



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 01:51 AM EDT

PDB ID : 3E3O  
Title : Glycogen phosphorylase R state-IMP complex  
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.  
Deposited on : unknown  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

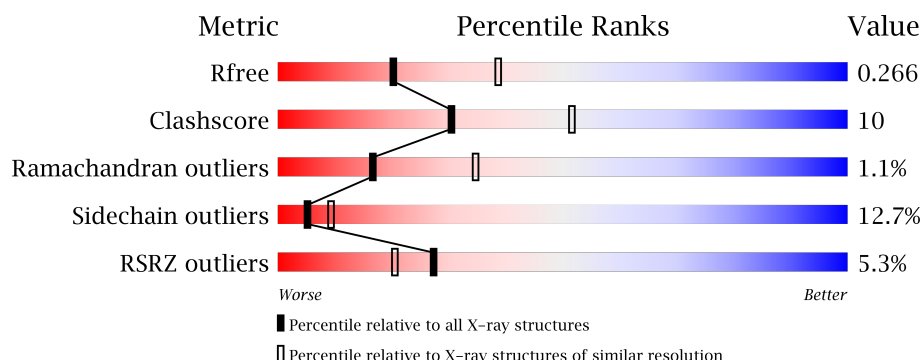
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	842	<div> <div>3%</div> <div>67%</div> <div>25%</div> <div>• •</div> </div>
1	B	842	<div> <div>5%</div> <div>69%</div> <div>22%</div> <div>5%</div> <div>•</div> </div>
1	C	842	<div> <div>5%</div> <div>69%</div> <div>24%</div> <div>• •</div> </div>
1	D	842	<div> <div>7%</div> <div>66%</div> <div>23%</div> <div>6%</div> <div>•</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IMP	A	920	-	-	-	X
3	IMP	B	920	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26630 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 phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	0	0
			6601	4206	1164	1201	1	29			
1	B	812	Total	C	N	O	P	S	0	0	0
			6616	4215	1167	1204	1	29			
1	C	808	Total	C	N	O	P	S	0	0	0
			6589	4198	1165	1196	1	29			
1	D	806	Total	C	N	O	P	S	0	0	0
			6576	4190	1159	1197	1	29			

There are 4 discrepancies between the modelled and reference sequences:

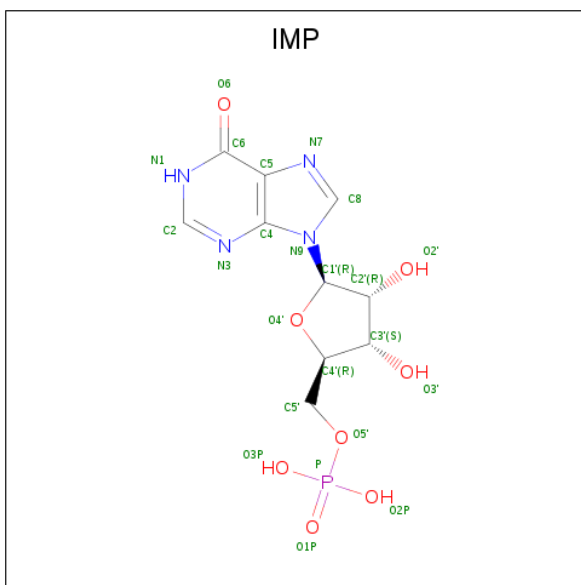
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489

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



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

- Molecule 3 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).

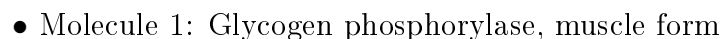


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	33	Total	O	0	0
			33	33		
4	C	33	Total	O	0	0
			33	33		
4	D	20	Total	O	0	0
			20	20		

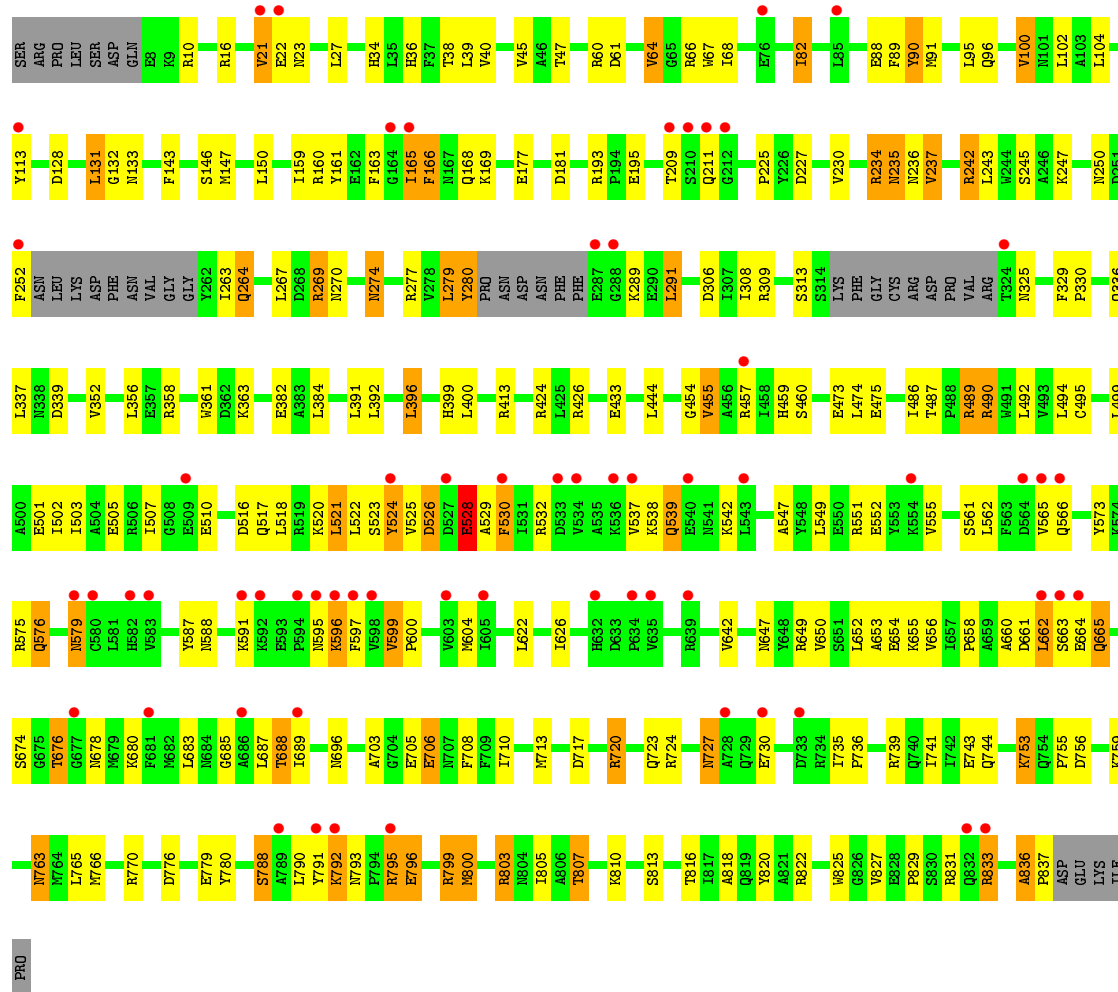








● Molecule 1: Glycogen phosphorylase, muscle form



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.68Å 188.45Å 87.85Å 90.00° 109.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.60) 99.3 (29.67-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.201 , 0.267 0.201 , 0.266	Depositor DCC
$R_{free}$ test set	5572 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, LLP, 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	0.55	3/6721 (0.0%)	0.71	8/9091 (0.1%)
1	B	0.48	0/6736	0.65	2/9110 (0.0%)
1	C	0.49	0/6708	0.65	1/9072 (0.0%)
1	D	0.66	16/6695 (0.2%)	0.67	5/9055 (0.1%)
All	All	0.55	19/26860 (0.1%)	0.67	16/36328 (0.0%)

