28,30,34	0
4	1PE	B	606	10/16	0.22	0.50	24,35,37,37	0

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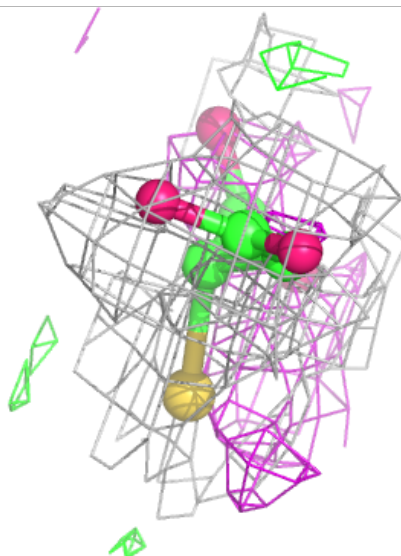
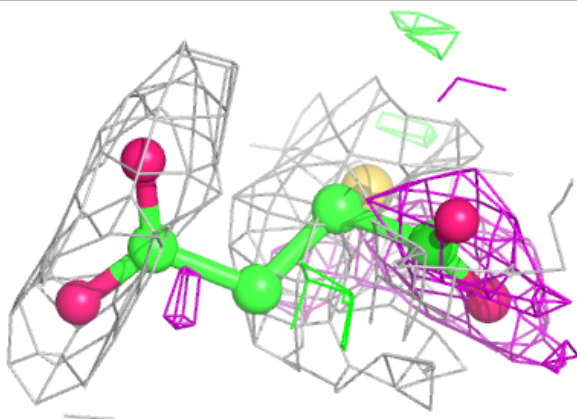
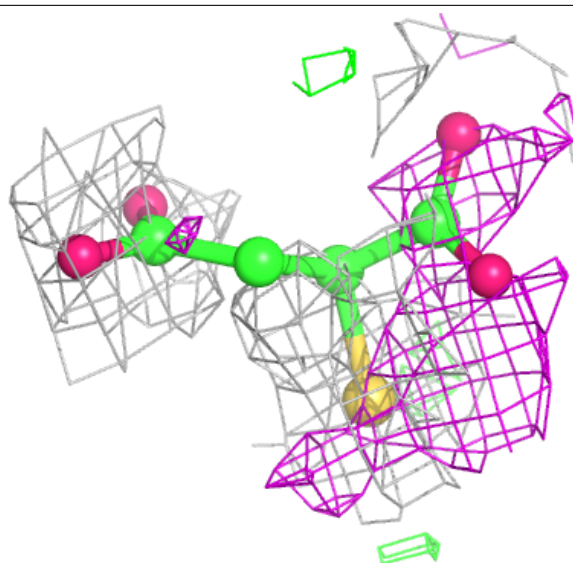
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	602	6/6	0.31	0.42	40,42,43,43	0
4	1PE	B	605	13/16	0.33	0.48	15,17,23,24	0
4	1PE	C	603	7/16	0.36	0.31	27,28,30,31	0
5	JYD	C	604	9/9	0.38	0.89	30,35,42,45	0
4	1PE	A	611	10/16	0.40	0.27	29,31,34,34	0
4	1PE	C	605	10/16	0.42	0.36	30,37,41,42	0
3	GOL	A	605	6/6	0.43	0.44	26,31,34,34	0
4	1PE	C	606	10/16	0.47	0.36	26,32,35,35	0
4	1PE	A	607	7/16	0.48	0.46	28,29,32,36	0
4	1PE	D	603	16/16	0.50	0.35	26,32,35,35	0
3	GOL	A	603	6/6	0.53	0.28	24,26,32,34	0
4	1PE	A	609	13/16	0.53	0.24	14,21,27,30	0
3	GOL	A	604	6/6	0.55	0.42	27,33,37,38	0
2	SF4	D	601	8/8	0.56	0.20	23,32,34,39	0
5	JYD	D	602	9/9	0.57	0.32	22,32,34,36	0
5	JYD	B	604[B]	9/9	0.60	0.34	9,10,12,14	9
5	JYD	B	604[A]	9/9	0.60	0.34	9,11,13,16	9
4	1PE	A	610	10/16	0.60	0.27	10,29,36,39	0
2	SF4	A	601	8/8	0.62	0.22	15,19,22,22	0
3	GOL	B	603	6/6	0.64	0.21	22,25,26,27	0
3	GOL	B	602	6/6	0.65	0.32	26,27,29,30	0
2	SF4	C	601	8/8	0.67	0.17	24,30,31,31	0
2	SF4	B	601	8/8	0.68	0.20	14,21,23,24	0
3	GOL	A	602	6/6	0.75	0.23	21,25,29,31	0
5	JYD	A	608[A]	9/9	0.81	0.30	17,17,18,21	9
5	JYD	A	608[B]	9/9	0.81	0.30	16,17,18,18	9

