



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 AM GMT

PDB ID : 3NCH  
Title : Yeast Glycogen Synthase (Gsy2p) Basal State Conformation  
Authors : Baskaran, S.; Hurley, T.D.  
Deposited on : 2010-06-04  
Resolution : 2.88 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

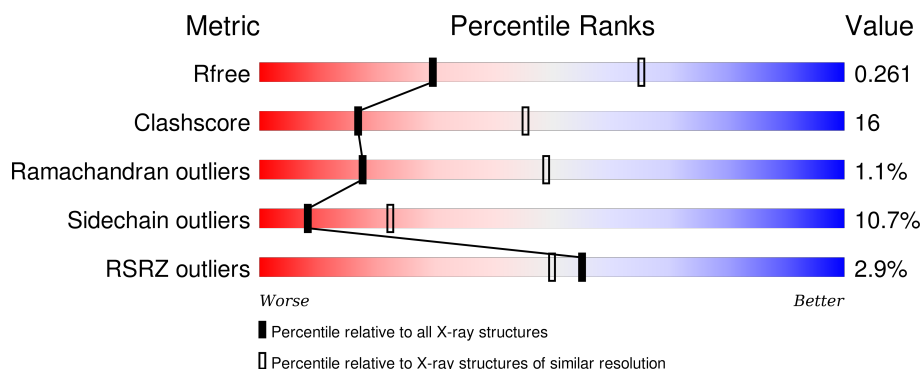
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	725	<div> <div>3%</div> <div>53%</div> <div>27%</div> <div>•</div> <div>16%</div> </div>
1	B	725	<div> <div>3%</div> <div>52%</div> <div>28%</div> <div>5%</div> <div>16%</div> </div>
1	C	725	<div> <div>3%</div> <div>58%</div> <div>22%</div> <div>5%</div> <div>15%</div> </div>
1	D	725	<div> <div>%</div> <div>57%</div> <div>23%</div> <div>•</div> <div>16%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	801	-	-	-	X
2	SO4	D	801	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19787 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4923	3148	857	899	19			
1	B	612	Total	C	N	O	S	0	0	0
			4927	3150	858	900	19			
1	C	613	Total	C	N	O	S	0	0	0
			4935	3154	860	902	19			
1	D	612	Total	C	N	O	S	0	0	0
			4927	3150	858	900	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27472
A	-18	GLY	-	EXPRESSION TAG	UNP P27472
A	-17	SER	-	EXPRESSION TAG	UNP P27472
A	-16	SER	-	EXPRESSION TAG	UNP P27472
A	-15	HIS	-	EXPRESSION TAG	UNP P27472
A	-14	HIS	-	EXPRESSION TAG	UNP P27472
A	-13	HIS	-	EXPRESSION TAG	UNP P27472
A	-12	HIS	-	EXPRESSION TAG	UNP P27472
A	-11	HIS	-	EXPRESSION TAG	UNP P27472
A	-10	HIS	-	EXPRESSION TAG	UNP P27472
A	-9	SER	-	EXPRESSION TAG	UNP P27472
A	-8	SER	-	EXPRESSION TAG	UNP P27472
A	-7	GLY	-	EXPRESSION TAG	UNP P27472
A	-6	LEU	-	EXPRESSION TAG	UNP P27472
A	-5	VAL	-	EXPRESSION TAG	UNP P27472
A	-4	PRO	-	EXPRESSION TAG	UNP P27472
A	-3	ARG	-	EXPRESSION TAG	UNP P27472
A	-2	GLY	-	EXPRESSION TAG	UNP P27472
A	-1	SER	-	EXPRESSION TAG	UNP P27472
A	0	HIS	-	EXPRESSION TAG	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	EXPRESSION TAG	UNP P27472
B	-14	HIS	-	EXPRESSION TAG	UNP P27472
B	-13	HIS	-	EXPRESSION TAG	UNP P27472
B	-12	HIS	-	EXPRESSION TAG	UNP P27472
B	-11	HIS	-	EXPRESSION TAG	UNP P27472
B	-10	HIS	-	EXPRESSION TAG	UNP P27472
B	-9	SER	-	EXPRESSION TAG	UNP P27472
B	-8	SER	-	EXPRESSION TAG	UNP P27472
B	-7	GLY	-	EXPRESSION TAG	UNP P27472
B	-6	LEU	-	EXPRESSION TAG	UNP P27472
B	-5	VAL	-	EXPRESSION TAG	UNP P27472
B	-4	PRO	-	EXPRESSION TAG	UNP P27472
B	-3	ARG	-	EXPRESSION TAG	UNP P27472
B	-2	GLY	-	EXPRESSION TAG	UNP P27472
B	-1	SER	-	EXPRESSION TAG	UNP P27472
B	0	HIS	-	EXPRESSION TAG	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	UNP P27472
C	-18	GLY	-	EXPRESSION TAG	UNP P27472
C	-17	SER	-	EXPRESSION TAG	UNP P27472
C	-16	SER	-	EXPRESSION TAG	UNP P27472
C	-15	HIS	-	EXPRESSION TAG	UNP P27472
C	-14	HIS	-	EXPRESSION TAG	UNP P27472
C	-13	HIS	-	EXPRESSION TAG	UNP P27472
C	-12	HIS	-	EXPRESSION TAG	UNP P27472
C	-11	HIS	-	EXPRESSION TAG	UNP P27472
C	-10	HIS	-	EXPRESSION TAG	UNP P27472
C	-9	SER	-	EXPRESSION TAG	UNP P27472
C	-8	SER	-	EXPRESSION TAG	UNP P27472
C	-7	GLY	-	EXPRESSION TAG	UNP P27472
C	-6	LEU	-	EXPRESSION TAG	UNP P27472
C	-5	VAL	-	EXPRESSION TAG	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP P27472
C	-3	ARG	-	EXPRESSION TAG	UNP P27472
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	UNP P27472
D	-18	GLY	-	EXPRESSION TAG	UNP P27472
D	-17	SER	-	EXPRESSION TAG	UNP P27472
D	-16	SER	-	EXPRESSION TAG	UNP P27472
D	-15	HIS	-	EXPRESSION TAG	UNP P27472
D	-14	HIS	-	EXPRESSION TAG	UNP P27472
D	-13	HIS	-	EXPRESSION TAG	UNP P27472
D	-12	HIS	-	EXPRESSION TAG	UNP P27472
D	-11	HIS	-	EXPRESSION TAG	UNP P27472
D	-10	HIS	-	EXPRESSION TAG	UNP P27472
D	-9	SER	-	EXPRESSION TAG	UNP P27472
D	-8	SER	-	EXPRESSION TAG	UNP P27472
D	-7	GLY	-	EXPRESSION TAG	UNP P27472
D	-6	LEU	-	EXPRESSION TAG	UNP P27472
D	-5	VAL	-	EXPRESSION TAG	UNP P27472
D	-4	PRO	-	EXPRESSION TAG	UNP P27472
D	-3	ARG	-	EXPRESSION TAG	UNP P27472
D	-2	GLY	-	EXPRESSION TAG	UNP P27472
D	-1	SER	-	EXPRESSION TAG	UNP P27472
D	0	HIS	-	EXPRESSION TAG	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	580	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	581	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	583	ALA	ARG	ENGINEERED MUTATION	UNP P27472

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



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

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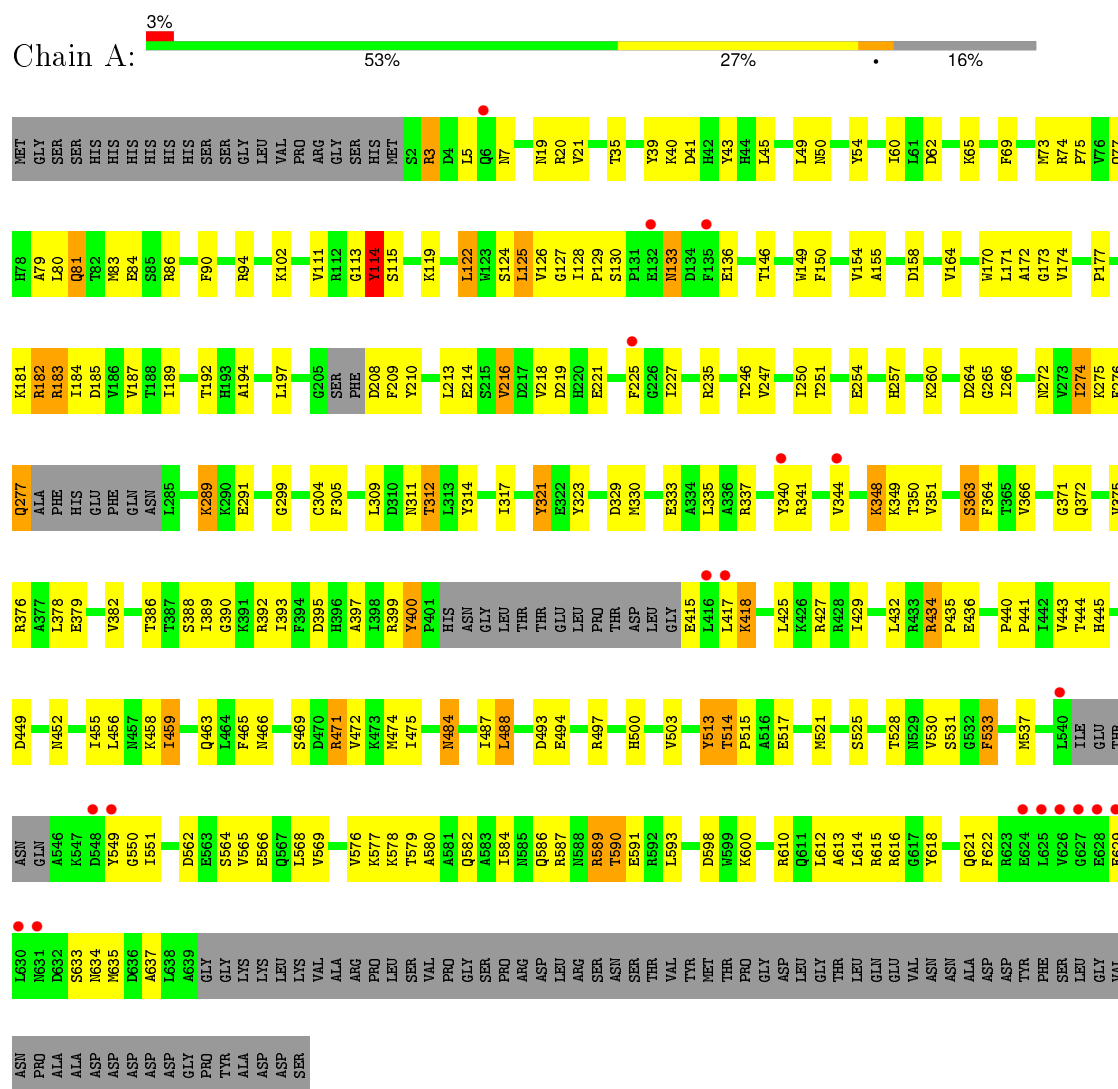
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		



