



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:09 PM GMT

PDB ID : 1IXE  
Title : Crystal structure of citrate synthase from *Thermus thermophilus* HB8  
Authors : Murakami, M.; Kanamori, E.; Kawaguchi, S.; Kuramitsu, S.; Kouyama, T.;  
RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-06-20  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

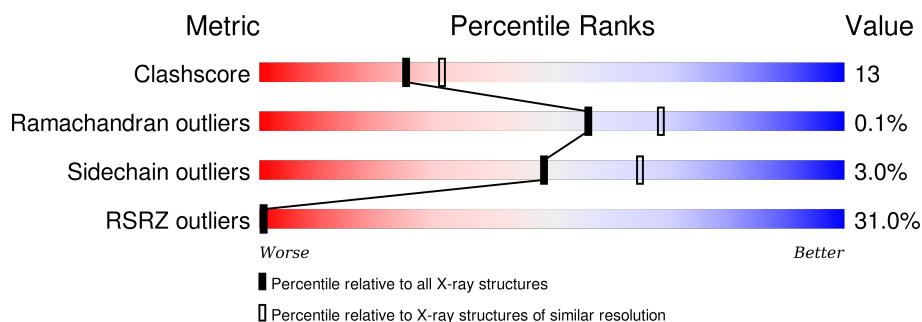
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	377	
1	B	377	
1	C	377	
1	D	377	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	383	-	-	-	X
2	SO4	C	390	-	-	-	X
2	SO4	D	389	-	-	-	X
3	COA	D	404	-	-	-	X
4	CIT	B	406	-	-	-	X
4	CIT	D	408	-	-	X	-
5	GOL	A	411	-	-	-	X
5	GOL	B	412	-	-	-	X
5	GOL	C	413	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12452 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 citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2920	1870	508	532	10			
1	B	370	Total	C	N	O	S	0	0	0
			2922	1871	507	534	10			
1	C	366	Total	C	N	O	S	0	0	0
			2887	1851	499	527	10			
1	D	366	Total	C	N	O	S	0	0	0
			2888	1851	501	526	10			

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



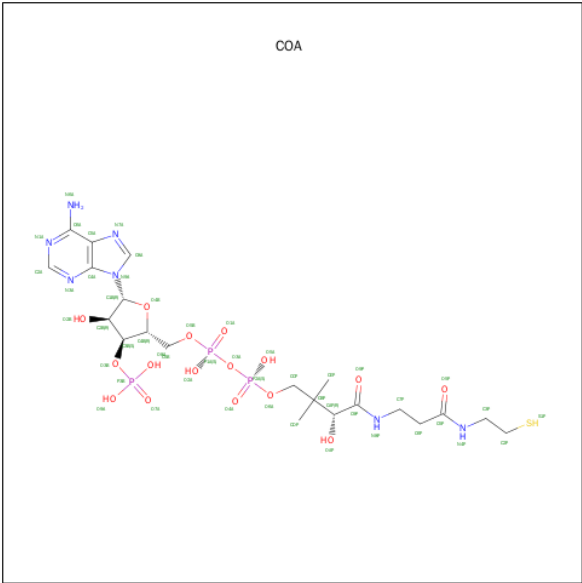
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



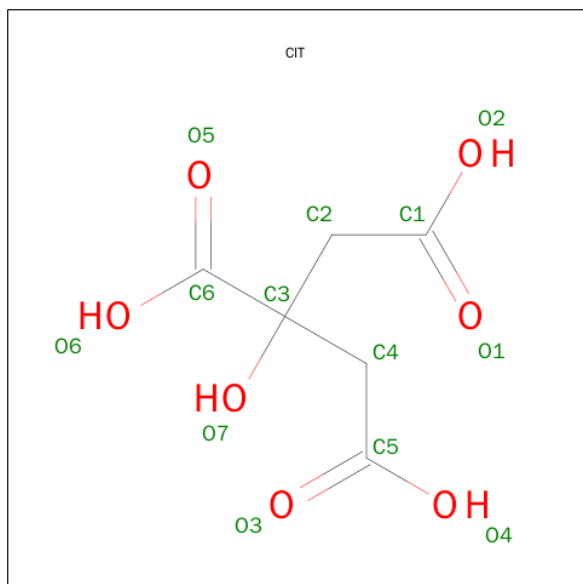
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

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



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

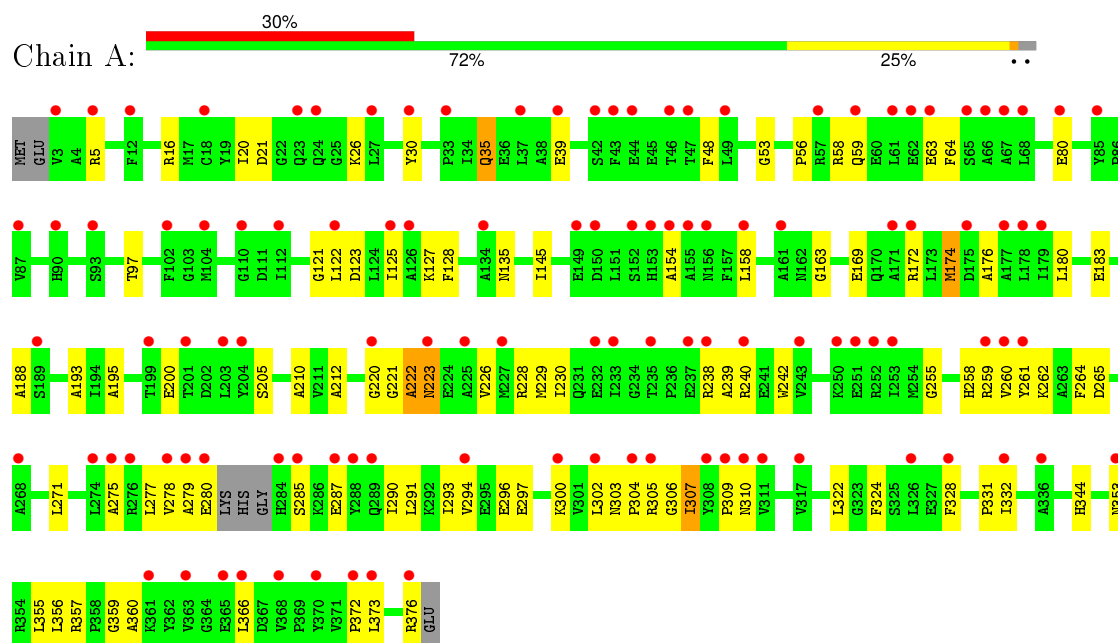
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	138	Total	O	0	0
			138	138		
6	C	120	Total	O	0	0
			120	120		
6	D	134	Total	O	0	0
			134	134		