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	C	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	528	GLU	CG-CD	11.22	1.68	1.51
1	D	524	TYR	CG-CD2	10.60	1.52	1.39
1	D	524	TYR	CE1-CZ	10.11	1.51	1.38
1	D	796	GLU	CD-OE2	9.90	1.36	1.25
1	D	661	ASP	CG-OD2	7.83	1.43	1.25
1	A	828	GLU	CD-OE2	7.54	1.33	1.25
1	D	528	GLU	CD-OE2	-7.51	1.17	1.25
1	A	464	LYS	CE-NZ	6.94	1.66	1.49
1	D	799	ARG	CZ-NH2	6.79	1.41	1.33
1	D	524	TYR	CB-CG	6.68	1.61	1.51
1	D	542	LYS	CE-NZ	6.53	1.65	1.49
1	D	796	GLU	CD-OE1	6.36	1.32	1.25
1	D	803	ARG	CZ-NH1	6.28	1.41	1.33
1	D	524	TYR	C-N	6.26	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	706	GLU	CD-OE2	6.11	1.32	1.25
1	D	800	MET	C-O	5.48	1.33	1.23
1	D	561	SER	C-O	5.46	1.33	1.23
1	D	706	GLU	CD-OE1	5.39	1.31	1.25
1	A	480	GLN	CD-OE1	5.33	1.35	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLY	N-CA-C	-9.41	89.57	113.10
1	D	799	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	D	524	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	D	803	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	16	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	16	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	395	LEU	CA-CB-CG	6.95	131.29	115.30
1	A	203	TYR	CB-CA-C	6.32	123.03	110.40
1	D	524	TYR	CB-CG-CD1	6.10	124.66	121.00
1	C	325	ASN	N-CA-C	-5.84	95.22	111.00
1	A	430	LEU	CA-CB-CG	5.69	128.38	115.30
1	A	395	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	131	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	203	TYR	CA-C-N	5.47	127.15	116.20
1	D	279	LEU	CA-CB-CG	5.12	127.06	115.30
1	A	683	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	324	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6601	0	6554	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6616	0	6572	139	0
1	C	6589	0	6550	134	0
1	D	6576	0	6528	151	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	23	0	11	1	0
3	B	23	0	11	0	0
3	C	23	0	11	0	0
3	D	23	0	11	1	0
4	A	30	0	0	0	0
4	B	33	0	0	2	0
4	C	33	0	0	2	0
4	D	20	0	0	1	0
All	All	26630	0	26248	552	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 10.