### 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 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.

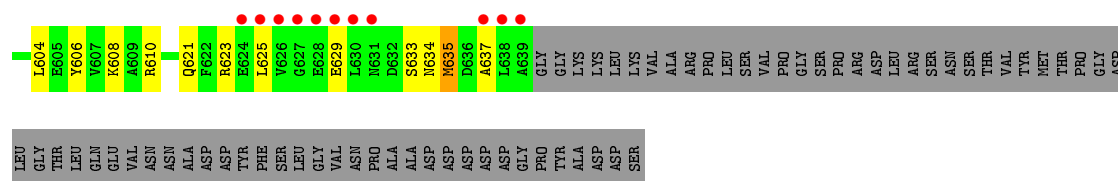
- Molecule 1: Glycogen [starch] synthase isoform 2



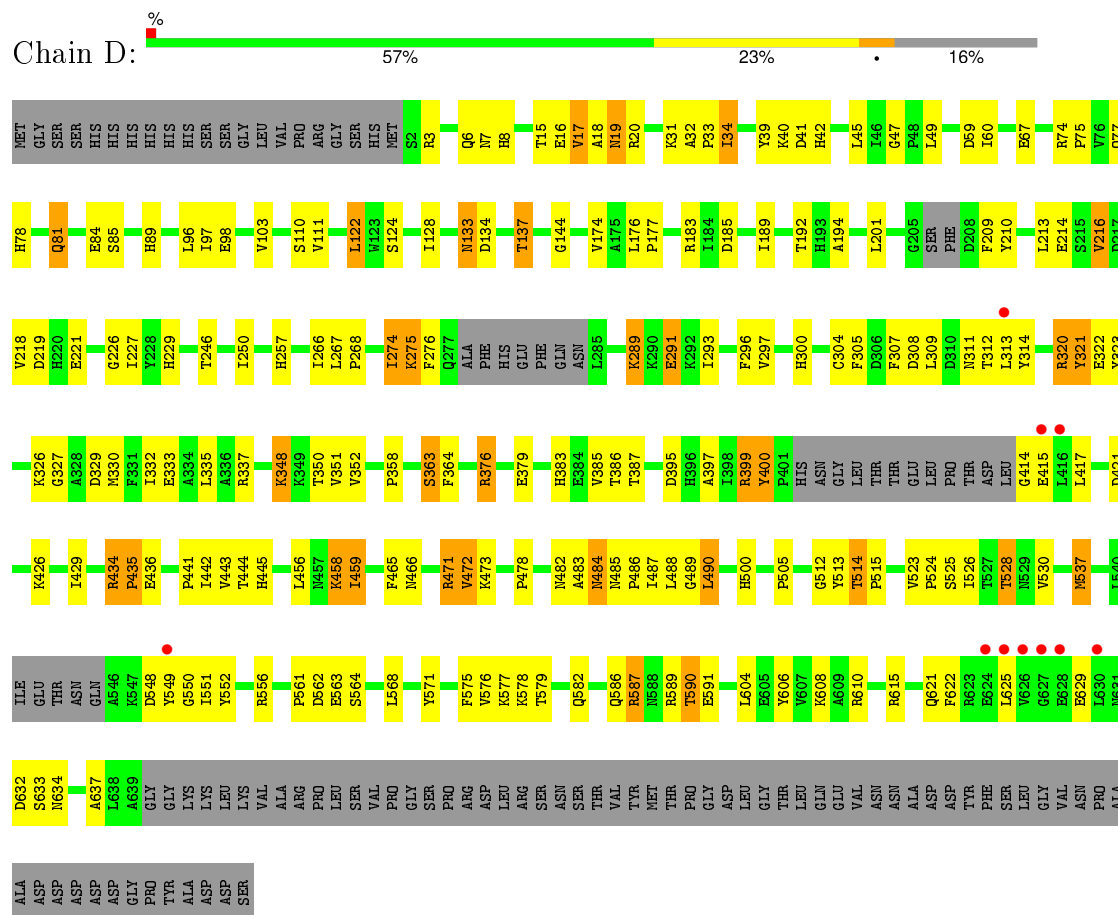
- Molecule 1: Glycogen [starch] synthase isoform 2







- Molecule 1: Glycogen [starch] synthase isoform 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.94Å 161.84Å 121.62Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	46.73 – 2.88 46.73 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.73-2.88) 98.3 (46.73-2.88)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.213 , 0.265 0.213 , 0.261	Depositor DCC
$R_{free}$ test set	4043 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 80328 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/5038	0.59	0/6819
1	B	0.44	0/5042	0.58	0/6824
1	C	0.41	0/5050	0.58	0/6835
1	D	0.43	0/5042	0.58	0/6824
All	All	0.43	0/20172	0.58	0/27302

There are no bond length outliers.

There are no bond angle outliers.

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	4923	0	4850	171	0
1	B	4927	0	4853	182	0
1	C	4935	0	4859	148	0
1	D	4927	0	4853	155	0
2	A	20	0	0	1	0
2	B	15	0	0	1	0
2	C	20	0	0	0	0
2	D	20	0	0	1	0
All	All	19787	0	19415	642	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 16.