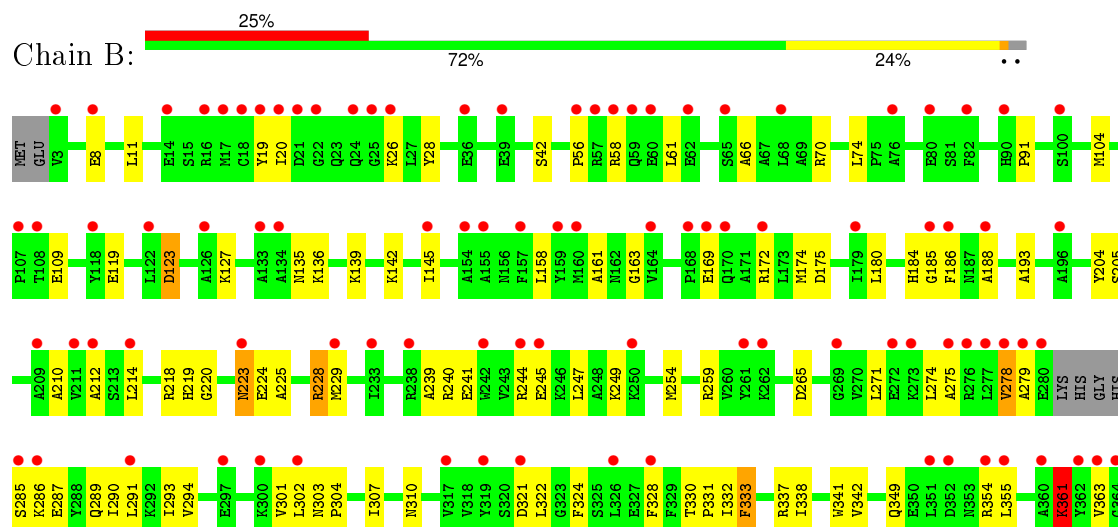
### 3 Residue-property plots

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

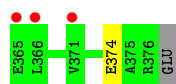
#### • Molecule 1: citrate synthase



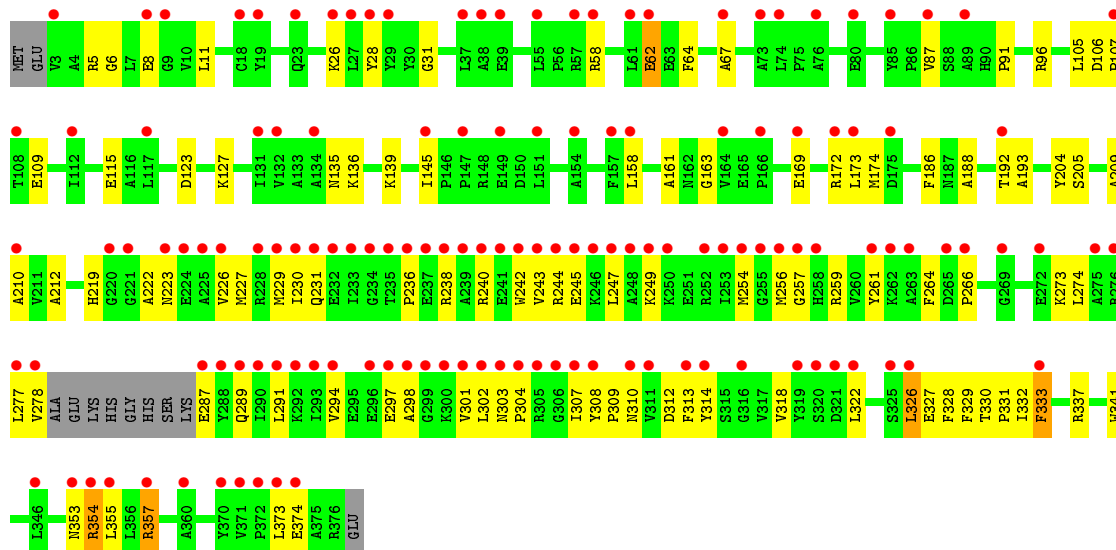
#### • Molecule 1: citrate synthase



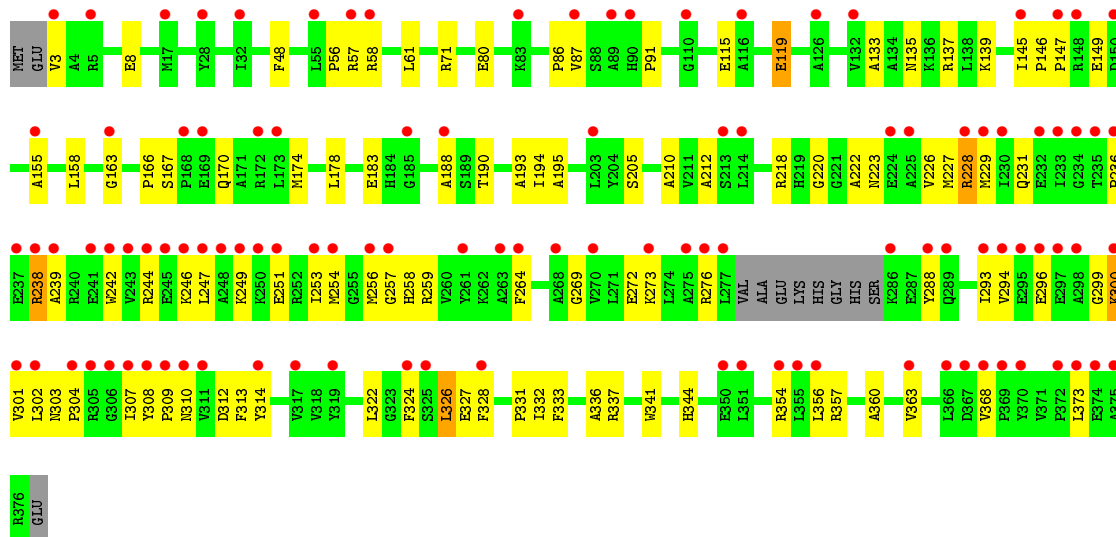




• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.01Å 110.63Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.79 – 2.30 14.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (14.79-2.30) 90.7 (14.79-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.177 , 0.217 0.185 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 66309 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, GOL, SO4, CIT

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	0.33	0/2986	0.47	0/4036
1	B	0.37	0/2987	0.51	0/4035
1	C	0.34	0/2952	0.48	0/3990
1	D	0.41	0/2953	0.54	0/3990
All	All	0.36	0/11878	0.50	0/16051

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LYS	Mainchain

### 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	2920	0	2911	81	0
1	B	2922	0	2924	76	0
1	C	2887	0	2884	87	0
1	D	2888	0	2888	89	0
2	A	10	0	0	0	0
2	B	15	0	0	2	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
3	C	48	0	32	1	0
3	D	48	0	32	11	0
4	A	13	0	5	1	0
4	B	13	0	5	1	0
4	C	13	0	5	0	0
4	D	13	0	5	6	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	125	0	0	1	0
6	B	138	0	0	6	0
6	C	120	0	0	1	0
6	D	134	0	0	3	0
All	All	12452	0	11787	302	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 13.