All (552) 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:D:836:ALA:HB1	1:D:837:PRO:HA	1.30	1.06
1:A:395:LEU:HD12	1:A:396:LEU:HD22	1.38	1.02
1:A:455:VAL:H	1:A:459:HIS:HD2	1.15	0.94
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.49	0.94
1:A:783:CYS:SG	1:A:786:ARG:NH2	2.42	0.93
1:B:455:VAL:H	1:B:459:HIS:HD2	1.13	0.91
1:A:168:GLN:HE21	1:A:647:ASN:H	1.14	0.88
1:C:292:ARG:HB3	1:C:292:ARG:HH11	1.39	0.88
1:B:168:GLN:HE21	1:B:647:ASN:H	1.21	0.88
1:A:33:ARG:HD2	1:B:33:ARG:HH21	1.40	0.86
1:C:455:VAL:H	1:C:459:HIS:HD2	1.25	0.84
1:B:211:GLN:HG2	1:B:358:ARG:HE	1.40	0.84
1:D:539:GLN:HA	1:D:539:GLN:HE21	1.42	0.83
1:C:168:GLN:HE21	1:C:647:ASN:H	1.24	0.83
1:A:18:LEU:HB3	1:B:37:PHE:HZ	1.43	0.83
1:D:227:ASP:OD1	1:D:242:ARG:HD3	1.79	0.82
1:B:486:ILE:HD11	1:B:676:THR:HG23	1.61	0.82
1:B:22:GLU:HG3	1:B:104:LEU:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:ARG:O	1:A:799:ARG:HG3	1.81	0.81
1:C:676:THR:HG22	1:C:680:LLP:H4'1	1.62	0.81
1:D:836:ALA:HB1	1:D:837:PRO:CA	2.10	0.81
1:A:292:ARG:CG	1:A:292:ARG:HH11	1.95	0.80
1:B:47:THR:HG22	1:B:49:ARG:H	1.50	0.78
1:C:63:LEU:HD13	1:C:229:PRO:HG2	1.66	0.78
1:A:168:GLN:NE2	1:A:647:ASN:H	1.82	0.77
1:A:455:VAL:H	1:A:459:HIS:CD2	2.01	0.76
1:D:88:GLU:HG2	1:D:132:GLY:HA2	1.68	0.76
1:B:455:VAL:H	1:B:459:HIS:CD2	2.02	0.76
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.51	0.75
1:C:355:ASP:OD2	1:C:398:ARG:HD3	1.87	0.75
1:A:290:GLU:HG2	1:A:391:LEU:HD21	1.67	0.75
1:B:836:ALA:HB1	1:B:837:PRO:HA	1.69	0.75
1:C:574:LYS:HB2	1:C:576:GLN:HE22	1.50	0.74
1:C:455:VAL:HG13	1:C:674:SER:HB2	1.68	0.74
1:A:395:LEU:HD12	1:A:396:LEU:CD2	2.16	0.74
1:A:23:ASN:HD22	1:A:26:GLU:HG2	1.52	0.74
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.36	0.73
1:B:386:ARG:HD3	1:B:432:GLU:OE1	1.88	0.73
1:D:143:PHE:O	1:D:147:MET:HG3	1.89	0.73
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.23	0.73
1:B:72:GLN:O	1:B:76:GLU:HG2	1.88	0.73
1:D:720:ARG:HH11	1:D:720:ARG:HB3	1.54	0.72
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.38	0.72
1:C:486:ILE:HD11	1:C:676:THR:HG23	1.70	0.72
1:C:87:LEU:HD21	1:C:292:ARG:HH22	1.54	0.72
1:A:93:ARG:O	1:A:490:ARG:NH2	2.21	0.72
1:C:336:GLN:HE21	1:C:825:TRP:HE1	1.38	0.71
1:D:264:GLN:HA	1:D:264:GLN:OE1	1.90	0.71
1:C:292:ARG:HB3	1:C:292:ARG:NH1	2.06	0.71
1:A:309:ARG:NH2	3:A:920:IMP:O3P	2.24	0.70
1:C:225:PRO:CB	1:C:242:ARG:HD2	2.21	0.69
1:B:168:GLN:NE2	1:B:647:ASN:H	1.89	0.69
1:C:783:CYS:O	1:C:787:VAL:HG23	1.91	0.69
1:D:227:ASP:OD1	1:D:242:ARG:CD	2.41	0.68
1:B:235:ASN:HA	1:B:833:ARG:HG3	1.75	0.68
1:D:274:ASN:C	1:D:274:ASN:HD22	1.97	0.68
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.57	0.68
1:B:502:ILE:HG23	4:B:948:HOH:O	1.94	0.67
1:D:424:ARG:NH2	1:D:473:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.77	0.67
1:C:486:ILE:CD1	1:C:676:THR:HG23	2.26	0.66
1:B:292:ARG:HH21	1:B:341:HIS:CD2	2.14	0.66
1:D:836:ALA:CB	1:D:837:PRO:HA	2.18	0.66
1:A:88:GLU:HG2	1:A:279:LEU:HD11	1.77	0.66
1:D:538:LYS:NZ	1:D:660:ALA:O	2.19	0.66
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.79	0.66
1:C:157:TYR:CE2	1:C:242:ARG:HG2	2.29	0.66
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.78	0.65
1:A:18:LEU:HB3	1:B:37:PHE:CZ	2.28	0.65
1:A:21:VAL:C	1:A:23:ASN:H	2.00	0.65
1:A:458:ILE:O	1:A:462:ILE:HG23	1.96	0.65
1:C:162:GLU:HA	1:C:183:LEU:HD12	1.79	0.65
1:C:455:VAL:H	1:C:459:HIS:CD2	2.13	0.65
1:A:615:MET:CE	1:A:761:ILE:HG12	2.27	0.65
1:C:308:ILE:HD13	1:C:352:VAL:HG11	1.79	0.65
1:B:703:ALA:HA	1:B:807:THR:HG21	1.79	0.64
1:D:23:ASN:O	1:D:27:LEU:HG	1.98	0.64
1:D:455:VAL:H	1:D:459:HIS:HD2	1.45	0.64
1:A:353:LEU:HA	1:A:357:GLU:HB2	1.80	0.64
1:C:87:LEU:CD2	1:C:292:ARG:HH22	2.10	0.63
1:B:588:ASN:HD21	1:B:744:GLN:HE22	1.45	0.63
1:D:495:CYS:HB3	1:D:654:GLU:HB2	1.79	0.63
1:A:96:GLN:HG2	1:A:494:LEU:HG	1.80	0.63
1:A:727:ASN:ND2	1:A:729:GLN:H	1.96	0.63
1:D:264:GLN:HG3	1:D:267:LEU:HG	1.80	0.63
1:A:142:CYS:SG	1:A:487:THR:HG22	2.39	0.63
1:B:571:HIS:H	1:B:576:GLN:NE2	1.97	0.63
1:C:235:ASN:HD22	1:C:235:ASN:H	1.46	0.63
1:C:270:ASN:HD22	1:D:269:ARG:HH21	1.45	0.63
1:D:487:THR:HG23	1:D:490:ARG:HB3	1.81	0.62
1:A:21:VAL:HG12	1:A:22:GLU:H	1.65	0.62
1:B:138:ARG:HD3	1:B:138:ARG:O	1.99	0.62
1:C:227:ASP:OD1	1:C:242:ARG:HD3	2.00	0.62
1:C:663:SER:OG	1:C:665:GLN:NE2	2.32	0.62
1:D:665:GLN:HE21	1:D:678:ASN:HA	1.64	0.62
1:B:22:GLU:HG3	1:B:104:LEU:CD1	2.30	0.62
1:D:413:ARG:NH2	1:D:475:GLU:OE2	2.27	0.61
1:D:525:VAL:HG11	1:D:803:ARG:NH1	2.15	0.61
1:D:588:ASN:HD21	1:D:744:GLN:HE22	1.48	0.61
1:B:571:HIS:H	1:B:576:GLN:HE22	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD13	1:B:475:GLU:HG3	1.82	0.61
1:B:274:ASN:HB3	1:B:277:ARG:HE	1.64	0.61
1:A:21:VAL:HG12	1:A:22:GLU:N	2.15	0.61
1:D:21:VAL:HG21	1:D:66:ARG:NH2	2.16	0.60
1:A:64:VAL:O	1:A:68:ILE:HG12	2.01	0.60
1:C:579:ASN:HB2	1:C:666:ILE:HD11	1.83	0.60
1:D:662:LEU:HD21	1:D:689:ILE:HB	1.83	0.60
1:A:594:PRO:O	1:A:639:ARG:NH2	2.33	0.60
1:A:18:LEU:CB	1:B:37:PHE:HZ	2.14	0.60
1:C:21:VAL:O	1:C:23:ASN:N	2.31	0.60
1:D:566:GLN:HE22	1:D:576:GLN:HA	1.66	0.60
1:D:599:VAL:HG12	1:D:600:PRO:HD2	1.82	0.60
1:C:66:ARG:HD3	1:C:236:ASN:OD1	2.00	0.60
1:A:47:THR:HG23	1:A:48:PRO:HD2	1.84	0.59
1:D:727:ASN:O	1:D:730:GLU:HG2	2.02	0.59
1:A:672:GLU:HB2	1:A:693:ASP:OD2	2.02	0.59
1:A:336:GLN:NE2	1:A:373:ALA:HB3	2.17	0.59
1:C:138:ARG:HD3	1:C:138:ARG:O	2.02	0.59
1:A:615:MET:HE2	1:A:761:ILE:HG12	1.84	0.59
1:B:87:LEU:HD13	1:B:341:HIS:HB3	1.85	0.59
1:D:82:ILE:HD11	1:D:147:MET:SD	2.43	0.59
1:C:571:HIS:ND1	1:C:573:TYR:HD1	2.00	0.59
1:D:507:ILE:HD12	1:D:517:GLN:HG2	1.84	0.59
1:A:47:THR:HG22	1:A:49:ARG:H	1.68	0.58
1:C:34:HIS:HE1	1:C:61:ASP:OD2	1.86	0.58
1:C:574:LYS:HB2	1:C:576:GLN:NE2	2.19	0.58
1:D:539:GLN:HA	1:D:539:GLN:NE2	2.15	0.58
1:B:729:GLN:HG2	1:C:724:ARG:HA	1.83	0.58
1:C:225:PRO:HB3	1:C:242:ARG:HD2	1.85	0.58
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.68	0.58
1:A:727:ASN:C	1:A:727:ASN:HD22	2.06	0.58
1:B:687:LEU:HD13	1:B:800:MET:CE	2.33	0.58
1:C:49:ARG:HA	1:C:125:ILE:HG21	1.85	0.58
1:A:168:GLN:HE21	1:A:647:ASN:N	1.94	0.58
1:D:664:GLU:OE1	1:D:780:TYR:OH	2.21	0.58
1:A:361:TRP:HH2	1:A:406:ILE:HG13	1.70	0.57
1:A:663:SER:HB2	1:A:681:PHE:CG	2.39	0.57
1:A:21:VAL:CG1	1:A:22:GLU:N	2.67	0.57