All (642) 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:B:312:THR:HG22	1:B:350:THR:HB	1.15	1.13
1:B:125:LEU:HD21	1:B:181:LYS:HG3	1.40	1.04
1:B:382:VAL:O	1:B:386:THR:HG23	1.58	1.03
1:B:493:ASP:HB2	1:B:521:MET:HE2	1.40	1.02
1:A:589:ARG:HG3	1:A:589:ARG:HH11	1.21	1.00
1:A:312:THR:CG2	1:A:350:THR:HB	1.92	0.99
1:D:314:TYR:H	1:D:500:HIS:HD2	1.07	0.99
1:A:351:VAL:HB	1:A:472:VAL:HG12	1.44	0.97
1:A:133:ASN:H	1:A:133:ASN:HD22	1.14	0.95
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.51	0.93
1:D:312:THR:HG22	1:D:350:THR:HB	1.50	0.92
1:C:314:TYR:H	1:C:500:HIS:HD2	1.16	0.92
1:C:589:ARG:HG3	1:C:589:ARG:HH11	1.33	0.92
1:B:312:THR:CG2	1:B:350:THR:HB	1.99	0.91
1:A:312:THR:HG22	1:A:350:THR:HB	1.50	0.90
1:C:312:THR:HG22	1:C:350:THR:HB	1.53	0.90
1:C:133:ASN:HD22	1:C:133:ASN:H	1.20	0.89
1:A:125:LEU:HD21	1:A:181:LYS:HG3	1.53	0.89
1:B:493:ASP:HB2	1:B:521:MET:CE	2.04	0.87
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.59	0.85
1:B:585:ASN:HB3	1:B:589:ARG:HH12	1.42	0.83
1:A:348:LYS:HE2	1:A:349:LYS:HE2	1.60	0.83
1:C:549:TYR:CD2	1:C:589:ARG:HB3	2.14	0.83
1:A:528:THR:HG22	1:A:530:VAL:H	1.44	0.82
1:D:122:LEU:HD13	1:D:128:ILE:HB	1.61	0.82
1:B:122:LEU:HD13	1:B:128:ILE:HB	1.61	0.81
1:A:390:GLY:HA2	1:C:386:THR:HG21	1.63	0.81
1:C:528:THR:HG22	1:C:530:VAL:H	1.44	0.80
1:A:309:LEU:HA	1:A:312:THR:OG1	1.80	0.79
1:D:74:ARG:HH21	1:D:77:GLN:HE22	1.29	0.79
1:A:122:LEU:HD13	1:A:128:ILE:HB	1.63	0.79
1:C:549:TYR:O	1:C:590:THR:HG22	1.83	0.79
1:A:62:ASP:OD2	1:A:65:LYS:HG3	1.83	0.78
1:A:314:TYR:H	1:A:500:HIS:HD2	1.32	0.78
1:D:589:ARG:HH11	1:D:589:ARG:HG3	1.47	0.78
1:C:579:THR:OG1	1:C:582:GLN:HG3	1.85	0.77
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ASN:H	1:B:484:ASN:HD22	1.31	0.76
1:A:133:ASN:ND2	1:A:133:ASN:H	1.82	0.76
1:C:434:ARG:NH2	1:C:440:PRO:HA	2.00	0.76
1:B:551:ILE:HD12	1:B:593:LEU:HD13	1.68	0.76
1:A:75:PRO:HG2	1:A:158:ASP:OD2	1.86	0.76
1:B:390:GLY:HA2	1:D:386:THR:HG21	1.68	0.75
1:A:81:GLN:HE21	1:A:81:GLN:HA	1.51	0.75
1:C:549:TYR:HD2	1:C:589:ARG:HB3	1.47	0.75
1:B:549:TYR:CE2	1:B:589:ARG:HD3	2.22	0.75
1:B:528:THR:HG22	1:B:530:VAL:H	1.52	0.74
1:C:434:ARG:HH21	1:C:440:PRO:HA	1.51	0.74
1:D:550:GLY:HA3	1:D:590:THR:CG2	2.18	0.74
1:C:6:GLN:NE2	1:C:625:LEU:HD21	2.03	0.74
1:B:589:ARG:HH11	1:B:589:ARG:HG3	1.52	0.73
1:D:214:GLU:HG2	1:D:257:HIS:CE1	2.23	0.73
1:B:174:VAL:O	1:B:177:PRO:HD2	1.88	0.72
1:C:74:ARG:HE	1:C:77:GLN:NE2	1.87	0.72
1:D:214:GLU:HG2	1:D:257:HIS:ND1	2.05	0.72
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.54	0.71
1:A:289:LYS:HG2	1:A:494:GLU:HB3	1.71	0.71
1:D:549:TYR:O	1:D:590:THR:HG22	1.90	0.71
1:B:75:PRO:HG2	1:B:158:ASP:OD2	1.89	0.71
1:A:382:VAL:O	1:A:386:THR:HG23	1.90	0.71
1:D:133:ASN:HD22	1:D:133:ASN:H	1.39	0.70
1:A:589:ARG:NH1	1:A:589:ARG:HG3	2.01	0.70
1:B:445:HIS:CD2	1:B:478:PRO:HD2	2.26	0.70
1:C:589:ARG:HG3	1:C:589:ARG:NH1	2.04	0.70
1:C:286:HIS:HB2	1:C:587:ARG:HH12	1.56	0.70
1:A:390:GLY:CA	1:C:386:THR:HG21	2.20	0.70
1:C:399:ARG:O	1:C:400:TYR:C	2.30	0.70
1:B:80:LEU:HD22	1:B:90:PHE:CE1	2.27	0.69
1:A:111:VAL:O	1:A:111:VAL:HG12	1.92	0.69
1:D:314:TYR:H	1:D:500:HIS:CD2	2.00	0.69
1:D:383:HIS:O	1:D:387:THR:HG23	1.92	0.69
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.28	0.68
1:C:32:ALA:HB3	1:C:33:PRO:HD3	1.75	0.68
1:C:443:VAL:HG22	1:C:456:LEU:HD21	1.76	0.67
1:A:314:TYR:H	1:A:500:HIS:CD2	2.12	0.67
1:B:484:ASN:HD22	1:B:484:ASN:N	1.93	0.67
1:A:5:LEU:HD21	1:A:618:TYR:HD1	1.59	0.67
1:B:125:LEU:HD21	1:B:181:LYS:CG	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ARG:HH21	1:B:260:LYS:HG3	1.60	0.67
1:B:125:LEU:CD2	1:B:181:LYS:HG3	2.23	0.66
1:D:323:TYR:CZ	1:D:329:ASP:HB3	2.30	0.66
1:C:314:TYR:H	1:C:500:HIS:CD2	2.05	0.66
1:D:122:LEU:CD1	1:D:128:ILE:HB	2.25	0.66
1:A:493:ASP:HB2	1:A:521:MET:CE	2.26	0.66
1:D:615:ARG:HD3	1:D:622:PHE:CD1	2.31	0.66
1:C:286:HIS:HB2	1:C:587:ARG:NH1	2.11	0.65
1:D:6:GLN:NE2	1:D:625:LEU:HD21	2.11	0.65
1:B:549:TYR:O	1:B:590:THR:HG22	1.97	0.65
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.62	0.65
1:D:74:ARG:HE	1:D:77:GLN:NE2	1.94	0.65
1:A:449:ASP:OD2	1:A:452:ASN:HB2	1.97	0.65
1:A:312:THR:HG23	1:A:350:THR:HB	1.75	0.65
1:C:133:ASN:HD22	1:C:133:ASN:N	1.90	0.65
1:C:383:HIS:O	1:C:387:THR:HG23	1.97	0.64
1:B:143:LEU:O	1:B:147:VAL:HG23	1.97	0.64
1:B:314:TYR:H	1:B:500:HIS:CD2	2.16	0.64
1:B:309:LEU:HA	1:B:312:THR:OG1	1.96	0.64
1:D:550:GLY:HA3	1:D:590:THR:HG21	1.80	0.64
1:C:634:ASN:HB2	1:C:637:ALA:H	1.62	0.63
1:A:305:PHE:HZ	1:A:309:LEU:HG	1.62	0.63
1:B:133:ASN:H	1:B:133:ASN:ND2	1.97	0.63
1:C:227:ILE:HG22	1:C:227:ILE:O	1.99	0.63
1:A:589:ARG:HH11	1:A:589:ARG:CG	2.02	0.63
1:D:483:ALA:HA	1:D:490:LEU:N	2.14	0.63
1:B:484:ASN:ND2	1:B:484:ASN:H	1.97	0.63
1:A:340:TYR:CE2	1:A:344:VAL:HG21	2.34	0.63
1:A:125:LEU:HD21	1:A:181:LYS:CG	2.27	0.62
1:B:340:TYR:CE2	1:B:344:VAL:HG21	2.35	0.62
1:D:589:ARG:NH1	1:D:589:ARG:HG3	2.15	0.62
1:D:550:GLY:HA3	1:D:590:THR:HG22	1.82	0.62
1:D:216:VAL:HG23	1:D:221:GLU:HG3	1.80	0.62
1:B:351:VAL:HB	1:B:472:VAL:CG1	2.29	0.62
1:A:579:THR:HG23	1:A:582:GLN:OE1	1.99	0.62
1:B:348:LYS:HE2	1:B:349:LYS:HE2	1.82	0.61
1:B:213:LEU:HD11	1:B:253:PHE:CE1	2.35	0.61
1:D:444:THR:OG1	1:D:445:HIS:HD2	1.82	0.61
1:C:307:PHE:HD1	1:C:312:THR:HG21	1.65	0.61
1:C:17:VAL:HG23	1:C:18:ALA:H	1.65	0.61
1:D:634:ASN:HB2	1:D:637:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.33	0.61
1:A:444:THR:OG1	1:A:445:HIS:HD2	1.83	0.61
1:D:323:TYR:CE1	1:D:329:ASP:HB3	2.35	0.61
1:A:122:LEU:CD1	1:A:128:ILE:HB	2.30	0.61
1:C:493:ASP:HB2	1:C:521:MET:CE	2.29	0.61
1:A:493:ASP:HB2	1:A:521:MET:HE2	1.81	0.60
1:C:133:ASN:H	1:C:133:ASN:ND2	1.97	0.60
1:A:5:LEU:HD21	1:A:618:TYR:CD1	2.36	0.60
1:C:340:TYR:CE2	1:C:344:VAL:HG21	2.36	0.60
1:D:385:VAL:HG22	1:D:421:ASP:HB3	1.82	0.60
1:B:548:ASP:O	1:B:589:ARG:HD2	2.02	0.60
1:B:390:GLY:CA	1:D:386:THR:HG21	2.30	0.60
1:B:549:TYR:HB3	1:B:593:LEU:HD11	1.82	0.60
1:C:234:GLU:HG2	1:C:259:LEU:HD21	1.82	0.60
1:B:133:ASN:HD22	1:B:133:ASN:H	1.50	0.60
1:A:528:THR:CG2	1:A:530:VAL:HG22	2.32	0.59
1:C:216:VAL:HG23	1:C:221:GLU:HG3	1.83	0.59
1:B:623:ARG:HE	1:B:629:GLU:HB3	1.67	0.59
1:D:307:PHE:CD1	1:D:312:THR:HG21	2.37	0.59
1:A:634:ASN:HB2	1:A:637:ALA:H	1.67	0.59
1:B:620:ASP:O	1:B:624:GLU:HG2	2.03	0.59
1:A:309:LEU:HA	1:A:312:THR:HG1	1.67	0.59
1:D:275:LYS:O	1:D:275:LYS:HG2	2.03	0.59
1:D:548:ASP:O	1:D:589:ARG:HD2	2.03	0.59
1:A:289:LYS:CG	1:A:494:GLU:HB3	2.33	0.59
1:B:327:GLY:HA3	1:B:505:PRO:O	2.03	0.58
1:D:89:HIS:HD2	1:D:110:SER:HB2	1.67	0.58
1:A:111:VAL:O	1:A:111:VAL:CG1	2.51	0.58
1:B:266:ILE:HG22	1:B:268:PRO:HG3	1.85	0.58
1:C:332:ILE:HG12	1:C:474:MET:HE2	1.84	0.58
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.02	0.58
1:B:606:TYR:O	1:B:610:ARG:HG3	2.03	0.58
1:B:414:GLY:HA2	1:D:414:GLY:N	2.18	0.58
1:A:213:LEU:HD12	1:A:214:GLU:N	2.18	0.58
1:C:17:VAL:HG23	1:C:18:ALA:N	2.17	0.58
1:C:266:ILE:HG22	1:C:268:PRO:HD3	1.85	0.58
1:D:445:HIS:CD2	1:D:478:PRO:HD2	2.38	0.58
1:C:21:VAL:HG12	1:C:21:VAL:O	2.03	0.58
1:C:307:PHE:CD1	1:C:312:THR:HG21	2.38	0.57
1:D:67:GLU:CD	1:D:67:GLU:H	2.07	0.57
1:B:11:PHE:HD1	1:B:46:ILE:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:ARG:HG3	1:B:589:ARG:NH1	2.19	0.57
1:A:615:ARG:HD3	1:A:622:PHE:CD1	2.40	0.57
1:C:552:TYR:HD1	1:C:571:TYR:CD2	2.22	0.57
1:D:45:LEU:HB2	1:D:103:VAL:HG12	1.86	0.57
1:D:308:ASP:O	1:D:312:THR:HG23	2.04	0.57
1:D:17:VAL:HG23	1:D:18:ALA:H	1.70	0.57
1:C:189:ILE:HD11	1:C:610:ARG:HA	1.87	0.57
1:C:3:ARG:NH1	1:C:185:ASP:OD2	2.37	0.57
1:D:17:VAL:HG22	1:D:47:GLY:HA3	1.87	0.57
1:B:399:ARG:NH2	1:D:308:ASP:HA	2.20	0.57
1:D:305:PHE:HZ	1:D:309:LEU:HG	1.69	0.57
1:A:375:VAL:O	1:A:379:GLU:HG3	2.05	0.56
1:B:235:ARG:NH2	1:B:260:LYS:HG3	2.19	0.56
1:B:271:LEU:HD13	1:B:520:VAL:HG21	1.87	0.56
1:C:425:LEU:O	1:C:429:ILE:HG13	2.05	0.56
1:A:225:PHE:O	1:A:227:ILE:HG12	2.05	0.56
1:D:81:GLN:CA	1:D:81:GLN:HE21	2.19	0.56
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.39	0.56
1:D:484:ASN:H	1:D:484:ASN:ND2	2.03	0.56
1:D:216:VAL:CG2	1:D:221:GLU:HG3	2.36	0.56
1:B:74:ARG:HE	1:B:77:GLN:NE2	2.04	0.56
1:C:213:LEU:HA	1:C:216:VAL:CG1	2.36	0.56
1:D:314:TYR:N	1:D:500:HIS:HD2	1.90	0.56
1:B:89:HIS:O	1:B:107:ASP:HB3	2.06	0.56
1:C:308:ASP:O	1:C:312:THR:HG23	2.06	0.56
1:A:181:LYS:C	1:A:183:ARG:H	2.09	0.56
1:A:119:LYS:HB3	1:A:130:SER:OG	2.05	0.56
1:C:443:VAL:CG2	1:C:456:LEU:HD21	2.36	0.56
1:D:358:PRO:HA	1:D:478:PRO:O	2.06	0.56
1:B:579:THR:HG23	1:B:582:GLN:OE1	2.05	0.56
1:D:3:ARG:HH12	1:D:185:ASP:HB3	1.71	0.56
1:D:174:VAL:O	1:D:177:PRO:HD2	2.06	0.55
1:A:434:ARG:NH2	1:A:440:PRO:HA	2.21	0.55
1:D:213:LEU:HD12	1:D:214:GLU:N	2.21	0.55
1:A:79:ALA:O	1:A:83:MET:HG2	2.06	0.55
1:C:234:GLU:HG2	1:C:259:LEU:CD2	2.37	0.55
1:A:218:VAL:HG23	1:A:219:ASP:N	2.21	0.55
1:A:350:THR:OG1	1:A:471:ARG:NH1	2.36	0.55
1:B:210:TYR:CZ	1:B:530:VAL:HB	2.41	0.55
1:D:31:LYS:HE2	1:D:606:TYR:CE1	2.41	0.55
1:C:350:THR:OG1	1:C:471:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:ALA:HA	1:D:490:LEU:H	1.70	0.55
1:B:463:GLN:HG2	1:B:465:PHE:HE2	1.72	0.55
1:B:62:ASP:OD2	1:B:65:LYS:HG3	2.07	0.55
1:A:379:GLU:HG2	1:C:394:PHE:CE1	2.42	0.55
1:A:565:VAL:O	1:A:569:VAL:HG23	2.07	0.55
1:D:213:LEU:HA	1:D:216:VAL:CG1	2.37	0.55
1:B:528:THR:CG2	1:B:530:VAL:HG22	2.36	0.54
1:B:493:ASP:CB	1:B:521:MET:HE2	2.25	0.54
1:D:19:ASN:HD22	1:D:19:ASN:N	2.05	0.54
1:D:528:THR:HG22	1:D:530:VAL:H	1.73	0.54
1:D:579:THR:OG1	1:D:582:GLN:HG3	2.07	0.54
1:D:17:VAL:CG2	1:D:47:GLY:HA3	2.37	0.54
1:D:134:ASP:OD2	1:D:229:HIS:NE2	2.39	0.54
1:D:332:ILE:HD13	1:D:459:ILE:HG23	1.90	0.54