All (302) 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)
3:D:404:COA:H21	4:D:408:CIT:O4	1.53	1.06
3:D:404:COA:H21	4:D:408:CIT:C5	1.94	0.97
1:A:35:GLN:HE21	1:A:35:GLN:H	1.16	0.88
1:A:35:GLN:NE2	1:A:35:GLN:H	1.73	0.87
3:D:404:COA:C2P	4:D:408:CIT:O4	2.26	0.83
1:C:236:PRO:HG3	1:C:289:GLN:NE2	1.92	0.83
1:C:229:MET:HE1	1:C:254:MET:N	1.93	0.82
1:B:169:GLU:HG3	1:B:172:ARG:HH22	1.45	0.81
1:C:236:PRO:HG3	1:C:289:GLN:HE21	1.46	0.81
1:C:229:MET:HE1	1:C:254:MET:H	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD13	1:B:301:VAL:HG21	1.64	0.78
1:B:169:GLU:HG3	1:B:172:ARG:NH2	2.00	0.76
1:A:20:ILE:HG21	1:A:260:VAL:HG21	1.67	0.76
1:C:355:LEU:HD23	3:D:404:COA:H132	1.68	0.75
1:D:246:LYS:HE2	1:D:251:GLU:HB2	1.71	0.72
1:B:123:ASP:O	1:B:127:LYS:HG3	1.88	0.72
1:B:274:LEU:O	1:B:278:VAL:HG12	1.92	0.70
1:C:245:GLU:O	1:C:249:LYS:HD3	1.91	0.70
1:C:169:GLU:HG3	1:C:172:ARG:NH1	2.07	0.70
1:D:229:MET:HE1	1:D:254:MET:N	2.08	0.69
1:C:58:ARG:HA	1:D:373:LEU:HD11	1.74	0.68
1:C:357:ARG:HB3	1:D:259:ARG:HG2	1.75	0.67
1:A:200:GLU:HG3	1:B:218:ARG:HG3	1.76	0.67
1:B:142:LYS:HE3	6:B:896:HOH:O	1.94	0.67
1:C:205:SER:HB3	1:D:212:ALA:HB1	1.76	0.67
1:C:169:GLU:HG3	1:C:172:ARG:HH12	1.58	0.66
1:A:258:HIS:CE1	1:A:260:VAL:HG22	2.30	0.66
1:D:310:ASN:ND2	3:D:404:COA:H31	2.11	0.66
1:C:328:PHE:C	1:C:331:PRO:HD2	2.16	0.65
1:A:58:ARG:HH22	1:B:374:GLU:HA	1.62	0.65
1:B:193:ALA:HB2	1:B:210:ALA:HB2	1.79	0.65
1:B:229:MET:HE1	1:B:254:MET:H	1.62	0.64
1:A:222:ALA:HB2	3:A:401:COA:H31	1.79	0.64
1:C:354:ARG:HB2	1:C:354:ARG:HH11	1.63	0.64
1:D:149:GLU:HG3	6:D:589:HOH:O	1.97	0.64
1:D:324:PHE:CG	1:D:332:ILE:HD11	2.33	0.63
3:D:404:COA:C3P	4:D:408:CIT:O4	2.46	0.63
3:B:402:COA:H21	6:B:601:HOH:O	1.99	0.63
1:C:26:LYS:HE2	1:C:28:TYR:OH	1.99	0.63
1:D:363:VAL:O	1:D:363:VAL:HG12	1.98	0.63
1:A:5:ARG:NE	1:B:354:ARG:HH11	1.96	0.62
1:D:8:GLU:HG3	1:D:259:ARG:HD2	1.80	0.62
1:B:285:SER:O	1:B:289:GLN:HG3	2.00	0.62
3:D:404:COA:H22	6:D:801:HOH:O	2.00	0.62
1:D:174:MET:HE2	1:D:322:LEU:HD13	1.82	0.62
1:A:174:MET:HG2	1:A:322:LEU:HD13	1.82	0.62
1:D:294:VAL:HG23	1:D:313:PHE:HZ	1.64	0.61
1:B:302:LEU:HB3	1:B:307:ILE:HB	1.82	0.61
1:A:35:GLN:HE21	1:A:35:GLN:N	1.93	0.61
1:A:328:PHE:C	1:A:331:PRO:HD2	2.21	0.60
1:B:328:PHE:C	1:B:331:PRO:HD2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:O	1:D:226:VAL:HG23	2.02	0.60
1:A:297:GLU:O	1:A:300:LYS:HG2	2.00	0.60
1:D:167:SER:OG	1:D:170:GLN:HG3	2.02	0.60
1:A:324:PHE:CG	1:A:332:ILE:HD11	2.37	0.60
1:C:259:ARG:HG2	1:D:357:ARG:HB3	1.83	0.59
1:D:246:LYS:HE2	1:D:251:GLU:CB	2.31	0.59
1:B:158:LEU:HD21	1:B:174:MET:HE2	1.83	0.59
1:B:241:GLU:HG2	6:B:696:HOH:O	2.03	0.58
1:B:278:VAL:HG21	1:B:321:ASP:HB2	1.86	0.58
1:D:228:ARG:NH2	1:D:228:ARG:HB3	2.18	0.58
1:A:212:ALA:HB1	1:B:205:SER:HB3	1.86	0.57
1:B:66:ALA:O	1:B:70:ARG:HG3	2.04	0.57
1:A:145:ILE:CD1	1:A:163:GLY:HA2	2.33	0.57
1:C:5:ARG:HG2	1:D:354:ARG:HD3	1.86	0.57
1:B:275:ALA:O	1:B:278:VAL:HG13	2.04	0.57
1:B:337:ARG:HG3	1:B:341:TRP:CE2	2.40	0.57
1:B:245:GLU:O	1:B:249:LYS:HG2	2.05	0.57
1:D:308:TYR:HB3	1:D:309:PRO:HD2	1.87	0.57
1:D:229:MET:HE1	1:D:254:MET:H	1.69	0.56
1:A:303:ASN:N	1:A:304:PRO:HD2	2.20	0.56
1:C:226:VAL:O	1:C:229:MET:HB3	2.05	0.56
1:B:42:SER:HA	1:B:175:ASP:OD2	2.05	0.56
1:A:372:PRO:O	1:A:376:ARG:HG3	2.06	0.56
1:B:109:GLU:HG3	1:B:204:TYR:CD1	2.41	0.56
1:D:190:THR:O	1:D:194:ILE:HG12	2.05	0.56
1:C:212:ALA:HB1	1:D:205:SER:HB3	1.88	0.56
1:D:326:LEU:HD13	1:D:327:GLU:H	1.70	0.56
1:D:56:PRO:HG3	1:D:61:LEU:HD13	1.88	0.56
1:B:225:ALA:HB1	1:B:254:MET:HG3	1.87	0.56
1:B:8:GLU:HG3	1:B:259:ARG:HD2	1.86	0.56
1:D:299:GLY:O	1:D:303:ASN:HB2	2.06	0.55
1:B:229:MET:HE1	1:B:254:MET:N	2.21	0.55
1:D:276:ARG:HG3	1:D:288:TYR:CZ	2.42	0.55
1:A:302:LEU:O	1:A:307:ILE:HG23	2.06	0.55
1:C:373:LEU:HD23	1:D:58:ARG:HH11	1.72	0.55
1:A:275:ALA:O	1:A:278:VAL:HG22	2.06	0.55
1:D:91:PRO:HB2	1:D:331:PRO:HG2	1.88	0.55
1:C:222:ALA:HB3	1:C:312:ASP:OD1	2.06	0.54
1:D:247:LEU:HD13	1:D:301:VAL:HG11	1.88	0.54
1:A:305:ARG:HH21	1:A:305:ARG:HG2	1.71	0.54
1:D:220:GLY:O	1:D:223:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ALA:HB2	1:D:210:ALA:HB2	1.89	0.54
1:B:174:MET:HE2	1:B:322:LEU:HD13	1.90	0.54
1:C:226:VAL:O	1:C:230:ILE:HG13	2.07	0.54
1:D:87:VAL:HG23	1:D:139:LYS:HA	1.90	0.53
1:C:11:LEU:O	1:D:3:VAL:HB	2.08	0.53
1:A:183:GLU:OE1	1:A:344:HIS:NE2	2.35	0.53
1:A:353:ASN:ND2	1:B:218:ARG:HH12	2.06	0.53
1:D:183:GLU:OE1	1:D:344:HIS:NE2	2.36	0.53
1:D:326:LEU:HD13	1:D:327:GLU:N	2.23	0.53
1:A:264:PHE:CE2	1:A:309:PRO:HG2	2.43	0.53
1:C:173:LEU:HD11	1:C:318:VAL:HG13	1.91	0.53
1:A:324:PHE:CD1	1:A:332:ILE:HD11	2.44	0.53
1:C:257:GLY:N	1:C:307:ILE:HG23	2.24	0.53
1:C:223:ASN:HD21	1:C:333:PHE:HD2	1.56	0.53
1:C:223:ASN:HD22	1:C:330:THR:HA	1.73	0.53