1:A:386:ARG:HG2	1:A:440:ASN:HA	1.86	0.57
1:B:730:GLU:HG3	1:B:734:ARG:HH21	1.68	0.57
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:MET:CE	1:C:774:PHE:HE2	2.18	0.57
1:D:741:ILE:HA	1:D:744:GLN:HE21	1.68	0.57
1:A:361:TRP:CH2	1:A:406:ILE:HG13	2.39	0.57
1:D:524:TYR:HD2	1:D:528:GLU:OE1	1.87	0.57
1:D:235:ASN:HA	1:D:833:ARG:HG3	1.86	0.57
1:B:536:LYS:NZ	1:B:540:GLU:OE1	2.35	0.56
1:B:336:GLN:NE2	1:B:373:ALA:HB3	2.20	0.56
1:C:170:ILE:HA	1:C:174:TRP:O	2.05	0.56
1:D:34:HIS:HE1	1:D:61:ASP:OD2	1.87	0.56
1:D:689:ILE:HG23	1:D:689:ILE:O	2.05	0.56
1:B:118:ASP:HB3	1:B:121:GLU:HG3	1.87	0.56
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.05	0.56
1:A:703:ALA:HA	1:A:807:THR:HG21	1.87	0.56
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.89	0.56
1:B:426:ARG:CZ	1:C:755:PRO:HD2	2.36	0.56
1:C:262:TYR:HB2	4:C:926:HOH:O	2.04	0.56
1:C:475:GLU:HB3	1:C:478:LYS:HG3	1.88	0.56
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.54	0.56
1:B:233:TYR:CZ	1:B:234:ARG:HD2	2.41	0.56
1:A:803:ARG:O	1:A:807:THR:HG22	2.06	0.56
1:B:348:GLU:OE1	1:B:399:HIS:CE1	2.58	0.56
1:D:34:HIS:HD2	1:D:38:THR:OG1	1.89	0.56
1:B:727:ASN:HD21	1:C:725:GLY:HA3	1.71	0.55
1:A:103:ALA:HB2	1:A:234:ARG:NE	2.22	0.55
1:A:692:MET:HB3	1:A:714:ARG:HG3	1.89	0.55
1:C:600:PRO:HA	1:C:639:ARG:O	2.06	0.55
1:D:306:ASP:OD1	1:D:309:ARG:NH1	2.39	0.55
1:D:274:ASN:HA	1:D:277:ARG:HB2	1.88	0.55
1:D:795:ARG:HG2	1:D:796:GLU:N	2.21	0.55
1:A:676:THR:HG22	1:A:680:LLP:H5'1	1.88	0.55
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.87	0.55
1:B:455:VAL:HG13	1:B:484:ASN:ND2	2.22	0.54
1:D:165:ILE:HD12	1:D:166:PHE:CD1	2.42	0.54
1:D:503:ILE:HG23	1:D:521:LEU:HD11	1.88	0.54
1:A:748:GLY:HA3	1:A:755:PRO:HA	1.88	0.54
1:D:21:VAL:HG13	1:D:22:GLU:H	1.72	0.54
1:D:309:ARG:NH2	3:D:920:IMP:O3P	2.40	0.54
1:D:308:ILE:HD13	1:D:352:VAL:HG11	1.87	0.54
1:D:791:TYR:C	1:D:793:ASN:H	2.10	0.54
1:A:21:VAL:HG22	1:A:62:HIS:CD2	2.42	0.54
1:B:396:LEU:HB3	1:B:399:HIS:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:MET:HB3	1:D:717:ASP:HB2	1.89	0.54
1:B:803:ARG:O	1:B:807:THR:HG22	2.07	0.54
1:B:292:ARG:NH2	1:B:341:HIS:CD2	2.75	0.54
1:B:730:GLU:HG3	1:B:734:ARG:NH2	2.23	0.54
1:B:88:GLU:HG2	1:B:132:GLY:HA2	1.88	0.54
1:D:150:LEU:HB3	1:D:829:PRO:HB3	1.90	0.54
1:A:503:ILE:HG12	1:A:521:LEU:HD21	1.89	0.54
1:D:329:PHE:HB3	1:D:330:PRO:HD3	1.88	0.54
1:D:665:GLN:NE2	1:D:678:ASN:HA	2.22	0.54
1:B:665:GLN:HB3	1:B:696:ASN:HD21	1.72	0.54
1:C:336:GLN:NE2	1:C:373:ALA:HB3	2.23	0.54
1:C:575:ARG:HD3	1:C:666:ILE:O	2.07	0.54
1:D:547:ALA:O	1:D:551:ARG:HG2	2.08	0.54
1:A:130:GLY:O	1:A:164:GLY:HA2	2.08	0.54
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.90	0.54
1:C:269:ARG:NH1	1:C:273:GLU:OE1	2.41	0.54
1:D:454:GLY:HA3	1:D:460:SER:OG	2.08	0.54
1:A:34:HIS:CD2	1:A:38:THR:OG1	2.59	0.53
1:C:279:LEU:HD22	1:C:280:TYR:H	1.73	0.53
1:C:565:VAL:HG11	1:C:681:PHE:CE1	2.43	0.53
1:D:685:GLY:HA2	1:D:805:ILE:HD11	1.90	0.53
1:A:712:GLY:H	1:A:779:GLU:HG2	1.74	0.53
1:A:12:GLN:HE22	1:B:28:LYS:NZ	2.06	0.53
1:A:232:GLY:HA3	1:A:235:ASN:HD21	1.72	0.53
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.89	0.53
1:C:455:VAL:CG1	1:C:674:SER:HB2	2.37	0.53
1:A:235:ASN:HD22	1:A:236:ASN:N	2.06	0.53
1:A:589:ARG:HD2	1:A:737:GLU:OE2	2.08	0.53
1:D:551:ARG:HG3	1:D:552:GLU:H	1.73	0.53
1:A:263:ILE:O	1:A:263:ILE:HG13	2.09	0.53
1:B:435:ALA:O	1:B:436:VAL:HB	2.09	0.53
1:B:584:ILE:HG22	1:B:741:ILE:HG22	1.91	0.53
1:C:581:LEU:HD22	1:C:741:ILE:HD12	1.90	0.53
1:C:161:TYR:CE2	1:C:279:LEU:HG	2.43	0.53
1:C:492:LEU:HB2	1:C:683:LEU:HD13	1.91	0.53
1:A:157:TYR:CE1	1:A:242:ARG:HG2	2.44	0.53
1:A:426:ARG:NH2	1:D:755:PRO:HG3	2.23	0.53
1:D:165:ILE:HD12	1:D:166:PHE:HD1	1.74	0.52
1:A:630:VAL:HG21	1:A:642:VAL:HG23	1.92	0.52
1:A:727:ASN:HD22	1:A:729:GLN:H	1.57	0.52
1:B:583:VAL:HG11	1:B:642:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:ALA:HB1	1:B:837:PRO:CA	2.38	0.52
1:C:47:THR:HG22	1:C:49:ARG:H	1.74	0.52
1:A:703:ALA:CB	1:A:807:THR:HG21	2.39	0.52
1:C:727:ASN:O	1:C:730:GLU:HG2	2.10	0.52
1:A:138:ARG:O	1:A:138:ARG:HD3	2.09	0.52
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.91	0.52
1:A:791:TYR:HA	1:A:797:TRP:CD1	2.45	0.52
1:B:348:GLU:OE1	1:B:399:HIS:HE1	1.92	0.52
1:C:727:ASN:HD21	1:C:729:GLN:HB3	1.75	0.52
1:B:395:LEU:HD12	1:B:396:LEU:HD22	1.91	0.52
1:B:455:VAL:N	1:B:459:HIS:HD2	1.95	0.52
1:A:568:LYS:HB3	1:A:574:LYS:HG2	1.92	0.52
1:C:424:ARG:NH2	1:C:473:GLU:OE1	2.43	0.52
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.91	0.52
1:D:64:VAL:HA	1:D:67:TRP:HB3	1.92	0.52
1:B:47:THR:HG22	1:B:49:ARG:N	2.21	0.52
1:D:133:ASN:OD1	1:D:165:ILE:HG21	2.10	0.52
1:A:615:MET:HE1	1:A:761:ILE:HG12	1.92	0.52
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.75	0.52
1:C:680:LLP:O3	1:C:680:LLP:NZ	2.43	0.52
1:D:163:PHE:CE1	1:D:181:ASP:HB3	2.44	0.52
1:C:348:GLU:OE1	1:C:399:HIS:HE1	1.92	0.51
1:C:336:GLN:NE2	1:C:825:TRP:HE1	2.05	0.51
1:D:495:CYS:HB2	1:D:654:GLU:O	2.10	0.51
1:A:733:ASP:O	1:A:739:ARG:NH1	2.43	0.51
1:B:379:VAL:HG21	1:B:670:GLY:O	2.09	0.51
1:D:455:VAL:N	1:D:459:HIS:HD2	2.09	0.51
1:B:289:LYS:NZ	4:B:929:HOH:O	2.43	0.51
1:A:739:ARG:O	1:A:743:GLU:HG2	2.11	0.51
1:D:96:GLN:O	1:D:100:VAL:HG13	2.11	0.51
1:D:562:LEU:HD21	1:D:662:LEU:HB2	1.92	0.51
1:D:595:ASN:O	1:D:596:LYS:C	2.48	0.51
1:A:574:LYS:O	1:A:575:ARG:HB2	2.11	0.51
1:A:741:ILE:HA	1:A:744:GLN:HE21	1.76	0.51
1:B:389:VAL:HG12	1:B:439:ILE:HG12	1.92	0.51
1:A:727:ASN:HD22	1:A:728:ALA:N	2.10	0.51
1:C:741:ILE:HA	1:C:744:GLN:NE2	2.23	0.51
1:C:748:GLY:HA3	1:C:755:PRO:HA	1.92	0.51
1:C:144:LEU:HD23	1:C:147:MET:HE3	1.93	0.50
1:C:39:LEU:HD21	1:C:53:PHE:HB3	1.91	0.50
1:B:460:SER:OG	1:B:481:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:HG2	1:A:825:TRP:HE1	1.76	0.50
1:B:566:GLN:NE2	1:B:576:GLN:HB3	2.26	0.50
1:B:503:ILE:HG23	1:B:521:LEU:HD11	1.93	0.50
1:D:455:VAL:H	1:D:459:HIS:CD2	2.28	0.50
1:D:510:GLU:HG2	1:D:831:ARG:HH22	1.75	0.50
1:B:739:ARG:O	1:B:743:GLU:HG2	2.11	0.50
1:C:85:LEU:HD12	1:C:335:ILE:HG23	1.93	0.50
1:D:524:TYR:CD2	1:D:528:GLU:OE1	2.65	0.50
1:A:680:LLP:O3	1:A:680:LLP:NZ	2.45	0.50
1:D:163:PHE:CD1	1:D:181:ASP:HB3	2.47	0.50
1:D:274:ASN:ND2	1:D:291:LEU:HD21	2.27	0.50
1:A:389:VAL:HG12	1:A:439:ILE:HG12	1.94	0.50