1:C:82:THR:O	1:C:85:SER:HB2	2.08	0.54
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.90	0.54
1:D:274:ILE:O	1:D:276:PHE:N	2.34	0.54
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.07	0.54
1:A:487:ILE:HG22	1:A:488:LEU:N	2.22	0.54
1:C:31:LYS:O	1:C:35:THR:HG23	2.08	0.54
1:A:146:THR:O	1:A:149:TRP:HB3	2.08	0.54
1:C:81:GLN:HE21	1:C:81:GLN:CA	2.20	0.54
1:B:549:TYR:CD2	1:B:589:ARG:HD3	2.42	0.53
1:B:444:THR:OG1	1:B:445:HIS:HD2	1.91	0.53
1:D:526:ILE:HG12	1:D:552:TYR:HB2	1.90	0.53
1:D:333:GLU:HG3	1:D:337:ARG:HH11	1.73	0.53
1:B:227:ILE:HG22	1:B:227:ILE:O	2.06	0.53
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.42	0.53
1:B:8:HIS:CE1	1:B:39:TYR:HE1	2.26	0.53
1:C:216:VAL:CG2	1:C:221:GLU:HG3	2.38	0.53
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.91	0.53
1:A:235:ARG:HH21	1:A:260:LYS:HG3	1.74	0.53
1:B:317:ILE:HG13	1:B:503:VAL:O	2.09	0.53
1:C:554:VAL:HG12	1:C:555:ASP:N	2.24	0.53
1:C:586:GLN:O	1:C:590:THR:HG23	2.09	0.53
1:B:314:TYR:H	1:B:500:HIS:HD2	1.52	0.53
1:B:332:ILE:HD13	1:B:459:ILE:HG23	1.90	0.53
1:B:351:VAL:HB	1:B:472:VAL:HG13	1.90	0.53
1:B:465:PHE:O	1:B:466:ASN:HB2	2.09	0.53
1:A:39:TYR:HB2	1:A:43:TYR:HB2	1.90	0.53
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:ILE:HD12	1:D:459:ILE:HG13	1.91	0.52
1:C:302:HIS:O	1:C:302:HIS:CG	2.62	0.52
1:B:221:GLU:O	1:B:224:ARG:HB3	2.10	0.52
1:A:371:GLY:O	1:A:375:VAL:HG23	2.09	0.52
1:B:150:PHE:O	1:B:154:VAL:HG23	2.08	0.52
1:B:585:ASN:HB3	1:B:589:ARG:NH1	2.19	0.52
1:B:3:ARG:NH1	1:B:185:ASP:OD2	2.39	0.52
1:D:274:ILE:C	1:D:276:PHE:H	2.11	0.52
1:A:341:ARG:NH2	1:A:566:GLU:OE1	2.42	0.52
1:A:49:LEU:HD11	1:A:54:TYR:CG	2.44	0.52
1:A:443:VAL:HG22	1:A:456:LEU:HD21	1.91	0.52
1:A:20:ARG:NH1	2:A:802:SO4:O3	2.26	0.52
1:C:550:GLY:HA3	1:C:590:THR:CG2	2.40	0.52
1:B:259:LEU:O	1:B:260:LYS:HB2	2.10	0.52
1:A:372:GLN:HG3	1:A:487:ILE:HG12	1.92	0.52
1:A:187:VAL:HG21	1:A:614:LEU:HD23	1.91	0.52
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.75	0.52
1:A:174:VAL:O	1:A:177:PRO:HD2	2.10	0.52
1:A:264:ASP:O	1:A:635:MET:HG3	2.09	0.52
1:B:114:TYR:HD1	1:B:114:TYR:H	1.56	0.52
1:A:386:THR:HG21	1:C:390:GLY:HA2	1.91	0.52
1:D:528:THR:CG2	1:D:530:VAL:H	2.23	0.52
1:B:8:HIS:HE1	1:B:39:TYR:CE1	2.28	0.52
1:A:586:GLN:O	1:A:590:THR:HG23	2.11	0.52
1:C:66:PRO:O	1:C:74:ARG:NH2	2.43	0.51
1:A:213:LEU:HA	1:A:216:VAL:HG12	1.91	0.51
1:C:122:LEU:HD13	1:C:128:ILE:HB	1.91	0.51
1:D:266:ILE:HG22	1:D:268:PRO:HD3	1.91	0.51
1:A:311:ASN:HD21	1:A:348:LYS:HD2	1.75	0.51
1:B:586:GLN:O	1:B:590:THR:HG23	2.08	0.51
1:B:20:ARG:NH1	2:B:802:SO4:O2	2.34	0.51
1:C:265:GLY:HA3	1:C:635:MET:HG3	1.93	0.51
1:B:383:HIS:O	1:B:387:THR:HG23	2.11	0.51
1:A:549:TYR:HB3	1:A:593:LEU:HD11	1.92	0.51
1:C:74:ARG:HH21	1:C:77:GLN:HE22	1.58	0.51
1:B:351:VAL:HB	1:B:472:VAL:HG12	1.92	0.51
1:A:192:THR:HG22	1:A:246:THR:HG22	1.92	0.51
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.91	0.51
1:B:213:LEU:HA	1:B:216:VAL:CG1	2.40	0.51
1:A:317:ILE:HG13	1:A:503:VAL:O	2.11	0.51
1:D:192:THR:HG22	1:D:246:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:580:ALA:O	1:C:584:ILE:HG13	2.11	0.51
1:A:528:THR:HG21	1:A:530:VAL:HG22	1.93	0.51
1:D:227:ILE:HG22	1:D:227:ILE:O	2.11	0.51
1:C:623:ARG:HE	1:C:629:GLU:HB3	1.76	0.51
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.46	0.51
1:B:79:ALA:O	1:B:83:MET:HG2	2.11	0.51
1:B:493:ASP:CB	1:B:521:MET:CE	2.82	0.51
1:A:81:GLN:HE21	1:A:81:GLN:CA	2.22	0.51
1:B:634:ASN:HB2	1:B:637:ALA:H	1.76	0.51
1:D:307:PHE:HD1	1:D:312:THR:HG21	1.75	0.50
1:B:400:TYR:CG	1:B:401:PRO:HA	2.45	0.50
1:B:423:VAL:HG12	1:B:424:MET:N	2.25	0.50
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.93	0.50
1:B:17:VAL:HG23	1:B:18:ALA:N	2.27	0.50
1:B:17:VAL:O	1:B:95:TRP:CZ2	2.64	0.50
1:B:94:ARG:HD3	1:B:100:ALA:HB1	1.92	0.50
1:A:170:TRP:O	1:A:173:GLY:N	2.42	0.50
1:A:21:VAL:O	1:A:21:VAL:CG1	2.59	0.50
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.34	0.50
1:B:113:GLY:C	1:B:115:SER:H	2.15	0.50
1:D:586:GLN:O	1:D:590:THR:HG23	2.12	0.50
1:C:330:MET:HE2	1:C:568:LEU:HD22	1.93	0.50
1:C:17:VAL:HG22	1:C:47:GLY:HA3	1.93	0.50
1:D:267:LEU:HD22	1:D:606:TYR:CD2	2.47	0.50
1:A:235:ARG:NH2	1:A:260:LYS:HG3	2.27	0.50
1:B:501:LEU:HD12	1:B:524:PRO:HB2	1.94	0.50
1:C:442:ILE:HD12	1:C:459:ILE:HG13	1.94	0.49
1:A:276:PHE:O	1:A:277:GLN:HG3	2.12	0.49
1:A:576:VAL:C	1:A:578:LYS:H	2.14	0.49
1:B:126:VAL:HB	1:B:128:ILE:HD12	1.94	0.49
1:A:73:MET:C	1:A:75:PRO:HD2	2.32	0.49
1:B:506:SER:O	1:B:528:THR:HG21	2.11	0.49
1:A:415:GLU:HG2	1:A:417:LEU:O	2.13	0.49
1:B:425:LEU:O	1:B:429:ILE:HG13	2.12	0.49
1:A:213:LEU:C	1:A:213:LEU:HD12	2.33	0.49
1:A:39:TYR:CB	1:A:43:TYR:HB2	2.41	0.49
1:C:463:GLN:HG2	1:C:465:PHE:HE2	1.77	0.49
1:A:580:ALA:O	1:A:584:ILE:HG13	2.12	0.49
1:D:74:ARG:HE	1:D:77:GLN:HE21	1.60	0.49
1:A:216:VAL:CG2	1:A:221:GLU:HG3	2.43	0.49
1:B:126:VAL:HB	1:B:128:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:250:ILE:HD11	2.47	0.49
1:C:320:ARG:O	1:C:322:GLU:N	2.44	0.49
1:D:352:VAL:HG22	1:D:473:LYS:HB2	1.95	0.49
1:C:31:LYS:HZ3	1:C:35:THR:HG21	1.78	0.49
1:A:378:LEU:HD22	1:A:432:LEU:HD11	1.95	0.49
1:C:267:LEU:HD22	1:C:606:TYR:CD2	2.48	0.49
1:D:489:GLY:O	1:D:490:LEU:HG	2.13	0.48
1:A:21:VAL:HG12	1:A:21:VAL:O	2.12	0.48
1:D:6:GLN:HE21	1:D:625:LEU:HD21	1.77	0.48
1:B:434:ARG:HD2	1:B:435:PRO:HD2	1.93	0.48
1:A:351:VAL:CB	1:A:472:VAL:HG12	2.30	0.48
1:D:20:ARG:NH1	2:D:802:SO4:O3	2.45	0.48
1:C:549:TYR:HE2	1:C:589:ARG:HG2	1.78	0.48
1:A:276:PHE:O	1:A:497:ARG:NH2	2.46	0.48
1:D:512:GLY:O	1:D:515:PRO:HD2	2.13	0.48
1:A:125:LEU:CD2	1:A:181:LYS:HG3	2.34	0.48
1:B:551:ILE:HD12	1:B:593:LEU:CD1	2.39	0.48
1:D:266:ILE:HG22	1:D:268:PRO:HG3	1.96	0.48
1:B:31:LYS:O	1:B:35:THR:HG23	2.14	0.48
1:D:289:LYS:N	1:D:289:LYS:HD2	2.27	0.48
1:A:598:ASP:OD2	1:A:600:LYS:HG3	2.12	0.48
1:C:213:LEU:C	1:C:213:LEU:HD12	2.34	0.48
1:A:214:GLU:HG2	1:A:257:HIS:CE1	2.49	0.48
1:B:113:GLY:O	1:B:115:SER:N	2.47	0.48
1:A:182:ARG:HB2	1:A:184:ILE:HG13	1.95	0.48
1:C:351:VAL:HB	1:C:472:VAL:HG13	1.95	0.48
1:A:528:THR:HG22	1:A:530:VAL:N	2.22	0.48
1:A:187:VAL:HB	1:A:613:ALA:HB1	1.96	0.47
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.14	0.47
1:A:50:ASN:C	1:A:50:ASN:OD1	2.52	0.47
1:B:3:ARG:NH2	1:B:158:ASP:O	2.46	0.47
1:D:176:LEU:HB2	1:D:177:PRO:HD3	1.96	0.47
1:B:8:HIS:CE1	1:B:39:TYR:CE1	3.02	0.47
1:C:79:ALA:O	1:C:83:MET:HG2	2.14	0.47
1:D:312:THR:HA	1:D:350:THR:O	2.14	0.47
1:C:589:ARG:NH1	1:C:589:ARG:CG	2.77	0.47
1:D:213:LEU:C	1:D:213:LEU:HD12	2.35	0.47
1:B:360:LYS:HB3	1:B:448:VAL:HB	1.97	0.47
1:A:484:ASN:ND2	1:A:484:ASN:N	2.63	0.47
1:C:527:THR:OG1	1:C:528:THR:N	2.47	0.47
1:B:430:LEU:HD12	1:C:96:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:O	1:B:128:ILE:HG13	2.14	0.47
1:A:133:ASN:HD22	1:A:133:ASN:N	1.97	0.47
1:A:528:THR:CG2	1:A:530:VAL:H	2.23	0.47
1:B:484:ASN:ND2	1:B:484:ASN:N	2.58	0.47
1:B:176:LEU:HB2	1:B:177:PRO:HD3	1.97	0.47
1:B:476:PHE:O	1:B:478:PRO:HD3	2.15	0.47
1:D:291:GLU:HA	1:D:291:GLU:OE1	2.15	0.47
1:C:311:ASN:HD21	1:C:348:LYS:HD2	1.79	0.47
1:A:513:TYR:O	1:A:517:GLU:HG2	2.15	0.47
1:B:276:PHE:CD2	1:B:521:MET:HE3	2.50	0.47
1:A:392:ARG:NH1	1:A:418:LYS:HD3	2.30	0.47
1:A:349:LYS:O	1:A:471:ARG:HG3	2.15	0.47
1:C:10:LEU:HD23	1:C:43:TYR:CD1	2.50	0.47
1:A:183:ARG:HB2	1:A:183:ARG:HE	1.56	0.46
1:D:376:ARG:O	1:D:379:GLU:HB2	2.15	0.46
1:B:442:ILE:HD12	1:B:459:ILE:HG13	1.96	0.46
1:C:192:THR:HG22	1:C:246:THR:HG22	1.97	0.46
1:C:547:LYS:HB2	1:C:547:LYS:HE3	1.75	0.46
1:A:333:GLU:OE2	1:A:337:ARG:NH1	2.48	0.46
1:D:67:GLU:N	1:D:67:GLU:CD	2.69	0.46
1:D:549:TYR:C	1:D:590:THR:HG22	2.34	0.46
1:D:575:PHE:O	1:D:578:LYS:HB2	2.15	0.46
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.96	0.46
1:D:465:PHE:O	1:D:466:ASN:HB2	2.16	0.46
1:C:479:GLU:HG3	1:C:480:PHE:N	2.29	0.46
1:B:415:GLU:HG2	1:B:417:LEU:O	2.16	0.46
1:A:615:ARG:O	1:A:615:ARG:HD2	2.15	0.46
1:A:612:LEU:HD21	1:A:616:ARG:NH2	2.30	0.46
1:D:385:VAL:CG1	1:D:417:LEU:HD21	2.46	0.46
1:C:321:TYR:CD2	1:C:359:ALA:HB2	2.51	0.46
1:B:565:VAL:O	1:B:569:VAL:HG23	2.15	0.46
1:B:193:HIS:ND1	1:B:247:VAL:HG11	2.31	0.46
1:A:443:VAL:HG12	1:A:445:HIS:H	1.80	0.46
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.84	0.46
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.98	0.46
1:A:69:PHE:HD2	1:A:77:GLN:HE21	1.60	0.46
1:A:386:THR:HG21	1:C:390:GLY:CA	2.46	0.45
1:B:90:PHE:CD2	1:B:90:PHE:N	2.84	0.45
1:A:119:LYS:HZ2	1:A:130:SER:HB2	1.81	0.45
1:D:210:TYR:CZ	1:D:530:VAL:HB	2.51	0.45
1:C:81:GLN:HA	1:C:81:GLN:NE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASN:ND2	1:A:484:ASN:H	2.14	0.45
1:B:334:ALA:CB	1:B:568:LEU:HD23	2.46	0.45
1:D:443:VAL:HG22	1:D:456:LEU:HD21	1.97	0.45
1:D:576:VAL:C	1:D:578:LYS:H	2.19	0.45
1:C:12:GLU:HB3	1:C:45:LEU:HD23	1.98	0.45
1:D:17:VAL:HG23	1:D:18:ALA:N	2.32	0.45
1:C:479:GLU:HG3	1:C:480:PHE:H	1.81	0.45
1:B:514:THR:HB	1:B:515:PRO:HD3	1.98	0.45
1:D:40:LYS:HB3	1:D:41:ASP:H	1.52	0.45
1:A:210:TYR:CZ	1:A:530:VAL:HB	2.52	0.45
1:D:385:VAL:HG13	1:D:417:LEU:HD21	1.98	0.45
1:C:331:PHE:O	1:C:335:LEU:HB2	2.16	0.45
1:C:550:GLY:HA3	1:C:590:THR:HG22	1.99	0.45
1:D:3:ARG:NH1	1:D:185:ASP:OD2	2.49	0.45
1:D:134:ASP:CG	1:D:137:THR:HG23	2.37	0.45
1:B:332:ILE:HG12	1:B:474:MET:HE1	1.97	0.45
1:A:465:PHE:O	1:A:466:ASN:HB2	2.16	0.45
1:C:3:ARG:NH2	1:C:158:ASP:O	2.49	0.45
1:D:385:VAL:CG2	1:D:421:ASP:HB3	2.47	0.45
1:B:610:ARG:O	1:B:613:ALA:HB3	2.17	0.45
1:A:213:LEU:HA	1:A:216:VAL:CG1	2.46	0.45
1:C:264:ASP:O	1:C:635:MET:HG3	2.17	0.45
1:C:559:LYS:HB3	1:C:563:GLU:HB2	1.99	0.45
1:B:74:ARG:N	1:B:75:PRO:CD	2.80	0.45
1:D:275:LYS:O	1:D:275:LYS:CG	2.63	0.45