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

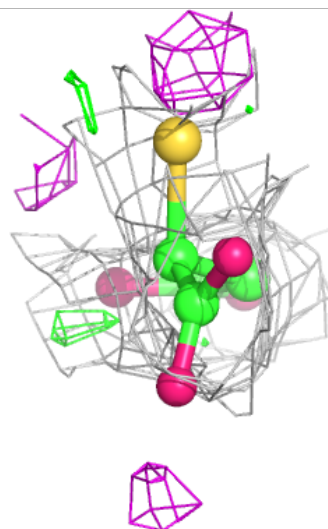
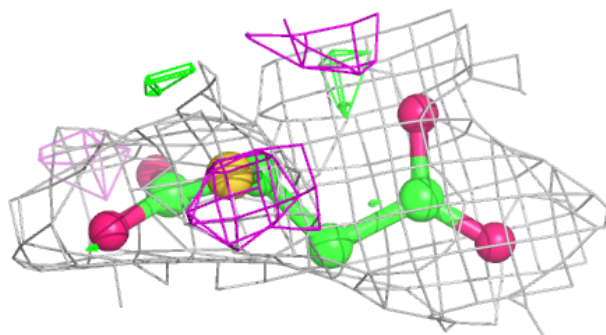
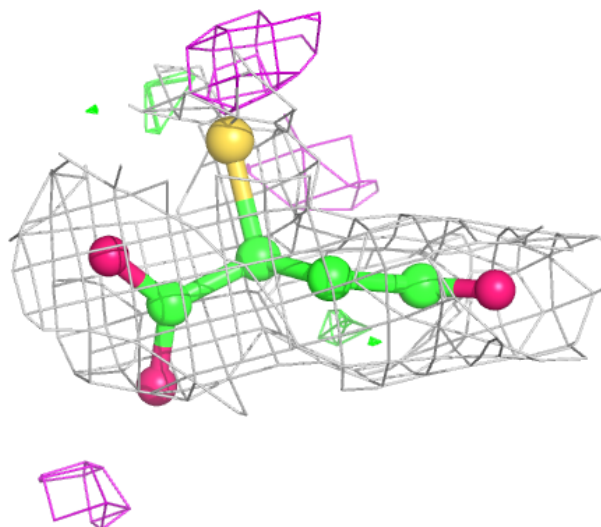
**Electron density around JYD C 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