1:C:521:LEU:HB2	1:C:806:ALA:HB2	1.93	0.50
1:D:90:TYR:CE2	1:D:680:LLP:H2'3	2.47	0.50
1:A:380:ILE:HG13	1:A:381:PRO:HD2	1.94	0.49
1:B:615:MET:HE3	1:B:761:ILE:HG12	1.94	0.49
1:C:163:PHE:CE1	1:C:181:ASP:HB3	2.46	0.49
1:A:82:ILE:C	1:A:82:ILE:HD13	2.32	0.49
1:B:337:LEU:HD22	1:B:373:ALA:O	2.12	0.49
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.78	0.49
1:D:588:ASN:ND2	1:D:741:ILE:HG22	2.28	0.49
1:C:566:GLN:HE22	1:C:576:GLN:HA	1.78	0.49
1:D:720:ARG:NH1	1:D:720:ARG:HB3	2.23	0.49
1:A:23:ASN:ND2	1:A:26:GLU:HG2	2.25	0.49
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.92	0.49
1:C:565:VAL:HG11	1:C:681:PHE:HE1	1.78	0.49
1:B:262:TYR:HB3	1:B:264:GLN:NE2	2.28	0.49
1:B:755:PRO:HD2	1:C:426:ARG:CZ	2.43	0.49
1:B:129:ALA:HB1	1:B:131:LEU:HD22	1.95	0.49
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.93	0.49
1:C:548:TYR:CE1	1:C:552:GLU:HG3	2.48	0.49
1:D:209:THR:C	1:D:211:GLN:H	2.15	0.49
1:C:47:THR:HG22	1:C:49:ARG:N	2.27	0.49
1:D:526:ASP:OD1	1:D:526:ASP:N	2.45	0.49
1:B:336:GLN:HG2	1:B:825:TRP:HE1	1.77	0.49
1:D:665:GLN:HB3	1:D:696:ASN:HD21	1.78	0.49
1:B:22:GLU:CG	1:B:104:LEU:HD12	2.40	0.49
1:D:818:ALA:O	1:D:822:ARG:HG3	2.13	0.49
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.13	0.48
1:C:525:VAL:HG12	1:C:526:ASP:OD1	2.13	0.48
1:C:804:ASN:O	1:C:807:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:VAL:HA	1:D:604:MET:O	2.14	0.48
1:D:676:THR:CG2	1:D:680:LLP:H4'1	2.43	0.48
1:A:549:LEU:O	1:A:552:GLU:O	2.31	0.48
1:B:262:TYR:HD1	1:B:264:GLN:HB3	1.79	0.48
1:D:597:PHE:HE2	1:D:792:LYS:HD2	1.74	0.48
1:A:580:CYS:O	1:A:584:ILE:HG13	2.13	0.48
1:A:833:ARG:HG2	1:A:834:LEU:N	2.28	0.48
1:B:36:HIS:O	1:B:40:VAL:HA	2.12	0.48
1:D:676:THR:HG22	1:D:680:LLP:H4'1	1.95	0.48
1:D:739:ARG:O	1:D:743:GLU:HG2	2.14	0.48
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.96	0.48
1:B:355:ASP:OD2	1:B:398:ARG:HD3	2.14	0.48
1:B:571:HIS:O	1:B:576:GLN:NE2	2.46	0.48
1:D:146:SER:OG	1:D:813:SER:OG	2.17	0.48
1:D:816:THR:HG22	1:D:820:TYR:HE1	1.79	0.48
1:A:270:ASN:HD22	1:B:269:ARG:HH21	1.62	0.48
1:C:168:GLN:HE21	1:C:647:ASN:N	2.03	0.48
1:C:597:PHE:HA	1:C:639:ARG:HH22	1.79	0.48
1:D:396:LEU:HB3	1:D:399:HIS:HB2	1.95	0.47
1:D:703:ALA:HA	1:D:807:THR:HG21	1.96	0.47
1:C:192:ALA:HB2	1:C:226:TYR:CE2	2.48	0.47
1:D:100:VAL:O	1:D:234:ARG:NH1	2.45	0.47
1:D:21:VAL:HG13	1:D:22:GLU:N	2.29	0.47
1:D:501:GLU:O	1:D:505:GLU:HG3	2.14	0.47
1:D:455:VAL:CG1	1:D:674:SER:HB2	2.44	0.47
1:A:129:ALA:HB1	1:A:131:LEU:HD22	1.96	0.47
1:B:564:ASP:HB3	1:B:603:VAL:HA	1.97	0.47
1:A:562:LEU:HD22	1:A:601:ARG:HG2	1.95	0.47
1:C:241:MET:HG2	1:C:243:LEU:HD13	1.96	0.47
1:C:455:VAL:HG22	1:C:484:ASN:OD1	2.15	0.47
1:C:335:ILE:HG22	1:C:337:LEU:HD13	1.96	0.47
1:C:386:ARG:HG2	1:C:440:ASN:HA	1.96	0.47
1:C:34:HIS:HD2	1:C:38:THR:OG1	1.98	0.47
1:D:279:LEU:HD23	1:D:280:TYR:N	2.30	0.47
1:B:566:GLN:HE22	1:B:576:GLN:HB3	1.80	0.47
1:A:264:GLN:O	1:A:264:GLN:HG2	2.15	0.46
1:A:30:ASN:OD1	1:B:33:ARG:NH2	2.49	0.46
1:B:663:SER:OG	1:B:665:GLN:NE2	2.48	0.46
1:C:163:PHE:HD2	1:C:277:ARG:HG2	1.81	0.46
1:A:395:LEU:O	1:A:396:LEU:HD13	2.15	0.46
1:B:163:PHE:HA	1:B:180:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:GLY:O	1:B:641:ARG:NH2	2.35	0.46
1:C:279:LEU:CD2	1:C:280:TYR:H	2.28	0.46
1:C:80:LYS:HE2	1:C:330:PRO:O	2.15	0.46
1:C:729:GLN:HE21	1:C:733:ASP:CG	2.19	0.46
1:D:487:THR:CG2	1:D:490:ARG:HB3	2.45	0.46
1:D:599:VAL:HG21	1:D:788:SER:O	2.15	0.46
1:C:571:HIS:ND1	1:C:573:TYR:CD1	2.82	0.46
1:D:289:LYS:HG3	1:D:291:LEU:H	1.81	0.46
1:D:502:ILE:HD12	1:D:537:VAL:CG2	2.46	0.46
1:C:455:VAL:N	1:C:459:HIS:HD2	2.03	0.46
1:A:392:LEU:HB3	1:A:400:LEU:HG	1.98	0.46
1:C:47:THR:HG23	1:C:48:PRO:HD2	1.98	0.46
1:A:161:TYR:CE2	1:A:279:LEU:HD12	2.51	0.46
1:A:687:LEU:CD2	1:A:800:MET:HG2	2.46	0.46
1:B:458:ILE:HD11	1:B:694:GLY:H	1.81	0.46
1:A:274:ASN:HB3	1:A:291:LEU:HD11	1.97	0.46
1:A:575:ARG:HD3	1:A:666:ILE:O	2.15	0.46
1:B:34:HIS:CE1	1:B:61:ASP:OD2	2.65	0.46
1:B:227:ASP:OD1	1:B:242:ARG:CD	2.64	0.46
1:A:346:ILE:HB	1:A:347:PRO:HD3	1.97	0.46
1:A:833:ARG:CG	1:A:834:LEU:H	2.30	0.45
1:A:386:ARG:HD3	1:A:432:GLU:OE2	2.16	0.45
1:A:833:ARG:CG	1:A:834:LEU:N	2.79	0.45
1:B:227:ASP:OD1	1:B:242:ARG:HD3	2.16	0.45
1:D:518:LEU:O	1:D:521:LEU:HB2	2.16	0.45
1:A:34:HIS:HE1	1:A:61:ASP:OD2	2.00	0.45
1:C:160:ARG:HB2	1:C:243:LEU:HB3	1.97	0.45
1:C:535:ALA:O	1:C:539:GLN:HB2	2.15	0.45
1:C:579:ASN:HB2	1:C:666:ILE:CD1	2.45	0.45
1:B:235:ASN:H	1:B:235:ASN:HD22	1.63	0.45
1:B:571:HIS:ND1	1:B:572:GLU:N	2.63	0.45
1:B:573:TYR:HB3	1:B:771:PHE:CE1	2.51	0.45
1:C:713:MET:HE3	1:C:718:VAL:HG22	1.98	0.45
1:A:687:LEU:HD21	1:A:800:MET:HG2	1.98	0.45
1:A:32:ASN:HB3	1:B:18:LEU:HD21	1.98	0.45
1:B:274:ASN:HA	1:B:277:ARG:HB2	1.98	0.45
1:B:67:TRP:HD1	1:B:238:VAL:HG12	1.82	0.45
1:D:502:ILE:HD12	1:D:537:VAL:HG21	1.99	0.45
1:D:21:VAL:HG21	1:D:66:ARG:HH22	1.81	0.45
1:D:687:LEU:HD13	1:D:800:MET:HE3	1.99	0.45
1:B:449:SER:O	1:B:478:LYS:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ASN:ND2	1:D:237:VAL:H	2.14	0.45
1:D:250:ASN:C	1:D:252:PHE:H	2.19	0.45
1:D:793:ASN:OD1	1:D:795:ARG:HD3	2.17	0.45
1:C:103:ALA:HA	1:C:234:ARG:NH1	2.32	0.45
1:D:60:ARG:O	1:D:64:VAL:HG13	2.16	0.45
1:B:615:MET:CE	1:B:761:ILE:HG12	2.47	0.45
1:C:618:MET:HB3	1:C:761:ILE:HD11	1.99	0.45
1:D:735:ILE:HA	1:D:736:PRO:HD3	1.82	0.45
1:A:426:ARG:HD2	1:D:753:LYS:O	2.17	0.45
1:C:738:LEU:O	1:C:742:ILE:HG12	2.16	0.45
1:C:766:MET:HE2	1:C:774:PHE:HE2	1.82	0.45
1:D:579:ASN:C	1:D:579:ASN:HD22	2.20	0.45
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.64	0.44
1:B:678:ASN:ND2	1:B:696:ASN:OD1	2.49	0.44
1:D:235:ASN:HD22	1:D:236:ASN:N	2.14	0.44
1:A:21:VAL:O	1:A:23:ASN:N	2.50	0.44
1:C:39:LEU:HD21	1:C:53:PHE:CB	2.47	0.44
1:D:168:GLN:NE2	1:D:647:ASN:H	2.15	0.44
1:A:225:PRO:HB2	1:A:242:ARG:HD2	2.00	0.44
1:A:348:GLU:OE1	1:A:399:HIS:HE1	2.01	0.44
1:D:678:ASN:ND2	1:D:696:ASN:OD1	2.50	0.44
1:D:663:SER:OG	1:D:688:THR:HG23	2.16	0.44
1:A:495:CYS:HB3	1:A:654:GLU:HB2	2.00	0.44
1:B:633:ASP:HA	1:B:634:PRO:HD3	1.87	0.44
1:B:699:MET:HB3	1:B:708:PHE:CZ	2.53	0.44
1:C:665:GLN:HB3	1:C:696:ASN:HD21	1.83	0.44
1:C:713:MET:HG2	1:C:717:ASP:HB3	2.00	0.44
1:C:129:ALA:HB1	1:C:131:LEU:HD22	2.00	0.44
1:B:379:VAL:HG23	1:B:462:ILE:CD1	2.48	0.44
1:D:551:ARG:HG3	1:D:552:GLU:N	2.32	0.44