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.51	0.45
1:A:330:MET:CE	1:A:568:LEU:HD22	2.46	0.45
1:B:181:LYS:C	1:B:183:ARG:H	2.20	0.45
1:C:471:ARG:HG3	1:C:471:ARG:HH11	1.81	0.45
1:C:21:VAL:CG1	1:C:21:VAL:O	2.64	0.45
1:B:8:HIS:CD2	1:B:614:LEU:HD11	2.52	0.45
1:A:550:GLY:HA3	1:A:590:THR:CG2	2.47	0.45
1:D:311:ASN:HD21	1:D:348:LYS:HD2	1.81	0.45
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.50	0.45
1:B:266:ILE:CG2	1:B:268:PRO:HG3	2.47	0.45
1:B:397:ALA:HB1	1:D:429:ILE:HG12	1.98	0.45
1:D:250:ILE:HG12	1:D:530:VAL:HA	1.99	0.45
1:D:434:ARG:O	1:D:435:PRO:C	2.56	0.45
1:A:150:PHE:O	1:A:154:VAL:HG23	2.17	0.45
1:A:113:GLY:C	1:A:115:SER:H	2.21	0.44
1:C:321:TYR:HD2	1:C:359:ALA:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:LEU:O	1:C:594:SER:C	2.56	0.44
1:A:208:ASP:OD2	1:A:209:PHE:N	2.49	0.44
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.78	0.44
1:A:170:TRP:O	1:A:172:ALA:N	2.51	0.44
1:D:399:ARG:O	1:D:400:TYR:C	2.55	0.44
1:A:114:TYR:HD1	1:A:114:TYR:H	1.65	0.44
1:D:484:ASN:N	1:D:484:ASN:ND2	2.65	0.44
1:C:604:LEU:O	1:C:608:LYS:HG3	2.18	0.44
1:A:471:ARG:NE	1:A:471:ARG:HA	2.33	0.44
1:B:537:MET:HG2	1:B:551:ILE:HD13	2.00	0.44
1:C:16:GLU:O	1:C:17:VAL:C	2.54	0.44
1:B:429:ILE:HG12	1:D:397:ALA:HB1	1.99	0.44
1:B:164:VAL:HA	1:B:187:VAL:HG23	1.99	0.44
1:B:227:ILE:CG2	1:B:227:ILE:O	2.65	0.44
1:B:193:HIS:O	1:B:194:ALA:HB2	2.18	0.44
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.63	0.44
1:C:213:LEU:HA	1:C:216:VAL:HG12	2.00	0.44
1:D:78:HIS:HA	1:D:81:GLN:HB2	2.00	0.44
1:D:514:THR:HB	1:D:515:PRO:HD3	2.00	0.44
1:A:587:ARG:O	1:A:591:GLU:HB2	2.18	0.44
1:C:296:PHE:CE2	1:C:354:PHE:HE1	2.36	0.44
1:C:31:LYS:NZ	1:C:35:THR:HG21	2.33	0.44
1:A:125:LEU:HD21	1:A:181:LYS:CB	2.47	0.44
1:C:528:THR:CG2	1:C:530:VAL:H	2.22	0.44
1:B:528:THR:HG21	1:B:530:VAL:HG22	1.99	0.44
1:C:81:GLN:CA	1:C:81:GLN:NE2	2.81	0.44
1:B:385:VAL:HG13	1:B:417:LEU:HD21	1.98	0.44
1:C:40:LYS:HB3	1:C:41:ASP:H	1.55	0.44
1:B:341:ARG:NH2	1:B:566:GLU:OE1	2.51	0.44
1:B:82:THR:O	1:B:85:SER:HB2	2.18	0.44
1:B:11:PHE:CD1	1:B:46:ILE:HD11	2.53	0.43
1:C:78:HIS:HA	1:C:81:GLN:HB2	1.99	0.43
1:B:39:TYR:CB	1:B:43:TYR:HB2	2.48	0.43
1:C:289:LYS:HD2	1:C:289:LYS:N	2.31	0.43
1:D:74:ARG:N	1:D:75:PRO:CD	2.81	0.43
1:A:427:ARG:HD2	1:D:96:LEU:O	2.18	0.43
1:C:291:GLU:OE1	1:C:291:GLU:HA	2.19	0.43
1:D:604:LEU:O	1:D:608:LYS:HG3	2.17	0.43
1:B:350:THR:HG1	1:B:471:ARG:HH12	1.60	0.43
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.99	0.43
1:B:443:VAL:HG22	1:B:456:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLY:HA3	1:B:590:THR:CG2	2.48	0.43
1:D:81:GLN:CA	1:D:81:GLN:NE2	2.81	0.43
1:D:266:ILE:HG22	1:D:268:PRO:CD	2.48	0.43
1:B:99:GLY:O	1:B:100:ALA:C	2.56	0.43
1:C:335:LEU:HA	1:C:335:LEU:HD12	1.68	0.43
1:D:296:PHE:CG	1:D:488:LEU:HD13	2.53	0.43
1:B:80:LEU:HB3	1:B:90:PHE:HZ	1.81	0.43
1:A:3:ARG:NH2	1:A:155:ALA:O	2.52	0.43
1:B:266:ILE:HG22	1:B:268:PRO:HD3	2.01	0.43
1:B:326:LYS:HE2	1:B:509:GLU:OE1	2.18	0.43
1:B:440:PRO:HA	1:B:441:PRO:HD3	1.90	0.43
1:B:538:GLU:HB2	1:B:553:ILE:HD13	2.00	0.43
1:D:97:ILE:O	1:D:98:GLU:C	2.56	0.43
1:B:167:PHE:N	1:B:167:PHE:CD2	2.87	0.43
1:C:75:PRO:HG2	1:C:158:ASP:OD2	2.19	0.43
1:D:333:GLU:CG	1:D:337:ARG:NH1	2.82	0.43
1:D:226:GLY:C	1:D:227:ILE:HD13	2.39	0.43
1:C:514:THR:N	1:C:515:PRO:CD	2.82	0.43
1:C:74:ARG:N	1:C:75:PRO:CD	2.82	0.43
1:D:210:TYR:CE1	1:D:250:ILE:HD11	2.53	0.43
1:C:348:LYS:H	1:C:348:LYS:HG3	1.57	0.43
1:A:265:GLY:O	1:A:266:ILE:HD13	2.19	0.43
1:C:36:VAL:O	1:C:36:VAL:HG12	2.18	0.43
1:B:549:TYR:HE2	1:B:589:ARG:HD3	1.77	0.43
1:C:265:GLY:O	1:C:266:ILE:HD13	2.19	0.43
1:B:13:THR:HA	1:B:46:ILE:O	2.18	0.43
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.01	0.43
1:C:528:THR:O	1:C:534:GLY:HA3	2.19	0.43
1:A:440:PRO:HA	1:A:441:PRO:HD3	1.93	0.43
1:B:456:LEU:HA	1:B:456:LEU:HD23	1.87	0.43
1:B:289:LYS:NZ	1:B:494:GLU:OE2	2.50	0.43
1:C:266:ILE:HG22	1:C:268:PRO:CD	2.48	0.42
1:B:20:ARG:HA	1:B:25:TYR:CD1	2.54	0.42
1:A:114:TYR:CD1	1:A:114:TYR:N	2.87	0.42
1:B:331:PHE:O	1:B:335:LEU:HB2	2.19	0.42
1:C:34:ILE:HA	1:C:34:ILE:HD12	1.66	0.42
1:D:351:VAL:HB	1:D:472:VAL:HG13	2.01	0.42
1:B:266:ILE:O	1:B:268:PRO:HD3	2.19	0.42
1:D:293:ILE:O	1:D:297:VAL:HG23	2.20	0.42
1:D:313:LEU:HA	1:D:500:HIS:CD2	2.54	0.42
1:A:299:GLY:HA2	1:A:375:VAL:CG2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:HB3	1:B:41:ASP:H	1.67	0.42
1:D:189:ILE:HD11	1:D:610:ARG:HA	2.00	0.42
1:B:378:LEU:O	1:B:382:VAL:HG23	2.19	0.42
1:A:589:ARG:NH1	1:A:589:ARG:CG	2.71	0.42
1:C:227:ILE:HG23	1:C:230:ARG:HB2	2.01	0.42
1:B:213:LEU:HD12	1:B:214:GLU:N	2.35	0.42
1:D:201:LEU:HD12	1:D:209:PHE:HE2	1.84	0.42
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.85	0.42
1:C:133:ASN:N	1:C:133:ASN:ND2	2.62	0.42
1:B:515:PRO:O	1:B:518:CYS:HB3	2.19	0.42
1:B:615:ARG:HD3	1:B:622:PHE:CD1	2.54	0.42
1:B:338:LEU:HG	1:B:338:LEU:O	2.20	0.42
1:A:80:LEU:O	1:A:83:MET:HB2	2.18	0.42
1:A:218:VAL:HG23	1:A:219:ASP:H	1.83	0.42
1:A:164:VAL:HA	1:A:187:VAL:HG23	2.02	0.42
1:B:81:GLN:O	1:B:85:SER:N	2.41	0.42
1:C:364:PHE:CE2	1:C:486:PRO:HD2	2.55	0.42
1:C:321:TYR:C	1:C:321:TYR:CD1	2.93	0.42
1:B:334:ALA:HB2	1:B:568:LEU:HD23	2.01	0.42
1:A:463:GLN:HG2	1:A:465:PHE:HE2	1.83	0.42
1:B:315:PHE:CE2	1:B:572:MET:HG2	2.55	0.42
1:B:560:ALA:O	1:B:561:PRO:C	2.58	0.42
1:D:561:PRO:O	1:D:564:SER:HB2	2.18	0.42
1:D:444:THR:OG1	1:D:445:HIS:CD2	2.69	0.42
1:A:216:VAL:HG21	1:A:221:GLU:HG3	2.02	0.42
1:A:533:PHE:O	1:A:537:MET:HB2	2.19	0.42
1:A:40:LYS:HB3	1:A:41:ASP:H	1.54	0.42
1:A:397:ALA:O	1:A:400:TYR:HB2	2.20	0.42
1:B:368:ALA:HB1	1:B:487:ILE:CD1	2.49	0.42
1:A:275:LYS:O	1:A:275:LYS:CG	2.68	0.42
1:A:455:ILE:O	1:A:459:ILE:HG12	2.20	0.42
1:C:181:LYS:HD3	1:C:181:LYS:O	2.20	0.42
1:B:5:LEU:HD23	1:B:5:LEU:N	2.34	0.42
1:D:552:TYR:HD1	1:D:571:TYR:CD2	2.39	0.41
1:C:321:TYR:C	1:C:321:TYR:HD1	2.23	0.41
1:A:127:GLY:O	1:A:129:PRO:HD3	2.20	0.41
1:A:181:LYS:O	1:A:183:ARG:N	2.53	0.41
1:A:459:ILE:H	1:A:459:ILE:HG12	1.71	0.41
1:B:332:ILE:HG23	1:B:459:ILE:HG22	2.01	0.41
1:A:551:ILE:HD12	1:A:593:LEU:HD13	2.02	0.41
1:D:587:ARG:O	1:D:591:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:VAL:O	1:D:524:PRO:C	2.59	0.41
1:C:271:LEU:HD21	1:C:513:TYR:CE2	2.55	0.41
1:C:301:PHE:HE1	1:C:473:LYS:HD2	1.85	0.41
1:D:385:VAL:HG13	1:D:417:LEU:CD2	2.51	0.41
1:D:333:GLU:HG3	1:D:337:ARG:NH1	2.35	0.41
1:A:389:ILE:O	1:A:393:ILE:HG13	2.20	0.41
1:B:547:LYS:HB2	1:B:547:LYS:HE3	1.65	0.41
1:C:25:TYR:CD2	1:C:25:TYR:C	2.94	0.41
1:B:471:ARG:HH11	1:B:471:ARG:HG3	1.84	0.41
1:C:344:VAL:C	1:C:346:GLY:H	2.24	0.41
1:B:266:ILE:HD13	1:B:266:ILE:HA	1.81	0.41
1:A:251:THR:O	1:A:254:GLU:HB2	2.21	0.41
1:A:429:ILE:HG12	1:C:397:ALA:HB1	2.02	0.41
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.86	0.41
1:B:128:ILE:HA	1:B:129:PRO:HD3	1.75	0.41
1:D:144:GLY:HA3	1:D:174:VAL:HB	2.02	0.41
1:B:612:LEU:HD11	1:B:616:ARG:HE	1.85	0.41
1:D:321:TYR:CD1	1:D:321:TYR:C	2.94	0.41
1:C:487:ILE:HG22	1:C:488:LEU:N	2.35	0.41
1:D:330:MET:CE	1:D:568:LEU:HD22	2.51	0.41
1:A:312:THR:HA	1:A:350:THR:O	2.21	0.41
1:A:74:ARG:N	1:A:75:PRO:CD	2.84	0.41
1:C:6:GLN:HB2	1:C:6:GLN:HE21	1.66	0.41
1:A:493:ASP:CB	1:A:521:MET:CE	2.97	0.41
1:A:514:THR:HB	1:A:515:PRO:HD3	2.03	0.41
1:B:125:LEU:O	1:B:126:VAL:HG22	2.19	0.41
1:D:74:ARG:NH2	1:D:77:GLN:HE22	2.08	0.41
1:C:213:LEU:HD12	1:C:214:GLU:N	2.36	0.41
1:D:528:THR:CG2	1:D:530:VAL:HG22	2.51	0.41
1:A:364:PHE:CD1	1:A:487:ILE:HD12	2.56	0.41
1:D:434:ARG:HA	1:D:434:ARG:HD2	1.61	0.41
1:D:320:ARG:O	1:D:322:GLU:N	2.52	0.41
1:A:474:MET:C	1:A:475:ILE:HG12	2.40	0.41
1:A:274:ILE:H	1:A:274:ILE:HG13	1.62	0.41
1:C:62:ASP:HB3	1:C:65:LYS:HG3	2.02	0.41
1:C:372:GLN:O	1:C:376:ARG:HB2	2.21	0.41
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.87	0.41
1:B:3:ARG:HH12	1:B:185:ASP:HB3	1.86	0.41
1:D:323:TYR:OH	1:D:458:LYS:HG3	2.21	0.41
1:C:554:VAL:CG1	1:C:555:ASP:N	2.84	0.41
1:A:41:ASP:OD1	1:A:102:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:PHE:CD1	1:D:487:ILE:HD12	2.55	0.41
1:D:218:VAL:HG23	1:D:219:ASP:H	1.85	0.41
1:C:621:GLN:HB3	1:C:621:GLN:HE21	1.68	0.41
1:C:565:VAL:O	1:C:569:VAL:HG23	2.21	0.41
1:D:3:ARG:NH1	1:D:185:ASP:CG	2.75	0.40
1:D:34:ILE:HD12	1:D:34:ILE:HA	1.67	0.40
1:A:81:GLN:NE2	1:A:81:GLN:HA	2.27	0.40
1:D:213:LEU:HA	1:D:216:VAL:HG12	2.02	0.40
1:A:418:LYS:HG2	1:A:418:LYS:H	1.76	0.40
1:C:316:PHE:CZ	1:C:496:VAL:HG22	2.56	0.40
1:C:14:ALA:HB2	1:C:168:HIS:HB2	2.02	0.40
1:B:19:ASN:N	1:B:19:ASN:HD22	2.19	0.40
1:A:312:THR:HG22	1:A:350:THR:CB	2.36	0.40
1:C:549:TYR:HA	1:C:549:TYR:HD2	1.67	0.40
1:C:309:LEU:HD23	1:C:309:LEU:HA	1.93	0.40
1:C:332:ILE:HG23	1:C:459:ILE:HG22	2.04	0.40
1:D:16:GLU:O	1:D:17:VAL:C	2.59	0.40
1:B:286:HIS:O	1:B:287:ALA:C	2.59	0.40
1:D:8:HIS:CE1	1:D:39:TYR:HE1	2.40	0.40
1:D:74:ARG:O	1:D:75:PRO:C	2.57	0.40
1:B:234:GLU:HG2	1:B:259:LEU:HD21	2.03	0.40
1:D:6:GLN:HE21	1:D:6:GLN:HB2	1.68	0.40
1:D:274:ILE:HG13	1:D:274:ILE:H	1.68	0.40
1:D:537:MET:HG2	1:D:551:ILE:HD13	2.04	0.40
1:D:300:HIS:HE1	1:D:441:PRO:O	2.04	0.40
1:B:259:LEU:O	1:B:260:LYS:CB	2.69	0.40
1:A:444:THR:OG1	1:A:445:HIS:CD2	2.70	0.40
1:A:550:GLY:HA3	1:A:590:THR:HG21	2.02	0.40
1:C:267:LEU:HD21	1:C:606:TYR:HA	2.03	0.40
1:A:321:TYR:CZ	1:A:455:ILE:HG13	2.57	0.40
1:D:327:GLY:HA3	1:D:505:PRO:O	2.20	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	601/725 (83%)	541 (90%)	51 (8%)	9 (2%)	13	40
1	B	602/725 (83%)	543 (90%)	55 (9%)	4 (1%)	26	61
1	C	603/725 (83%)	549 (91%)	49 (8%)	5 (1%)	24	58
1	D	602/725 (83%)	547 (91%)	46 (8%)	9 (2%)	13	40
All	All	2408/2900 (83%)	2180 (90%)	201 (8%)	27 (1%)	17	49