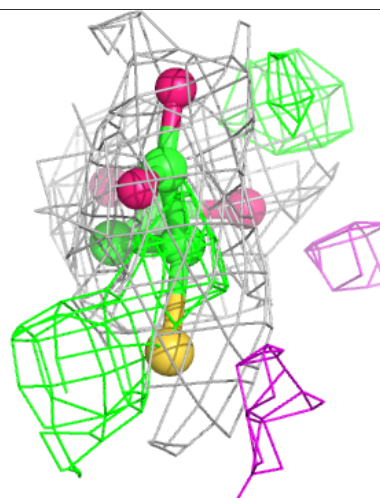
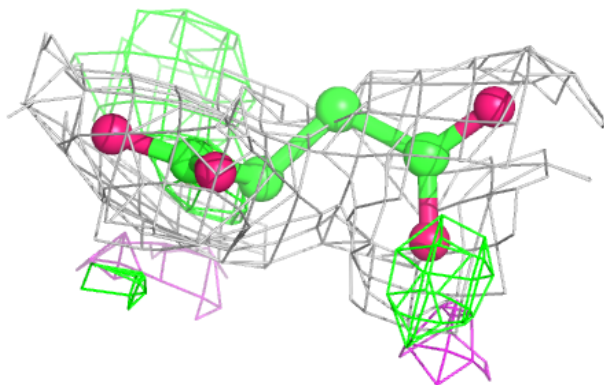
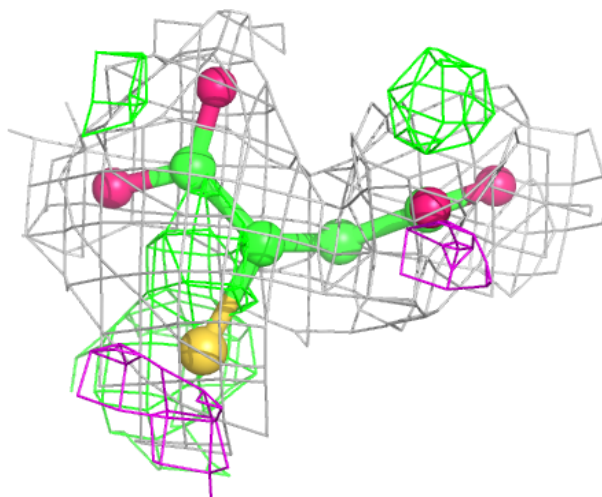
**Electron density around JYD D 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



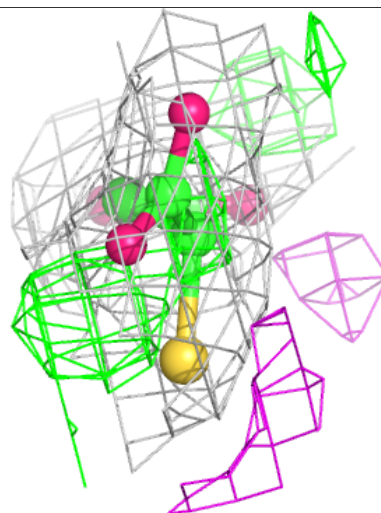
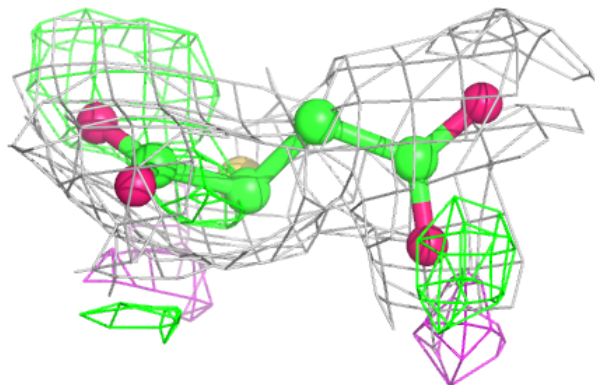
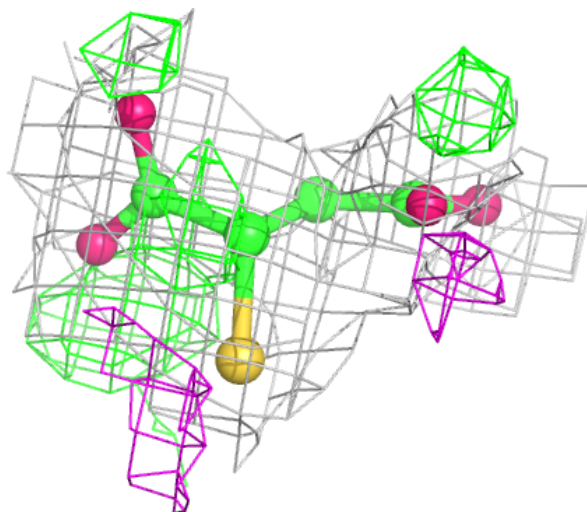
**Electron density around JYD B 604 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