1:D:575:ARG:NH2	1:D:776:ASP:HB2	2.33	0.44
1:B:600:PRO:HA	1:B:639:ARG:O	2.17	0.44
1:C:588:ASN:HD21	1:C:744:GLN:NE2	2.15	0.44
1:D:36:HIS:O	1:D:40:VAL:HA	2.17	0.44
1:A:18:LEU:CB	1:B:37:PHE:CZ	2.96	0.44
1:B:77:LYS:HG3	1:B:77:LYS:O	2.17	0.44
1:C:678:ASN:OD1	1:C:678:ASN:N	2.51	0.44
1:A:740:GLN:O	1:A:744:GLN:HG3	2.18	0.43
1:B:211:GLN:CG	1:B:358:ARG:HE	2.20	0.43
1:B:495:CYS:HB3	1:B:654:GLU:HB2	2.00	0.43
1:C:475:GLU:OE1	1:C:478:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:837:PRO:HG2	4:C:930:HOH:O	2.17	0.43
1:A:766:MET:HA	1:A:766:MET:HE3	2.01	0.43
1:B:651:SER:HA	1:B:654:GLU:HG2	1.98	0.43
1:D:676:THR:HG22	1:D:680:LLP:H5'1	2.00	0.43
1:D:816:THR:HG22	1:D:820:TYR:CE1	2.53	0.43
1:A:37:PHE:CD1	1:B:64:VAL:HG23	2.54	0.43
1:A:343:SER:OG	1:A:441:MET:HG3	2.19	0.43
1:B:381:PRO:HG3	1:B:467:ILE:HG13	2.00	0.43
1:C:699:MET:HB3	1:C:708:PHE:CZ	2.54	0.43
1:D:689:ILE:O	1:D:689:ILE:CG2	2.65	0.43
1:D:89:PHE:O	1:D:131:LEU:HB3	2.19	0.43
1:A:687:LEU:HD12	1:A:797:TRP:CE2	2.54	0.43
1:C:143:PHE:O	1:C:147:MET:HG3	2.19	0.43
1:A:21:VAL:C	1:A:23:ASN:N	2.68	0.43
1:B:15:VAL:HA	1:B:18:LEU:HD22	2.00	0.43
1:B:280:TYR:OH	1:B:291:LEU:HD12	2.17	0.43
1:B:619:ILE:O	1:B:623:ILE:HG13	2.19	0.43
1:D:159:ILE:HB	1:D:161:TYR:CZ	2.54	0.43
1:A:584:ILE:HG22	1:A:741:ILE:HG22	2.01	0.43
1:A:234:ARG:O	1:A:833:ARG:NH1	2.51	0.43
1:B:687:LEU:HD13	1:B:800:MET:HE2	1.99	0.43
1:D:650:VAL:HA	1:D:680:LLP:H2'1	1.99	0.43
1:B:118:ASP:HB3	1:B:121:GLU:CG	2.48	0.43
1:B:575:ARG:NH2	1:B:776:ASP:OD2	2.49	0.43
1:D:235:ASN:ND2	1:D:237:VAL:HG13	2.33	0.43
1:D:727:ASN:HD22	1:D:727:ASN:C	2.21	0.43
1:D:336:GLN:HG3	1:D:825:TRP:HZ2	1.83	0.43
1:A:743:GLU:O	1:A:747:SER:HB3	2.19	0.42
1:D:193:ARG:HB2	1:D:225:PRO:HG2	2.00	0.42
1:A:663:SER:HB2	1:A:681:PHE:CD1	2.54	0.42
1:B:232:GLY:HA3	1:B:235:ASN:HD21	1.84	0.42
1:C:36:HIS:O	1:C:40:VAL:HA	2.20	0.42
1:D:250:ASN:C	1:D:252:PHE:N	2.72	0.42
1:D:313:SER:HB2	4:D:925:HOH:O	2.19	0.42
1:A:769:ASP:C	1:A:771:PHE:H	2.21	0.42
1:B:790:LEU:CD2	1:B:800:MET:HE1	2.49	0.42
1:C:344:LEU:HA	1:C:347:PRO:HD2	2.02	0.42
1:D:336:GLN:HG3	1:D:825:TRP:CZ2	2.54	0.42
1:D:653:ALA:HA	1:D:656:VAL:HG12	2.00	0.42
1:B:338:ASN:OD1	1:B:377:HIS:CE1	2.72	0.42
1:B:676:THR:HG22	1:B:680:LLP:H4'1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:CYS:HB3	1:C:654:GLU:HB2	2.01	0.42
1:D:263:ILE:O	1:D:264:GLN:OE1	2.38	0.42
1:A:304:LEU:HD23	1:A:348:GLU:HG3	2.02	0.42
1:A:716:GLU:O	1:A:720:ARG:HG3	2.20	0.42
1:A:732:TYR:CE1	1:A:739:ARG:HG2	2.53	0.42
1:A:703:ALA:CA	1:A:807:THR:HG21	2.48	0.42
1:C:195:GLU:HG3	1:C:195:GLU:H	1.38	0.42
1:D:524:TYR:HA	1:D:528:GLU:OE2	2.20	0.42
1:A:600:PRO:HA	1:A:639:ARG:O	2.20	0.42
1:B:170:ILE:HG12	1:B:646:GLU:HG3	2.00	0.42
1:C:615:MET:HE3	1:C:761:ILE:HG12	2.01	0.42
1:C:727:ASN:HD22	1:C:727:ASN:C	2.22	0.42
1:C:528:GLU:OE2	1:C:795:ARG:NH1	2.52	0.42
1:C:336:GLN:HG2	1:C:825:TRP:HE1	1.85	0.42
1:D:433:GLU:H	1:D:433:GLU:HG2	1.71	0.42
1:A:296:GLU:OE2	1:A:385:GLU:OE2	2.37	0.42
1:C:430:LEU:HD22	1:C:443:HIS:HB3	2.02	0.42
1:D:759:LYS:O	1:D:763:ASN:HB2	2.20	0.42
1:A:557:ILE:HD11	1:A:643:ILE:CD1	2.50	0.42
1:C:235:ASN:N	1:C:235:ASN:HD22	2.12	0.42
1:D:507:ILE:HG21	1:D:520:LYS:HB2	2.02	0.41
1:A:292:ARG:HH11	1:A:292:ARG:HG3	1.82	0.41
1:B:408:GLN:HB3	1:B:408:GLN:HE21	1.53	0.41
1:C:791:TYR:HA	1:C:797:TRP:CD1	2.56	0.41
1:C:88:GLU:HG2	1:C:132:GLY:HA2	2.01	0.41
1:D:626:ILE:HG22	1:D:642:VAL:HG21	2.02	0.41
1:A:681:PHE:HB3	1:A:686:ALA:HB3	2.01	0.41
1:B:562:LEU:HD22	1:B:601:ARG:HG2	2.02	0.41
1:B:336:GLN:NE2	1:B:825:TRP:HE1	2.10	0.41
1:C:293:LEU:HD21	1:C:392:LEU:HD12	2.02	0.41
1:C:538:LYS:HE2	1:C:660:ALA:O	2.19	0.41
1:D:655:LYS:O	1:D:658:PRO:HD2	2.21	0.41
1:A:264:GLN:HE21	1:A:264:GLN:H	1.68	0.41
1:A:703:ALA:HB2	1:A:807:THR:HG21	2.01	0.41
1:A:148:ALA:O	1:A:237:VAL:HG22	2.19	0.41
1:A:163:PHE:HA	1:A:180:ASP:O	2.21	0.41
1:A:338:ASN:OD1	1:A:377:HIS:HE1	2.03	0.41
1:D:235:ASN:C	1:D:235:ASN:HD22	2.23	0.41
1:A:486:ILE:HD11	1:A:676:THR:HG23	2.02	0.41
1:D:494:LEU:C	1:D:494:LEU:HD23	2.41	0.41
1:B:157:TYR:CE2	1:B:242:ARG:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:GLY:HA3	1:B:776:ASP:OD1	2.21	0.41
1:C:556:HIS:HE1	1:C:638:ASP:HB3	1.85	0.41
1:A:12:GLN:HE22	1:B:28:LYS:HZ2	1.69	0.41
1:A:396:LEU:HB3	1:A:399:HIS:HB2	2.03	0.41
1:A:455:VAL:HG22	1:A:484:ASN:OD1	2.20	0.41
1:B:10:ARG:HG3	1:B:13:ILE:HD12	2.03	0.41
1:B:274:ASN:HB3	1:B:277:ARG:NE	2.34	0.41
1:C:460:SER:OG	1:C:481:ASN:ND2	2.53	0.41
1:D:247:LYS:HB2	1:D:247:LYS:NZ	2.36	0.41
1:D:680:LLP:O3	1:D:680:LLP:NZ	2.54	0.41
1:D:708:PHE:HB3	1:D:710:ILE:HG12	2.03	0.41
1:B:560:ASN:HD22	1:B:560:ASN:HA	1.58	0.41
1:A:782:LYS:HA	1:A:782:LYS:HE3	2.03	0.41
1:B:680:LLP:NZ	1:B:680:LLP:O3	2.52	0.41
1:B:706:GLU:CD	1:B:706:GLU:H	2.24	0.41
1:D:64:VAL:O	1:D:68:ILE:HG12	2.21	0.41
1:D:795:ARG:HG2	1:D:796:GLU:H	1.84	0.41
1:B:353:LEU:HB3	1:B:359:LEU:HD12	2.03	0.40
1:C:224:MET:HA	1:C:225:PRO:HD3	1.96	0.40
1:C:549:LEU:HB3	1:C:557:ILE:HG13	2.03	0.40
1:C:565:VAL:CG1	1:C:681:PHE:CE1	3.03	0.40
1:D:225:PRO:HB2	1:D:242:ARG:HD2	2.03	0.40
1:D:230:VAL:O	1:D:230:VAL:HG23	2.20	0.40
1:B:262:TYR:CD1	1:B:264:GLN:HB3	2.54	0.40
1:B:35:LEU:HA	1:B:39:LEU:HD23	2.03	0.40
1:C:557:ILE:HD11	1:C:643:ILE:HD12	2.04	0.40
1:D:267:LEU:C	1:D:269:ARG:H	2.24	0.40
1:D:530:PHE:C	1:D:532:ARG:N	2.74	0.40
1:D:587:TYR:CZ	1:D:591:LYS:HD2	2.55	0.40
1:A:67:TRP:HD1	1:A:238:VAL:HG12	1.86	0.40
1:C:23:ASN:ND2	1:C:26:GLU:HG2	2.37	0.40
1:C:586:LEU:HB3	1:C:640:LEU:HD22	2.03	0.40
1:C:714:ARG:O	1:C:718:VAL:HG23	2.20	0.40
1:A:573:TYR:HB3	1:A:771:PHE:CZ	2.56	0.40
1:B:717:ASP:HA	1:B:720:ARG:HB2	2.03	0.40
1:A:235:ASN:HD22	1:A:235:ASN:C	2.23	0.40
1:A:455:VAL:HA	1:A:482:LYS:O	2.21	0.40
1:B:143:PHE:CG	1:B:817:ILE:HD11	2.56	0.40
1:C:269:ARG:HH21	1:D:270:ASN:CG	2.24	0.40
1:C:687:LEU:HD22	1:C:800:MET:HE2	2.03	0.40
1:D:21:VAL:HG22	1:D:104:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:ARG:O	1:D:799:ARG:HG3	2.20	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	801/842 (95%)	744 (93%)	46 (6%)	11 (1%)	13	26
1	B	803/842 (95%)	758 (94%)	36 (4%)	9 (1%)	17	35
1	C	799/842 (95%)	751 (94%)	40 (5%)	8 (1%)	18	37
1	D	797/842 (95%)	724 (91%)	65 (8%)	8 (1%)	18	37
All	All	3200/3368 (95%)	2977 (93%)	187 (6%)	36 (1%)	17	35