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	SER
1	B	114	TYR
1	D	275	LYS
1	A	171	LEU
1	A	182	ARG
1	A	577	LYS
1	C	17	VAL
1	C	323	TYR
1	D	17	VAL
1	D	577	LYS
1	A	114	TYR
1	B	194	ALA
1	C	321	TYR
1	C	363	SER
1	D	415	GLU
1	A	194	ALA
1	C	594	SER
1	D	194	ALA
1	D	363	SER
1	A	435	PRO
1	D	490	LEU
1	A	274	ILE
1	B	126	VAL
1	B	363	SER
1	D	274	ILE
1	D	435	PRO
1	A	126	VAL

### 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	526/622 (85%)	470 (89%)	56 (11%)	8	23
1	B	526/622 (85%)	467 (89%)	59 (11%)	7	20
1	C	527/622 (85%)	469 (89%)	58 (11%)	8	21
1	D	526/622 (85%)	474 (90%)	52 (10%)	10	27
All	All	2105/2488 (85%)	1880 (89%)	225 (11%)	8	22

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	7	ASN
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	60	ILE
1	A	81	GLN
1	A	84	GLU
1	A	86	ARG
1	A	94	ARG
1	A	114	TYR
1	A	122	LEU
1	A	124	SER
1	A	125	LEU
1	A	133	ASN
1	A	136	GLU
1	A	183	ARG
1	A	216	VAL
1	A	247	VAL
1	A	272	ASN
1	A	277	GLN
1	A	289	LYS
1	A	291	GLU
1	A	304	CYS