1:D:87:VAL:CG2	1:D:139:LYS:HA	2.39	0.52
1:C:87:VAL:CG2	1:C:139:LYS:HA	2.39	0.52
3:D:404:COA:H32	4:D:408:CIT:O4	2.08	0.52
1:D:158:LEU:HD21	1:D:174:MET:HE2	1.92	0.52
1:D:229:MET:CE	1:D:254:MET:H	2.22	0.52
1:B:290:ILE:O	1:B:294:VAL:HG23	2.08	0.52
1:B:324:PHE:CG	1:B:332:ILE:HD11	2.45	0.52
1:C:337:ARG:HG3	1:C:341:TRP:CE2	2.45	0.52
1:A:226:VAL:O	1:A:230:ILE:HG13	2.10	0.52
1:C:115:GLU:H	1:C:115:GLU:CD	2.14	0.51
1:B:214:LEU:HA	1:B:219:HIS:CD2	2.45	0.51
1:C:193:ALA:HB2	1:C:210:ALA:HB2	1.93	0.51
1:C:8:GLU:OE1	1:D:354:ARG:NH2	2.42	0.51
1:C:303:ASN:N	1:C:304:PRO:HD2	2.25	0.51
1:C:374:GLU:CD	1:C:374:GLU:H	2.14	0.51
1:A:205:SER:HB3	1:B:212:ALA:HB1	1.92	0.51
1:B:145:ILE:CD1	1:B:163:GLY:HA2	2.41	0.51
1:A:35:GLN:O	1:A:39:GLU:HG3	2.11	0.50
1:D:303:ASN:N	1:D:304:PRO:HD2	2.25	0.50
1:C:109:GLU:HG3	1:C:204:TYR:CD1	2.46	0.50
1:C:247:LEU:HD13	1:C:301:VAL:HG11	1.93	0.50
1:C:326:LEU:HD23	1:C:327:GLU:N	2.26	0.50
1:A:265:ASP:HB2	1:A:310:ASN:HA	1.92	0.50
1:C:145:ILE:CD1	1:C:163:GLY:HA2	2.41	0.50
1:D:145:ILE:CD1	1:D:163:GLY:HA2	2.41	0.50
1:D:296:GLU:O	1:D:300:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASP:O	1:C:127:LYS:HG3	2.11	0.50
1:C:256:MET:HB3	1:C:307:ILE:CG2	2.42	0.50
3:D:404:COA:C2P	4:D:408:CIT:C5	2.81	0.50
1:A:20:ILE:HD12	2:B:382:SO4:O3	2.11	0.49
1:C:136:LYS:HD3	1:C:161:ALA:HB1	1.94	0.49
1:A:305:ARG:HH11	3:A:401:COA:H4B	1.77	0.49
1:A:240:ARG:NH2	1:A:296:GLU:OE2	2.46	0.49
1:A:80:GLU:OE2	1:D:80:GLU:OE1	2.30	0.49
1:A:359:GLY:O	1:B:11:LEU:HA	2.11	0.49
1:C:291:LEU:HD21	1:C:313:PHE:O	2.12	0.49
1:C:222:ALA:O	1:C:226:VAL:HG23	2.12	0.49
1:C:326:LEU:HD23	1:C:327:GLU:H	1.76	0.49
1:B:303:ASN:N	1:B:304:PRO:HD2	2.28	0.49
1:C:223:ASN:HB3	1:C:329:PHE:HB3	1.94	0.49
1:D:227:MET:O	1:D:231:GLN:HG3	2.13	0.48
1:D:302:LEU:HB3	1:D:307:ILE:HB	1.95	0.48
1:B:286:LYS:O	1:B:290:ILE:HG13	2.13	0.48
1:A:169:GLU:HG3	1:A:172:ARG:HH12	1.77	0.48
1:A:5:ARG:HB3	1:B:354:ARG:NE	2.28	0.48
1:A:5:ARG:HB3	1:B:354:ARG:HE	1.79	0.48
1:C:91:PRO:HB2	1:C:331:PRO:HG2	1.95	0.48
1:B:136:LYS:HE2	6:B:719:HOH:O	2.14	0.48
1:C:96:ARG:NH1	1:D:205:SER:OG	2.44	0.48
1:D:269:GLY:O	1:D:273:LYS:HG3	2.14	0.48
1:C:294:VAL:O	1:C:298:ALA:HB3	2.14	0.48
1:A:357:ARG:HB3	1:B:259:ARG:HG2	1.96	0.47
1:C:291:LEU:HD23	1:C:314:TYR:CD1	2.49	0.47
1:D:337:ARG:HG3	1:D:341:TRP:CE2	2.49	0.47
1:A:59:GLN:O	1:A:63:GLU:HG3	2.15	0.47
1:B:328:PHE:O	1:B:332:ILE:HG13	2.14	0.47
1:D:300:LYS:CA	1:D:300:LYS:HE3	2.45	0.47
1:B:180:LEU:HD13	1:B:271:LEU:HG	1.97	0.47
1:A:373:LEU:HD11	1:B:58:ARG:HA	1.96	0.47
1:B:240:ARG:O	1:B:244:ARG:HG2	2.15	0.47
1:B:275:ALA:HA	1:B:278:VAL:CG1	2.45	0.46
1:C:373:LEU:HD23	1:D:58:ARG:NH1	2.29	0.46
1:D:239:ALA:HB3	1:D:293:ILE:HG13	1.97	0.46
1:D:228:ARG:CZ	1:D:228:ARG:HB3	2.45	0.46
1:C:243:VAL:HG21	1:C:297:GLU:CB	2.45	0.46
1:C:353:ASN:ND2	1:D:218:ARG:HH12	2.13	0.46
1:C:302:LEU:HD13	1:C:307:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:VAL:HG23	1:C:313:PHE:HZ	1.79	0.46
1:B:26:LYS:HD3	1:B:28:TYR:OH	2.15	0.46
1:C:355:LEU:HD11	1:D:188:ALA:HB2	1.98	0.46
1:B:279:ALA:O	1:B:285:SER:HB3	2.15	0.46
1:A:302:LEU:HD13	1:A:307:ILE:CD1	2.46	0.46
1:A:221:GLY:O	1:A:223:ASN:N	2.48	0.46
1:C:240:ARG:HA	1:C:297:GLU:HG3	1.97	0.46
1:A:258:HIS:ND1	1:A:260:VAL:HG22	2.30	0.46
1:A:21:ASP:HB3	1:A:26:LYS:HB2	1.98	0.46
1:C:328:PHE:O	1:C:332:ILE:HG13	2.16	0.46
1:D:195:ALA:HA	1:D:356:LEU:HD12	1.98	0.46
1:C:210:ALA:HB1	1:C:341:TRP:CE2	2.51	0.46
1:D:71:ARG:HH21	1:D:119:GLU:CD	2.19	0.46
1:D:328:PHE:C	1:D:331:PRO:HD2	2.37	0.46
1:A:279:ALA:O	1:A:285:SER:OG	2.25	0.46
1:A:290:ILE:O	1:A:294:VAL:HG23	2.16	0.46
1:B:136:LYS:HA	1:B:328:PHE:CZ	2.51	0.45
1:B:224:GLU:OE1	1:B:228:ARG:NH1	2.49	0.45
1:C:174:MET:HE2	1:C:322:LEU:HD13	1.98	0.45
1:A:64:PHE:CE1	1:A:122:LEU:HD21	2.52	0.45
1:A:366:LEU:HD21	1:B:19:TYR:CG	2.52	0.45
1:A:220:GLY:H	4:A:405:CIT:C5	2.29	0.45
1:B:265:ASP:HB2	1:B:310:ASN:HA	1.98	0.45
1:A:277:LEU:O	1:A:280:GLU:HG2	2.16	0.45
1:A:58:ARG:NH2	1:B:374:GLU:HA	2.29	0.45
1:B:136:LYS:HD3	1:B:161:ALA:HB1	1.99	0.45
1:C:227:MET:O	1:C:231:GLN:HG3	2.16	0.45
1:A:58:ARG:NH2	1:A:58:ARG:HB2	2.31	0.45
1:C:354:ARG:HB2	1:C:354:ARG:NH1	2.29	0.45
1:B:330:THR:O	1:B:333:PHE:HB3	2.17	0.45
1:D:294:VAL:HG23	1:D:313:PHE:CZ	2.50	0.44
1:B:91:PRO:HB2	1:B:331:PRO:HG2	1.99	0.44
1:B:219:HIS:CE1	4:B:406:CIT:H41	2.52	0.44
1:A:193:ALA:HB2	1:A:210:ALA:HB2	1.99	0.44
1:A:188:ALA:HB2	1:B:355:LEU:HD11	1.98	0.44
1:B:56:PRO:HG3	1:B:61:LEU:HD13	1.99	0.44
1:A:355:LEU:HD11	1:B:188:ALA:HB2	2.00	0.44
1:C:264:PHE:CE1	1:C:309:PRO:HG2	2.52	0.44
1:D:242:TRP:CH2	1:D:246:LYS:HD2	2.53	0.44
1:A:200:GLU:HG2	6:A:820:HOH:O	2.17	0.44
1:D:236:PRO:O	1:D:293:ILE:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLY:HA3	1:D:368:VAL:HG23	1.99	0.44