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	PHE
1	C	21	VAL
1	C	22	GLU
1	C	166	PHE
1	A	166	PHE
1	A	210	SER
1	A	514	ASP
1	A	551	ARG
1	A	575	ARG
1	B	314	SER
1	C	16	ARG
1	C	264	GLN
1	C	807	THR
1	D	166	PHE

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Mol	Chain	Res	Type
1	D	523	SER
1	D	596	LYS
1	D	836	ALA
1	A	21	VAL
1	A	22	GLU
1	A	474	LEU
1	A	553	TYR
1	B	211	GLN
1	D	16	ARG
1	B	436	VAL
1	B	705	GLU
1	B	836	ALA
1	C	382	GLU
1	D	489	ARG
1	D	529	ALA
1	B	264	GLN
1	C	835	PRO
1	B	835	PRO
1	D	21	VAL
1	A	204	GLY
1	A	20	GLY
1	B	260	GLY

### 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	699/730 (96%)	604 (86%)	95 (14%)	4	7
1	B	701/730 (96%)	615 (88%)	86 (12%)	5	10
1	C	698/730 (96%)	617 (88%)	81 (12%)	6	11
1	D	697/730 (96%)	604 (87%)	93 (13%)	4	8
All	All	2795/2920 (96%)	2440 (87%)	355 (13%)	5	9