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Mol	Chain	Res	Type
1	A	312	THR
1	A	321	TYR
1	A	335	LEU
1	A	348	LYS
1	A	363	SER
1	A	366	VAL
1	A	376	ARG
1	A	388	SER
1	A	395	ASP
1	A	399	ARG
1	A	400	TYR
1	A	418	LYS
1	A	434	ARG
1	A	436	GLU
1	A	458	LYS
1	A	459	ILE
1	A	469	SER
1	A	471	ARG
1	A	484	ASN
1	A	488	LEU
1	A	513	TYR
1	A	514	THR
1	A	525	SER
1	A	531	SER
1	A	533	PHE
1	A	562	ASP
1	A	564	SER
1	A	589	ARG
1	A	590	THR
1	A	621	GLN
1	A	629	GLU
1	A	633	SER
1	B	3	ARG
1	B	7	ASN
1	B	19	ASN
1	B	35	THR
1	B	40	LYS
1	B	42	HIS
1	B	60	ILE
1	B	72	GLU
1	B	74	ARG
1	B	85	SER

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Mol	Chain	Res	Type
1	B	86	ARG
1	B	111	VAL
1	B	114	TYR
1	B	122	LEU
1	B	125	LEU
1	B	133	ASN
1	B	183	ARG
1	B	199	ARG
1	B	216	VAL
1	B	272	ASN
1	B	289	LYS
1	B	291	GLU
1	B	312	THR
1	B	320	ARG
1	B	321	TYR
1	B	326	LYS
1	B	348	LYS
1	B	366	VAL
1	B	376	ARG
1	B	387	THR
1	B	388	SER
1	B	395	ASP
1	B	399	ARG
1	B	400	TYR
1	B	418	LYS
1	B	423	VAL
1	B	426	LYS
1	B	434	ARG
1	B	436	GLU
1	B	443	VAL
1	B	448	VAL
1	B	458	LYS
1	B	459	ILE
1	B	469	SER
1	B	471	ARG
1	B	472	VAL
1	B	484	ASN
1	B	488	LEU
1	B	493	ASP
1	B	513	TYR
1	B	525	SER
1	B	548	ASP