1:C:62:GLU:HA	1:C:62:GLU:OE1	2.17	0.44
1:D:249:LYS:HG3	1:D:251:GLU:HG2	2.00	0.43
1:B:74:LEU:HD23	1:B:127:LYS:HD3	2.00	0.43
1:D:300:LYS:HE3	1:D:300:LYS:N	2.33	0.43
1:A:123:ASP:CG	1:A:127:LYS:HE2	2.38	0.43
1:C:238:ARG:O	1:C:242:TRP:HB2	2.18	0.43
1:C:58:ARG:HD3	1:D:373:LEU:HD21	2.01	0.43
1:C:307:ILE:N	1:C:307:ILE:HD12	2.33	0.43
1:B:338:ILE:O	1:B:342:VAL:HG23	2.17	0.43
1:A:302:LEU:HD13	1:A:307:ILE:HD11	1.99	0.43
1:B:220:GLY:O	1:B:223:ASN:HB2	2.18	0.43
1:A:305:ARG:NH2	1:A:305:ARG:HG2	2.33	0.43
1:C:308:TYR:HB3	1:C:309:PRO:HD2	2.00	0.43
1:A:123:ASP:O	1:A:127:LYS:HG3	2.19	0.43
1:C:6:GLY:HA2	1:D:356:LEU:HD23	1.99	0.43
1:C:158:LEU:HD21	1:C:174:MET:HE2	2.00	0.43
1:A:121:GLY:O	1:A:125:ILE:HG13	2.19	0.43
1:D:272:GLU:HG2	1:D:314:TYR:CZ	2.54	0.43
1:A:260:VAL:HG23	1:A:261:TYR:N	2.33	0.42
1:D:155:ALA:HA	1:D:166:PRO:HG3	2.01	0.42
1:D:229:MET:HE2	1:D:242:TRP:HH2	1.84	0.42
1:D:300:LYS:HE3	1:D:300:LYS:HA	1.99	0.42
1:C:273:LYS:O	1:C:277:LEU:HG	2.18	0.42
1:A:20:ILE:HG21	1:A:260:VAL:CG2	2.44	0.42
1:A:195:ALA:HA	1:A:356:LEU:HD12	2.01	0.42
1:A:287:GLU:H	1:A:287:GLU:HG2	1.69	0.42
1:A:158:LEU:HD21	1:A:174:MET:HG2	2.01	0.42
1:A:176:ALA:O	1:A:180:LEU:HG	2.19	0.42
1:D:178:LEU:O	1:D:336:ALA:HB1	2.20	0.42
1:C:302:LEU:HB3	1:C:307:ILE:HB	2.02	0.42
1:A:30:TYR:CD1	1:A:53:GLY:HA2	2.55	0.42
1:C:186:PHE:CE2	1:D:360:ALA:HB2	2.55	0.42
1:C:355:LEU:CD2	3:D:404:COA:H132	2.45	0.42
1:D:210:ALA:HB1	1:D:341:TRP:CE2	2.55	0.42
1:A:48:PHE:CG	1:A:56:PRO:HB3	2.54	0.42
1:B:239:ALA:HB3	1:B:293:ILE:HG21	2.02	0.42
1:B:361:LYS:C	1:B:361:LYS:HD3	2.40	0.42
1:A:262:LYS:HA	1:A:306:GLY:O	2.19	0.42
1:B:349:GLN:HG3	6:B:683:HOH:O	2.19	0.42
1:A:154:ALA:HB1	1:A:174:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ARG:HG3	1:D:288:TYR:CE1	2.54	0.42
1:D:236:PRO:C	1:D:238:ARG:H	2.23	0.42
1:B:139:LYS:HE2	6:B:451:HOH:O	2.20	0.42
1:C:192:THR:HG22	1:C:209:ALA:HB1	2.02	0.41
1:D:48:PHE:CD1	1:D:48:PHE:C	2.93	0.41
1:D:258:HIS:HA	3:D:404:COA:S1P	2.61	0.41
1:C:249:LYS:N	1:C:249:LYS:HD2	2.35	0.41
1:C:274:LEU:O	1:C:278:VAL:HG23	2.20	0.41
1:D:115:GLU:CD	1:D:115:GLU:H	2.23	0.41
1:C:310:ASN:ND2	3:C:403:COA:H31	2.35	0.41
1:B:123:ASP:OD1	1:B:127:LYS:HE2	2.20	0.41
1:D:246:LYS:HG2	1:D:253:ILE:HG12	2.01	0.41
1:D:324:PHE:CD2	1:D:332:ILE:HD11	2.56	0.41
1:D:139:LYS:HE2	6:D:662:HOH:O	2.21	0.41
1:A:229:MET:HG3	1:A:242:TRP:CH2	2.55	0.41
1:C:91:PRO:HG3	1:C:139:LYS:HE3	2.01	0.41
1:D:174:MET:CE	1:D:322:LEU:HD13	2.50	0.41
1:D:257:GLY:CA	1:D:307:ILE:HG23	2.50	0.41
1:A:35:GLN:NE2	1:A:35:GLN:N	2.54	0.41
1:C:87:VAL:HG22	1:C:139:LYS:HA	2.02	0.41
1:B:286:LYS:HD2	1:B:286:LYS:H	1.84	0.41
1:B:20:ILE:HD13	1:B:184:HIS:CE1	2.55	0.41
1:C:106:ASP:HA	1:C:107:PRO:HD2	1.93	0.41
1:A:16:ARG:HG2	1:B:363:VAL:HG23	2.03	0.41
1:D:264:PHE:CE1	1:D:309:PRO:HG2	2.56	0.41
1:D:146:PRO:HA	1:D:147:PRO:HD3	1.91	0.41
1:C:136:LYS:HA	1:C:328:PHE:CZ	2.56	0.41
1:A:5:ARG:HG3	1:B:354:ARG:NH1	2.35	0.41
1:D:226:VAL:HG21	1:D:312:ASP:O	2.21	0.41
1:A:48:PHE:CD1	1:A:56:PRO:HB3	2.56	0.41
1:C:261:TYR:CZ	1:C:266:PRO:HD2	2.55	0.41
1:C:287:GLU:N	6:C:572:HOH:O	2.53	0.41
1:B:185:GLY:HA3	2:B:383:SO4:O3	2.20	0.41
1:A:360:ALA:HB2	1:B:186:PHE:CE2	2.56	0.41
1:C:105:LEU:HD23	1:D:86:PRO:HG2	2.02	0.41
1:D:256:MET:HG2	1:D:309:PRO:HA	2.03	0.40
1:C:64:PHE:O	1:C:67:ALA:HB3	2.21	0.40
1:C:243:VAL:HG21	1:C:297:GLU:HB3	2.02	0.40
1:A:180:LEU:HD13	1:A:271:LEU:HG	2.02	0.40
1:A:97:THR:HG21	1:B:104:MET:CE	2.51	0.40
1:C:188:ALA:HB3	1:C:219:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:O	1:A:309:PRO:HA	2.21	0.40
1:D:178:LEU:HA	1:D:178:LEU:HD23	1.90	0.40
1:A:97:THR:HG21	1:B:104:MET:HE2	2.03	0.40
1:A:239:ALA:HB3	1:A:293:ILE:HG21	2.04	0.40
1:D:133:ALA:O	1:D:137:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/377 (97%)	356 (97%)	10 (3%)	1 (0%)	46	57
1	B	366/377 (97%)	356 (97%)	10 (3%)	0	100	100
1	C	362/377 (96%)	349 (96%)	13 (4%)	0	100	100
1	D	362/377 (96%)	350 (97%)	12 (3%)	0	100	100
All	All	1457/1508 (97%)	1411 (97%)	45 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/307 (97%)	288 (97%)	10 (3%)	44	59
1	B	300/307 (98%)	290 (97%)	10 (3%)	45	61
1	C	296/307 (96%)	289 (98%)	7 (2%)	57	74
1	D	296/307 (96%)	287 (97%)	9 (3%)	48	65
All	All	1190/1228 (97%)	1154 (97%)	36 (3%)	48	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	128	PHE
1	A	135	ASN
1	A	174	MET
1	A	223	ASN
1	A	228	ARG
1	A	238	ARG
1	A	259	ARG
1	A	291	LEU
1	A	307	ILE
1	B	119	GLU
1	B	123	ASP
1	B	135	ASN
1	B	223	ASN
1	B	228	ARG
1	B	278	VAL
1	B	287	GLU
1	B	291	LEU
1	B	333	PHE
1	B	361	LYS
1	C	62	GLU
1	C	135	ASN
1	C	244	ARG
1	C	326	LEU
1	C	333	PHE
1	C	354	ARG
1	C	357	ARG
1	D	57	ARG
1	D	119	GLU
1	D	135	ASN
1	D	228	ARG
1	D	238	ARG
1	D	244	ARG