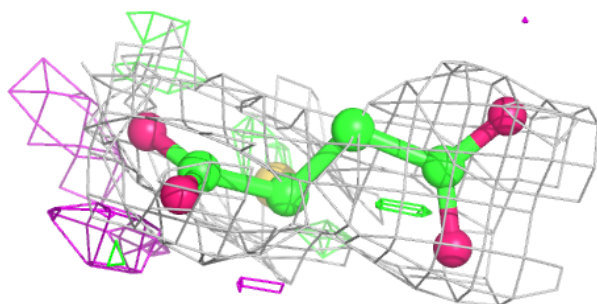
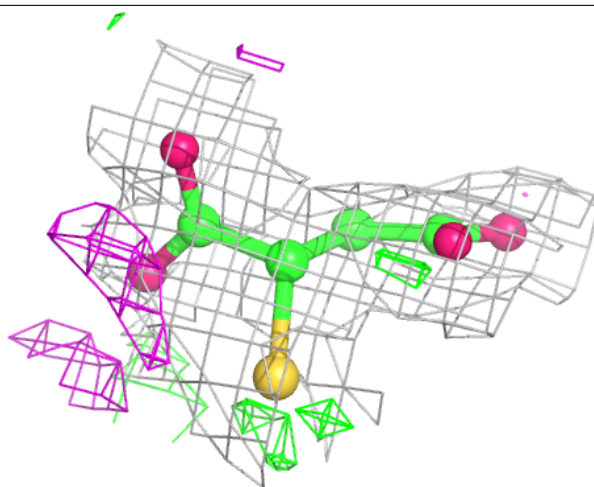
**Electron density around JYD B 604 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



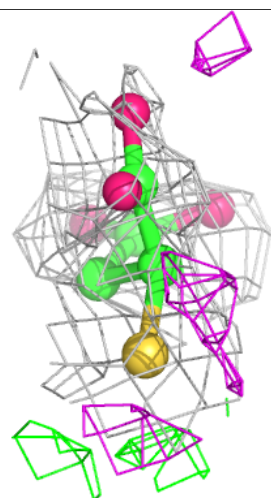
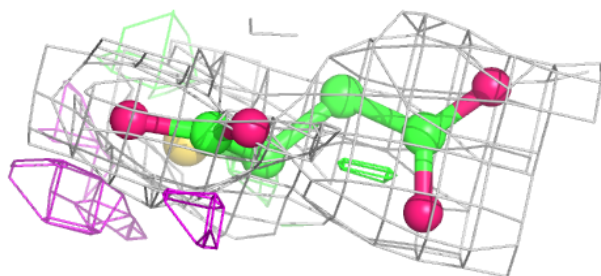
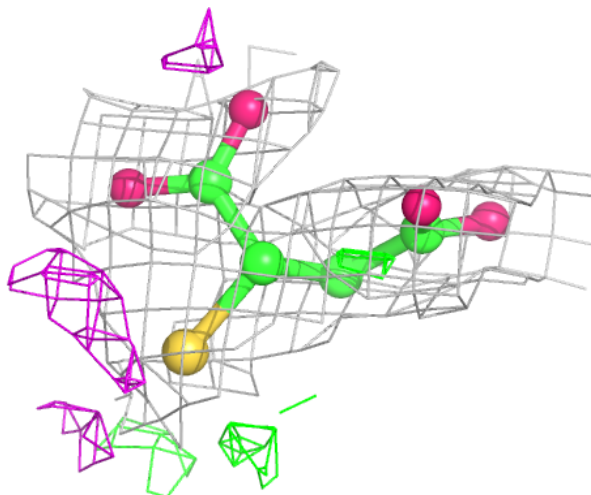
**Electron density around JYD A 608 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around JYD A 608 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.