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Mol	Chain	Res	Type
1	B	556	ARG
1	B	564	SER
1	B	574	GLU
1	B	590	THR
1	B	621	GLN
1	B	629	GLU
1	B	633	SER
1	C	6	GLN
1	C	7	ASN
1	C	19	ASN
1	C	34	ILE
1	C	40	LYS
1	C	42	HIS
1	C	60	ILE
1	C	72	GLU
1	C	74	ARG
1	C	81	GLN
1	C	84	GLU
1	C	111	VAL
1	C	122	LEU
1	C	133	ASN
1	C	136	GLU
1	C	183	ARG
1	C	199	ARG
1	C	213	LEU
1	C	216	VAL
1	C	289	LYS
1	C	291	GLU
1	C	320	ARG
1	C	321	TYR
1	C	326	LYS
1	C	335	LEU
1	C	343	LYS
1	C	348	LYS
1	C	363	SER
1	C	376	ARG
1	C	395	ASP
1	C	399	ARG
1	C	400	TYR
1	C	418	LYS
1	C	419	SER
1	C	426	LYS

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Mol	Chain	Res	Type
1	C	436	GLU
1	C	443	VAL
1	C	458	LYS
1	C	459	ILE
1	C	461	GLN
1	C	469	SER
1	C	471	ARG
1	C	472	VAL
1	C	482	ASN
1	C	488	LEU
1	C	490	LEU
1	C	513	TYR
1	C	514	THR
1	C	525	SER
1	C	537	MET
1	C	549	TYR
1	C	556	ARG
1	C	562	ASP
1	C	578	LYS
1	C	587	ARG
1	C	590	THR
1	C	633	SER
1	C	635	MET
1	D	7	ASN
1	D	15	THR
1	D	19	ASN
1	D	34	ILE
1	D	42	HIS
1	D	60	ILE
1	D	81	GLN
1	D	84	GLU
1	D	85	SER
1	D	111	VAL
1	D	122	LEU
1	D	124	SER
1	D	133	ASN
1	D	137	THR
1	D	183	ARG
1	D	216	VAL
1	D	289	LYS
1	D	291	GLU
1	D	304	CYS

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Mol	Chain	Res	Type
1	D	320	ARG
1	D	321	TYR
1	D	326	LYS
1	D	335	LEU
1	D	348	LYS
1	D	363	SER
1	D	376	ARG
1	D	395	ASP
1	D	399	ARG
1	D	400	TYR
1	D	426	LYS
1	D	434	ARG
1	D	436	GLU
1	D	458	LYS
1	D	459	ILE
1	D	471	ARG
1	D	472	VAL
1	D	482	ASN
1	D	484	ASN
1	D	513	TYR
1	D	514	THR
1	D	525	SER
1	D	528	THR
1	D	537	MET
1	D	556	ARG
1	D	562	ASP
1	D	563	GLU
1	D	587	ARG
1	D	590	THR
1	D	621	GLN
1	D	629	GLU
1	D	632	ASP
1	D	633	SER

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
1	A	81	GLN
1	A	133	ASN
1	A	239	HIS

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Mol	Chain	Res	Type
1	A	249	GLN
1	A	300	HIS
1	A	311	ASN
1	A	445	HIS
1	A	484	ASN
1	A	500	HIS
1	A	621	GLN
1	B	6	GLN
1	B	8	HIS
1	B	77	GLN
1	B	133	ASN
1	B	300	HIS
1	B	445	HIS
1	B	482	ASN
1	B	484	ASN
1	B	500	HIS
1	B	621	GLN
1	C	6	GLN
1	C	8	HIS
1	C	77	GLN
1	C	81	GLN
1	C	133	ASN
1	C	239	HIS
1	C	249	GLN
1	C	257	HIS
1	C	300	HIS
1	C	311	ASN
1	C	445	HIS
1	C	484	ASN
1	C	500	HIS
1	C	621	GLN
1	D	6	GLN
1	D	8	HIS
1	D	19	ASN
1	D	77	GLN
1	D	81	GLN
1	D	89	HIS
1	D	133	ASN
1	D	239	HIS
1	D	249	GLN
1	D	300	HIS
1	D	311	ASN

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Mol	Chain	Res	Type
1	D	445	HIS
1	D	477	HIS
1	D	484	ASN
1	D	500	HIS
1	D	621	GLN

### 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](#)

15 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	801	-	4,4,4	0.27	0	6,6,6	0.33	0
2	SO4	A	802	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.29	0
2	SO4	A	804	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	B	801	-	4,4,4	0.25	0	6,6,6	0.18	0
2	SO4	B	802	-	4,4,4	0.13	0	6,6,6	0.43	0
2	SO4	B	803	-	4,4,4	0.26	0	6,6,6	0.39	0
2	SO4	C	801	-	4,4,4	0.17	0	6,6,6	0.40	0
2	SO4	C	802	-	4,4,4	0.17	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	803	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	C	804	-	4,4,4	0.12	0	6,6,6	0.33	0
2	SO4	D	801	-	4,4,4	0.27	0	6,6,6	0.69	0
2	SO4	D	802	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	D	803	-	4,4,4	0.12	0	6,6,6	0.16	0
2	SO4	D	804	-	4,4,4	0.06	0	6,6,6	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	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	802	-	-	0/0/0/0	0/0/0/0
2	SO4	A	803	-	-	0/0/0/0	0/0/0/0
2	SO4	A	804	-	-	0/0/0/0	0/0/0/0
2	SO4	B	801	-	-	0/0/0/0	0/0/0/0
2	SO4	B	802	-	-	0/0/0/0	0/0/0/0
2	SO4	B	803	-	-	0/0/0/0	0/0/0/0
2	SO4	C	801	-	-	0/0/0/0	0/0/0/0
2	SO4	C	802	-	-	0/0/0/0	0/0/0/0
2	SO4	C	803	-	-	0/0/0/0	0/0/0/0
2	SO4	C	804	-	-	0/0/0/0	0/0/0/0
2	SO4	D	801	-	-	0/0/0/0	0/0/0/0
2	SO4	D	802	-	-	0/0/0/0	0/0/0/0
2	SO4	D	803	-	-	0/0/0/0	0/0/0/0
2	SO4	D	804	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	SO4	1	0
2	B	802	SO4	1	0
2	D	802	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	611/725 (84%)	0.21	19 (3%)	52 46	48, 69, 93, 123	0
1	B	612/725 (84%)	0.23	22 (3%)	46 40	53, 71, 93, 122	0
1	C	613/725 (84%)	0.10	21 (3%)	49 42	49, 68, 93, 120	0
1	D	612/725 (84%)	0.12	10 (1%)	74 73	44, 66, 93, 122	0
All	All	2448/2900 (84%)	0.16	72 (2%)	55 50	44, 69, 93, 123	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	630	LEU	5.2
1	B	416	LEU	5.1
1	B	630	LEU	4.8
1	D	416	LEU	4.7
1	C	414	GLY	4.7
1	A	630	LEU	4.0
1	D	630	LEU	4.0
1	C	415	GLU	3.9
1	C	417	LEU	3.8
1	A	416	LEU	3.8
1	D	625	LEU	3.7
1	A	549	TYR	3.7
1	B	627	GLY	3.7
1	B	549	TYR	3.6
1	B	414	GLY	3.6
1	B	581	ALA	3.5
1	A	624	GLU	3.5
1	C	624	GLU	3.4
1	C	416	LEU	3.3
1	B	135	PHE	3.2
1	C	629	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	627	GLY	3.2
1	A	629	GLU	3.2
1	C	549	TYR	3.2
1	A	625	LEU	3.1
1	B	628	GLU	3.1
1	D	627	GLY	3.1
1	D	549	TYR	3.0
1	C	638	LEU	3.0
1	B	631	ASN	3.0
1	C	626	VAL	3.0
1	B	626	VAL	2.9
1	A	628	GLU	2.9
1	C	313	LEU	2.9
1	B	580	ALA	2.9
1	A	548	ASP	2.8
1	C	436	GLU	2.8
1	A	631	ASN	2.7
1	B	624	GLU	2.7
1	A	417	LEU	2.6
1	A	132	GLU	2.6
1	B	622	PHE	2.6
1	B	629	GLU	2.6
1	A	344	VAL	2.6
1	C	628	GLU	2.6
1	B	623	ARG	2.5
1	D	313	LEU	2.5
1	C	631	ASN	2.5
1	D	626	VAL	2.5
1	C	581	ALA	2.4
1	B	305	PHE	2.4
1	D	415	GLU	2.4
1	D	624	GLU	2.4
1	B	225	PHE	2.4
1	B	342	LEU	2.3
1	A	135	PHE	2.3
1	C	625	LEU	2.3
1	C	6	GLN	2.3
1	A	626	VAL	2.3
1	C	627	GLY	2.3
1	D	628	GLU	2.2
1	A	340	TYR	2.2
1	A	6	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	637	ALA	2.2
1	B	132	GLU	2.2
1	B	131	PRO	2.1
1	B	133	ASN	2.1
1	A	225	PHE	2.1
1	C	639	ALA	2.1
1	C	548	ASP	2.1
1	A	540	LEU	2.1
1	B	344	VAL	2.1

## 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	D	801	5/5	0.75	0.30	4.08	82,84,92,103	0
2	SO4	A	801	5/5	0.90	0.24	2.25	71,76,84,92	0
2	SO4	C	804	5/5	0.82	0.28	0.19	103,109,110,117	0
2	SO4	C	801	5/5	0.90	0.20	0.17	85,86,90,103	0
2	SO4	D	803	5/5	0.92	0.18	-0.90	82,88,94,100	0
2	SO4	B	801	5/5	0.95	0.16	-2.56	72,77,83,91	0
2	SO4	A	803	5/5	0.90	0.17	-	76,80,85,91	0
2	SO4	C	802	5/5	0.96	0.15	-	76,77,90,91	0
2	SO4	D	802	5/5	0.92	0.14	-	77,79,87,92	0
2	SO4	A	802	5/5	0.96	0.18	-	68,71,75,77	0
2	SO4	B	802	5/5	0.97	0.12	-	71,75,81,82	0
2	SO4	D	804	5/5	0.86	0.27	-	105,108,116,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	803	5/5	0.87	0.17	-	77,86,88,97	0
2	SO4	C	803	5/5	0.91	0.19	-	90,91,97,105	0
2	SO4	A	804	5/5	0.92	0.17	-	100,101,104,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.