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Mol	Chain	Res	Type
1	D	300	LYS
1	D	326	LEU
1	D	333	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	59	GLN
1	A	162	ASN
1	A	170	GLN
1	A	223	ASN
1	A	231	GLN
1	B	23	GLN
1	B	289	GLN
1	C	23	GLN
1	C	289	GLN
1	D	353	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

22 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	SO4	A	387	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	391	-	4,4,4	0.19	0	6,6,6	0.12	0
3	COA	A	401	-	40,50,50	1.68	7 (17%)	50,75,75	1.92	11 (22%)
4	CIT	A	405	-	3,12,12	2.37	2 (66%)	3,17,17	7.32	3 (100%)
5	GOL	A	411	-	5,5,5	0.76	0	5,5,5	0.26	0
2	SO4	B	382	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	B	383	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	B	385	-	4,4,4	0.26	0	6,6,6	0.09	0
3	COA	B	402	-	40,50,50	1.66	9 (22%)	50,75,75	1.95	10 (20%)
4	CIT	B	406	-	3,12,12	1.77	1 (33%)	3,17,17	7.64	2 (66%)
5	GOL	B	412	-	5,5,5	0.77	0	5,5,5	0.34	0
2	SO4	C	381	-	4,4,4	0.10	0	6,6,6	0.15	0
2	SO4	C	388	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	C	390	-	4,4,4	0.16	0	6,6,6	0.10	0
3	COA	C	403	-	40,50,50	1.69	8 (20%)	50,75,75	1.94	12 (24%)
4	CIT	C	407	-	3,12,12	2.15	1 (33%)	3,17,17	7.09	2 (66%)
5	GOL	C	413	-	5,5,5	0.85	0	5,5,5	0.61	0
2	SO4	D	386	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	D	389	-	4,4,4	0.20	0	6,6,6	0.13	0
3	COA	D	404	-	40,50,50	2.19	13 (32%)	50,75,75	2.18	18 (36%)
4	CIT	D	408	-	3,12,12	2.30	1 (33%)	3,17,17	5.21	2 (66%)
5	GOL	D	414	-	5,5,5	0.69	0	5,5,5	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	387	-	-	0/0/0/0	0/0/0/0
2	SO4	A	391	-	-	0/0/0/0	0/0/0/0
3	COA	A	401	-	-	0/44/64/64	0/3/3/3
4	CIT	A	405	-	-	0/6/16/16	0/0/0/0
5	GOL	A	411	-	-	0/4/4/4	0/0/0/0
2	SO4	B	382	-	-	0/0/0/0	0/0/0/0
2	SO4	B	383	-	-	0/0/0/0	0/0/0/0
2	SO4	B	385	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	402	-	-	0/44/64/64	0/3/3/3
4	CIT	B	406	-	-	0/6/16/16	0/0/0/0
5	GOL	B	412	-	-	0/4/4/4	0/0/0/0
2	SO4	C	381	-	-	0/0/0/0	0/0/0/0
2	SO4	C	388	-	-	0/0/0/0	0/0/0/0
2	SO4	C	390	-	-	0/0/0/0	0/0/0/0
3	COA	C	403	-	-	0/44/64/64	0/3/3/3
4	CIT	C	407	-	-	0/6/16/16	0/0/0/0
5	GOL	C	413	-	-	0/4/4/4	0/0/0/0
2	SO4	D	386	-	-	0/0/0/0	0/0/0/0
2	SO4	D	389	-	-	0/0/0/0	0/0/0/0
3	COA	D	404	-	-	0/44/64/64	0/3/3/3
4	CIT	D	408	-	-	0/6/16/16	0/0/0/0
5	GOL	D	414	-	-	0/4/4/4	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	COA	C8A-N7A	-2.16	1.30	1.34
3	A	401	COA	O5P-C5P	2.01	1.27	1.23
3	D	404	COA	P3B-O9A	2.11	1.62	1.54
3	B	402	COA	C4A-N3A	2.14	1.38	1.35
3	B	402	COA	C3P-N4P	2.15	1.51	1.46
4	A	405	CIT	C4-C3	2.16	1.58	1.54
3	C	403	COA	O4B-C4B	2.18	1.50	1.45
3	B	402	COA	O4B-C4B	2.23	1.50	1.45
3	C	403	COA	O5P-C5P	2.29	1.28	1.23
3	B	402	COA	O5P-C5P	2.29	1.28	1.23
3	D	404	COA	OAP-CAP	2.49	1.47	1.42
3	A	401	COA	O4B-C4B	2.55	1.50	1.45
3	D	404	COA	C4A-N3A	2.60	1.39	1.35
3	D	404	COA	P3B-O3B	2.66	1.68	1.60
3	D	404	COA	P2A-O4A	2.67	1.60	1.51
3	C	403	COA	C4A-N3A	2.68	1.39	1.35
3	D	404	COA	O2B-C2B	2.71	1.49	1.43
3	D	404	COA	CEP-CBP	2.71	1.59	1.53
3	D	404	COA	C2A-N1A	2.74	1.39	1.33
4	B	406	CIT	C2-C3	2.78	1.58	1.54
3	B	402	COA	P3B-O3B	2.88	1.68	1.60
3	C	403	COA	P3B-O7A	2.96	1.60	1.51
3	A	401	COA	P3B-O7A	3.01	1.61	1.51
3	B	402	COA	P3B-O7A	3.16	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	COA	P3B-O3B	3.21	1.69	1.60
3	B	402	COA	C2A-N1A	3.29	1.40	1.33
3	A	401	COA	P3B-O3B	3.33	1.70	1.60
4	A	405	CIT	C2-C3	3.33	1.59	1.54
3	D	404	COA	P3B-O7A	3.34	1.62	1.51
3	A	401	COA	C2A-N1A	3.34	1.40	1.33
3	C	403	COA	O4B-C1B	3.36	1.45	1.41
4	C	407	CIT	C2-C3	3.38	1.59	1.54
3	D	404	COA	C3B-C4B	3.42	1.62	1.52
3	C	403	COA	C2A-N1A	3.51	1.40	1.33
4	D	408	CIT	C2-C3	3.59	1.60	1.54
3	A	401	COA	O4B-C1B	3.65	1.45	1.41
3	B	402	COA	O4B-C1B	3.71	1.45	1.41
3	B	402	COA	O9P-C9P	3.87	1.31	1.23
3	A	401	COA	O9P-C9P	4.26	1.31	1.23
3	C	403	COA	O9P-C9P	4.43	1.32	1.23
3	D	404	COA	O9P-C9P	5.40	1.34	1.23
3	D	404	COA	O4B-C1B	7.24	1.50	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	N3A-C2A-N1A	-8.06	122.73	128.89
3	D	404	COA	N3A-C2A-N1A	-7.66	123.03	128.89
3	C	403	COA	N3A-C2A-N1A	-7.31	123.30	128.89
3	A	401	COA	N3A-C2A-N1A	-6.79	123.69	128.89
3	B	402	COA	C2B-C1B-N9A	-4.77	107.00	114.29
3	A	401	COA	C2B-C1B-N9A	-4.75	107.03	114.29
3	D	404	COA	O4B-C1B-N9A	-4.63	98.41	108.10
3	C	403	COA	C2B-C1B-N9A	-4.47	107.46	114.29
3	D	404	COA	C4B-O4B-C1B	-4.06	105.26	109.72
3	A	401	COA	C4B-O4B-C1B	-3.68	105.67	109.72
3	D	404	COA	C2B-C1B-N9A	-3.66	108.70	114.29
3	C	403	COA	C4B-O4B-C1B	-3.31	106.08	109.72
3	D	404	COA	C7P-N8P-C9P	-3.24	116.12	122.53
3	B	402	COA	O4B-C1B-N9A	-3.09	101.62	108.10
3	C	403	COA	O4B-C1B-N9A	-2.62	102.61	108.10
3	A	401	COA	O4B-C1B-N9A	-2.52	102.83	108.10
3	D	404	COA	CEP-CBP-CCP	-2.47	105.30	108.50
3	B	402	COA	C4B-O4B-C1B	-2.37	107.12	109.72
3	B	402	COA	C6P-C7P-N8P	-2.22	107.00	111.88
3	C	403	COA	C6P-C7P-N8P	-2.17	107.12	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	COA	C7P-N8P-C9P	-2.11	118.36	122.53
3	D	404	COA	C6P-C7P-N8P	-2.07	107.33	111.88
3	A	401	COA	C7P-N8P-C9P	-2.07	118.43	122.53
3	A	401	COA	C6P-C7P-N8P	-2.02	107.44	111.88
3	D	404	COA	C1B-N9A-C4A	-2.00	123.92	126.94
3	A	401	COA	O5A-P2A-O3A	2.02	114.27	105.09
3	D	404	COA	O5A-P2A-O3A	2.05	114.39	105.09
3	B	402	COA	O5A-P2A-O3A	2.06	114.44	105.09
3	D	404	COA	O9A-P3B-O7A	2.12	117.42	110.58
4	A	405	CIT	C4-C3-C2	2.15	114.95	109.81
3	D	404	COA	CDP-CBP-CAP	2.20	113.37	109.34
3	C	403	COA	C2A-N1A-C6A	2.29	122.86	118.77
3	C	403	COA	O5A-P2A-O3A	2.30	115.54	105.09
3	D	404	COA	C2A-N1A-C6A	2.32	122.91	118.77
3	D	404	COA	P3B-O3B-C3B	2.46	127.47	121.56
3	D	404	COA	C4A-C5A-N7A	2.55	111.83	109.48
3	D	404	COA	CDP-CBP-CCP	2.56	111.82	108.50
3	A	401	COA	CDP-CBP-CAP	2.68	114.23	109.34
3	B	402	COA	CDP-CBP-CAP	2.71	114.30	109.34
3	C	403	COA	CDP-CBP-CAP	2.79	114.44	109.34
3	B	402	COA	CEP-CBP-CAP	2.92	114.67	109.34
3	C	403	COA	O3B-C3B-C4B	2.92	121.46	109.99
3	B	402	COA	O3B-C3B-C4B	2.97	121.63	109.99
3	D	404	COA	O3B-P3B-O7A	3.04	114.70	107.11
3	A	401	COA	CEP-CBP-CAP	3.11	115.02	109.34
3	C	403	COA	CEP-CBP-CAP	3.18	115.16	109.34
3	B	402	COA	O3B-P3B-O7A	3.21	115.12	107.11
3	D	404	COA	O3B-C3B-C4B	3.22	122.61	109.99
3	A	401	COA	O3B-C3B-C4B	3.22	122.62	109.99
3	C	403	COA	O3B-P3B-O7A	3.69	116.33	107.11
3	A	401	COA	O3B-P3B-O7A	3.78	116.54	107.11
3	D	404	COA	CEP-CBP-CAP	3.86	116.40	109.34
4	A	405	CIT	C3-C2-C1	4.61	122.32	114.96
4	C	407	CIT	C3-C2-C1	5.97	124.51	114.96
4	D	408	CIT	C3-C2-C1	6.25	124.96	114.96
4	D	408	CIT	C3-C4-C5	6.26	124.97	114.96
4	B	406	CIT	C3-C2-C1	7.00	126.16	114.96
4	C	407	CIT	C3-C4-C5	10.60	131.91	114.96
4	B	406	CIT	C3-C4-C5	11.16	132.80	114.96
4	A	405	CIT	C3-C4-C5	11.62	133.54	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	COA	2	0
4	A	405	CIT	1	0
2	B	382	SO4	1	0
2	B	383	SO4	1	0
3	B	402	COA	1	0
4	B	406	CIT	1	0
3	C	403	COA	1	0
3	D	404	COA	11	0
4	D	408	CIT	6	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	371/377 (98%)	1.72	113 (30%) 1 1	8, 21, 39, 57	21 (5%)
1	B	370/377 (98%)	1.58	96 (25%) 1 1	10, 21, 39, 55	24 (6%)
1	C	366/377 (97%)	1.96	139 (37%) 0 0	10, 25, 65, 79	30 (8%)
1	D	366/377 (97%)	1.76	109 (29%) 1 1	10, 23, 52, 64	28 (7%)
All	All	1473/1508 (97%)	1.75	457 (31%) 1 1	8, 22, 51, 79	103 (6%)

All (457) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	16.3
1	C	288	TYR	9.6
1	C	278	VAL	9.2
1	C	247	LEU	8.9
1	C	302	LEU	8.6
1	A	44	GLU	8.2
1	D	248	ALA	7.7
1	D	250	LYS	7.5
1	D	228	ARG	7.2
1	A	284	HIS	7.1
1	D	305	ARG	6.7
1	D	294	VAL	6.7
1	D	244	ARG	6.4
1	C	242	TRP	6.3
1	C	287	GLU	6.3
1	D	245	GLU	6.2
1	C	248	ALA	6.0
1	A	42	SER	5.9
1	A	279	ALA	5.9
1	C	250	LYS	5.6
1	C	245	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	306	GLY	5.6
1	C	303	ASN	5.4
1	C	262	LYS	5.4
1	D	301	VAL	5.3
1	C	314	TYR	5.3
1	C	254	MET	5.3
1	A	46	THR	5.3
1	D	237	GLU	5.3
1	B	169	GLU	5.3
1	C	298	ALA	5.3
1	C	232	GLU	5.3
1	C	231	GLN	5.3
1	D	293	ILE	5.2
1	C	293	ILE	5.2
1	C	297	GLU	5.1
1	C	9	GLY	5.1
1	A	156	ASN	5.1
1	A	178	LEU	5.0
1	B	280	GLU	5.0
1	A	153	HIS	4.9
1	C	237	GLU	4.9
1	C	249	LYS	4.8
1	D	249	LYS	4.7
1	A	23	GLN	4.6
1	D	110	GLY	4.6
1	D	286	LYS	4.5
1	A	285	SER	4.5
1	C	238	ARG	4.5
1	A	154	ALA	4.4
1	C	244	ARG	4.4
1	C	354	ARG	4.4
1	D	300	LYS	4.4
1	A	3	VAL	4.4
1	A	68	LEU	4.3
1	C	291	LEU	4.3
1	D	253	ILE	4.2
1	C	300	LYS	4.2
1	C	220	GLY	4.2
1	B	24	GLN	4.1
1	D	350	GLU	4.1
1	C	169	GLU	4.1
1	D	275	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	289	GLN	4.1
1	D	304	PRO	4.1
1	A	125	ILE	4.1
1	D	251	GLU	4.1
1	C	325	SER	4.0
1	A	220	GLY	4.0
1	C	301	VAL	4.0
1	D	308	TYR	4.0
1	D	289	GLN	3.9
1	C	307	ILE	3.9
1	A	250	LYS	3.8
1	B	168	PRO	3.8
1	D	233	ILE	3.8
1	C	28	TYR	3.8
1	B	36	GLU	3.8
1	D	373	LEU	3.8
1	C	246	LYS	3.7
1	D	311	VAL	3.7
1	A	238	ARG	3.7
1	C	172	ARG	3.7
1	A	59	GLN	3.7
1	B	275	ALA	3.7
1	C	87	VAL	3.6
1	D	375	ALA	3.6
1	A	310	ASN	3.6
1	C	360	ALA	3.6
1	A	287	GLU	3.6
1	D	247	LEU	3.6
1	B	279	ALA	3.6
1	B	20	ILE	3.6
1	C	236	PRO	3.6
1	B	126	ALA	3.6
1	A	150	ASP	3.6
1	C	353	ASN	3.6
1	D	230	ILE	3.5
1	D	254	MET	3.5
1	B	300	LYS	3.5
1	C	230	ILE	3.5
1	C	313	PHE	3.5
1	C	265	ASP	3.5
1	A	373	LEU	3.5
1	D	277	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	3.4
1	D	369	PRO	3.4
1	D	276	ARG	3.4
1	B	302	LEU	3.4
1	B	326	LEU	3.4
1	C	374	GLU	3.4
1	D	17	MET	3.4
1	B	273	LYS	3.4
1	D	246	LYS	3.4
1	C	269	GLY	3.4
1	B	277	LEU	3.4
1	D	172	ARG	3.4
1	D	297	GLU	3.4
1	A	300	LYS	3.4
1	A	126	ALA	3.3
1	D	263	ALA	3.3
1	A	308	TYR	3.3
1	A	63	GLU	3.3
1	B	250	LYS	3.3
1	B	58	ARG	3.3
1	C	234	GLY	3.3
1	B	133	ALA	3.3
1	A	372	PRO	3.3
1	C	57	ARG	3.3
1	B	262	LYS	3.3
1	C	23	GLN	3.3
1	A	328	PHE	3.3
1	A	259	ARG	3.3
1	C	19	TYR	3.3
1	A	232	GLU	3.2
1	C	304	PRO	3.2
1	C	308	TYR	3.2
1	A	223	ASN	3.2
1	A	110	GLY	3.2
1	D	243	VAL	3.2
1	C	239	ALA	3.2
1	C	261	TYR	3.2
1	B	100	SER	3.2
1	B	244	ARG	3.1
1	D	256	MET	3.1
1	D	295	GLU	3.1
1	C	290	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	65	SER	3.1
1	A	87	VAL	3.1
1	C	3	VAL	3.1
1	C	276	ARG	3.1
1	B	276	ARG	3.1
1	C	310	ASN	3.1
1	A	376	ARG	3.1
1	C	80	GLU	3.1
1	C	18	CYS	3.1
1	A	311	VAL	3.1
1	C	166	PRO	3.1
1	B	360	ALA	3.0
1	A	227	MET	3.0
1	D	173	LEU	3.0
1	A	18	CYS	3.0
1	A	175	ASP	3.0
1	A	280	GLU	3.0
1	D	302	LEU	3.0
1	D	355	LEU	3.0
1	B	19	TYR	3.0
1	C	225	ALA	3.0
1	C	294	VAL	3.0
1	B	261	TYR	3.0
1	A	268	ALA	3.0
1	A	361	LYS	3.0
1	A	317	VAL	3.0
1	B	76	ALA	3.0
1	D	298	ALA	3.0
1	B	285	SER	3.0
1	C	134	ALA	3.0
1	A	326	LEU	3.0
1	C	235	THR	3.0
1	C	256	MET	3.0
1	B	278	VAL	2.9
1	D	28	TYR	2.9
1	A	57	ARG	2.9
1	C	289	GLN	2.9
1	A	177	ALA	2.9
1	A	240	ARG	2.9
1	C	26	LYS	2.9
1	D	238	ARG	2.9
1	A	30	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	39	GLU	2.9
1	D	351	LEU	2.9
1	D	325	SER	2.9
1	C	241	GLU	2.9
1	D	5	ARG	2.9
1	B	179	ILE	2.9
1	D	257	GLY	2.9
1	A	278	VAL	2.9
1	C	243	VAL	2.9
1	C	321	ASP	2.9
1	D	314	TYR	2.8
1	C	221	GLY	2.8
1	C	132	VAL	2.8
1	B	319	TYR	2.8
1	A	225	ALA	2.8
1	B	26	LYS	2.8
1	B	159	TYR	2.8
1	B	272	GLU	2.8
1	D	268	ALA	2.8
1	D	354	ARG	2.8
1	C	372	PRO	2.8
1	D	372	PRO	2.7
1	B	90	HIS	2.7
1	A	368	VAL	2.7
1	B	18	CYS	2.7
1	A	67	ALA	2.7
1	C	319	TYR	2.7
1	B	59	GLN	2.7
1	C	76	ALA	2.7
1	D	213	SER	2.7
1	B	62	GLU	2.7
1	B	80	GLU	2.7
1	C	257	GLY	2.7
1	B	371	VAL	2.7
1	C	311	VAL	2.7
1	A	179	ILE	2.7
1	C	131	ILE	2.7
1	C	229	MET	2.7
1	C	157	PHE	2.7
1	D	264	PHE	2.7
1	C	296	GLU	2.7
1	A	366	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	37	LEU	2.7
1	C	346	LEU	2.7
1	A	332	ILE	2.7
1	A	5	ARG	2.7
1	C	58	ARG	2.7
1	C	89	ALA	2.6
1	C	299	GLY	2.6
1	D	368	VAL	2.6
1	B	22	GLY	2.6
1	B	25	GLY	2.6
1	B	8	GLU	2.6
1	B	291	LEU	2.6
1	B	352	ASP	2.6
1	C	333	PHE	2.6
1	D	309	PRO	2.6
1	B	17	MET	2.6
1	B	211	VAL	2.6
1	C	164	VAL	2.6
1	D	225	ALA	2.6
1	C	108	THR	2.6
1	B	186	PHE	2.6
1	A	305	ARG	2.6
1	D	236	PRO	2.6
1	C	253	ILE	2.6
1	D	307	ILE	2.6
1	C	320	SER	2.6
1	C	272	GLU	2.6
1	D	288	TYR	2.6
1	B	196	ALA	2.6
1	A	251	GLU	2.5
1	D	58	ARG	2.5
1	A	288	TYR	2.5
1	D	261	TYR	2.5
1	A	66	ALA	2.5
1	D	132	VAL	2.5
1	D	214	LEU	2.5
1	A	112	ILE	2.5
1	C	74	LEU	2.5
1	B	145	ILE	2.5
1	B	269	GLY	2.5
1	C	252	ARG	2.5
1	C	8	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	363	VAL	2.5
1	D	241	GLU	2.5
1	B	223	ASN	2.5
1	D	367	ASP	2.5
1	A	24	GLN	2.5
1	D	163	GLY	2.5
1	D	185	GLY	2.5
1	B	82	PHE	2.5
1	C	29	TYR	2.5
1	C	371	VAL	2.5
1	A	172	ARG	2.5
1	A	276	ARG	2.5
1	C	305	ARG	2.5
1	D	57	ARG	2.5
1	D	126	ALA	2.4
1	D	239	ALA	2.4
1	B	108	THR	2.4
1	C	223	ASN	2.4
1	C	277	LEU	2.4
1	C	373	LEU	2.4
1	B	286	LYS	2.4
1	B	365	GLU	2.4
1	C	263	ALA	2.4
1	B	16	ARG	2.4
1	D	150	ASP	2.4
1	A	309	PRO	2.4
1	B	229	MET	2.4
1	D	319	TYR	2.4
1	C	292	LYS	2.4
1	C	112	ILE	2.4
1	B	238	ARG	2.4
1	B	209	ALA	2.4
1	A	304	PRO	2.4
1	B	60	GLU	2.4
1	B	21	ASP	2.4
1	B	185	GLY	2.4
1	D	270	VAL	2.4
1	C	73	ALA	2.4
1	C	154	ALA	2.4
1	D	374	GLU	2.4
1	A	49	LEU	2.4
1	A	203	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	234	GLY	2.4
1	C	370	TYR	2.4
1	A	252	ARG	2.4
1	D	232	GLU	2.3
1	A	253	ILE	2.3
1	A	47	THR	2.3
1	A	171	ALA	2.3
1	A	104	MET	2.3
1	C	258	HIS	2.3
1	C	357	ARG	2.3
1	B	170	GLN	2.3
1	B	14	GLU	2.3
1	C	55	LEU	2.3
1	C	85	TYR	2.3
1	A	336	ALA	2.3
1	B	154	ALA	2.3
1	B	155	ALA	2.3
1	B	328	PHE	2.3
1	D	306	GLY	2.3
1	B	65	SER	2.3
1	C	275	ALA	2.3
1	B	321	ASP	2.3
1	D	273	LYS	2.3
1	D	3	VAL	2.3
1	D	235	THR	2.3
1	A	261	TYR	2.3
1	B	118	TYR	2.3
1	B	122	LEU	2.3
1	D	366	LEU	2.3
1	B	242	TRP	2.3
1	B	317	VAL	2.2
1	C	38	ALA	2.2
1	C	210	ALA	2.2
1	C	233	ILE	2.2
1	C	226	VAL	2.2
1	C	228	ARG	2.2
1	A	27	LEU	2.2
1	D	55	LEU	2.2
1	A	199	THR	2.2
1	A	243	VAL	2.2
1	A	365	GLU	2.2
1	B	3	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	370	TYR	2.2
1	B	354	ARG	2.2
1	D	328	PHE	2.2
1	B	214	LEU	2.2
1	C	158	LEU	2.2
1	C	39	GLU	2.2
1	A	274	LEU	2.2
1	C	67	ALA	2.2
1	D	310	ASN	2.2
1	B	233	ILE	2.2
1	A	149	GLU	2.2
1	B	366	LEU	2.2
1	C	326	LEU	2.2
1	A	93	SER	2.2
1	A	80	GLU	2.2
1	D	188	ALA	2.2
1	A	294	VAL	2.2
1	D	87	VAL	2.2
1	B	172	ARG	2.2
1	B	107	PRO	2.2
1	A	122	LEU	2.2
1	C	117	LEU	2.2
1	A	201	THR	2.2
1	A	134	ALA	2.2
1	A	155	ALA	2.2
1	B	188	ALA	2.2
1	D	317	VAL	2.1
1	C	147	PRO	2.1
1	D	296	GLU	2.1
1	A	12	PHE	2.1
1	A	204	TYR	2.1
1	A	158	LEU	2.1
1	B	68	LEU	2.1
1	B	351	LEU	2.1
1	C	27	LEU	2.1
1	C	192	THR	2.1
1	C	62	GLU	2.1
1	C	255	GLY	2.1
1	D	242	TRP	2.1
1	D	83	LYS	2.1
1	C	61	LEU	2.1
1	C	322	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	235	THR	2.1
1	B	212	ALA	2.1
1	C	149	GLU	2.1
1	A	33	PRO	2.1
1	A	85	TYR	2.1
1	C	175	ASP	2.1
1	D	169	GLU	2.1
1	C	173	LEU	2.1
1	B	134	ALA	2.1
1	D	116	ALA	2.1
1	B	56	PRO	2.1
1	D	32	ILE	2.1
1	D	148	ARG	2.1
1	D	168	PRO	2.1
1	A	260	VAL	2.1
1	D	324	PHE	2.1
1	A	161	ALA	2.1
1	A	275	ALA	2.1
1	D	155	ALA	2.1
1	C	240	ARG	2.1
1	D	145	ILE	2.1
1	B	164	VAL	2.1
1	B	157	PHE	2.1
1	A	237	GLU	2.1
1	A	302	LEU	2.1
1	B	297	GLU	2.1
1	C	151	LEU	2.1
1	D	356	LEU	2.1
1	C	107	PRO	2.1
1	D	147	PRO	2.1
1	A	353	ASN	2.0
1	B	364	GLY	2.0
1	C	355	LEU	2.0
1	D	203	LEU	2.0
1	D	229	MET	2.0
1	A	370	TYR	2.0
1	B	362	TYR	2.0
1	A	90	HIS	2.0
1	A	152	SER	2.0
1	A	189	SER	2.0
1	A	39	GLU	2.0
1	A	62	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	224	GLU	2.0
1	D	224	GLU	2.0
1	A	233	ILE	2.0
1	A	102	PHE	2.0
1	D	90	HIS	2.0
1	C	145	ILE	2.0
1	C	316	GLY	2.0
1	A	363	VAL	2.0
1	B	363	VAL	2.0
1	B	245	GLU	2.0
1	A	37	LEU	2.0
1	B	160	MET	2.0
1	B	355	LEU	2.0
1	D	89	ALA	2.0
1	B	57	ARG	2.0
1	C	266	PRO	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
2	SO4	C	390	5/5	0.79	0.52	10.40	80,82,83,83	0
5	GOL	C	413	6/6	0.63	0.56	7.74	43,47,50,51	0
2	SO4	B	383	5/5	0.83	0.50	4.53	59,62,63,64	0
5	GOL	A	411	6/6	0.80	0.39	3.47	22,30,31,36	0
4	CIT	B	406	13/13	0.77	0.32	3.44	22,31,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	412	6/6	0.59	0.37	3.29	35,39,40,42	0
2	SO4	D	389	5/5	0.85	0.39	3.02	70,70,72,73	0
3	COA	D	404	48/48	0.48	0.43	2.00	82,86,89,90	0
4	CIT	D	408	13/13	0.70	0.30	1.60	32,39,47,49	0
5	GOL	D	414	6/6	0.71	0.27	1.11	59,61,62,62	0
4	CIT	C	407	13/13	0.70	0.30	0.78	36,43,51,53	0
4	CIT	A	405	13/13	0.78	0.28	0.70	22,28,42,45	0
3	COA	A	401	48/48	0.65	0.32	0.67	42,52,62,65	0
3	COA	C	403	48/48	0.60	0.35	0.35	63,73,81,82	0
2	SO4	B	382	5/5	0.90	0.23	0.29	52,55,56,58	0
3	COA	B	402	48/48	0.79	0.22	0.01	18,25,43,45	0
2	SO4	C	381	5/5	0.95	0.14	-2.45	25,26,27,29	0
2	SO4	A	391	5/5	0.96	0.14	-2.69	15,16,17,19	0
2	SO4	A	387	5/5	0.89	0.30	-	42,43,43,46	0
2	SO4	D	386	5/5	0.83	0.22	-	42,43,44,45	0
2	SO4	B	385	5/5	0.92	0.25	-	43,43,44,45	0
2	SO4	C	388	5/5	0.90	0.14	-	49,50,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.