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	ARG
1	A	15	VAL
1	A	18	LEU
1	A	21	VAL
1	A	29	LYS
1	A	33	ARG
1	A	39	LEU
1	A	45	VAL
1	A	63	LEU
1	A	82	ILE
1	A	90	TYR
1	A	91	MET
1	A	95	LEU
1	A	100	VAL
1	A	128	ASP
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	165	ILE
1	A	169	LYS
1	A	184	ARG
1	A	191	LYS
1	A	214	LYS
1	A	216	VAL
1	A	230	VAL
1	A	234	ARG
1	A	235	ASN
1	A	237	VAL
1	A	242	ARG
1	A	243	LEU
1	A	247	LYS
1	A	251	ASP
1	A	262	TYR
1	A	264	GLN
1	A	278	VAL
1	A	290	GLU
1	A	291	LEU
1	A	292	ARG
1	A	304	LEU
1	A	306	ASP
1	A	325	ASN
1	A	332	LYS

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Mol	Chain	Res	Type
1	A	339	ASP
1	A	358	ARG
1	A	361	TRP
1	A	380	ILE
1	A	382	GLU
1	A	391	LEU
1	A	392	LEU
1	A	396	LEU
1	A	400	LEU
1	A	408	GLN
1	A	426	ARG
1	A	441	MET
1	A	444	LEU
1	A	453	ASN
1	A	455	VAL
1	A	486	ILE
1	A	490	ARG
1	A	492	LEU
1	A	506	ARG
1	A	516	ASP
1	A	522	LEU
1	A	540	GLU
1	A	554	LYS
1	A	555	VAL
1	A	565	VAL
1	A	575	ARG
1	A	576	GLN
1	A	579	ASN
1	A	598	VAL
1	A	622	LEU
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	676	THR
1	A	683	LEU
1	A	705	GLU
1	A	708	PHE
1	A	713	MET
1	A	714	ARG
1	A	724	ARG
1	A	727	ASN

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Mol	Chain	Res	Type
1	A	741	ILE
1	A	753	LYS
1	A	765	LEU
1	A	766	MET
1	A	778	GLU
1	A	782	LYS
1	A	797	TRP
1	A	827	VAL
1	A	830	SER
1	A	831	ARG
1	B	10	ARG
1	B	15	VAL
1	B	21	VAL
1	B	33	ARG
1	B	39	LEU
1	B	82	ILE
1	B	85	LEU
1	B	87	LEU
1	B	90	TYR
1	B	91	MET
1	B	95	LEU
1	B	104	LEU
1	B	112	THR
1	B	128	ASP
1	B	131	LEU
1	B	136	LEU
1	B	165	ILE
1	B	176	MET
1	B	235	ASN
1	B	237	VAL
1	B	242	ARG
1	B	243	LEU
1	B	251	ASP
1	B	259	VAL
1	B	262	TYR
1	B	274	ASN
1	B	277	ARG
1	B	278	VAL
1	B	279	LEU
1	B	291	LEU
1	B	304	LEU
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	339	ASP
1	B	358	ARG
1	B	378	THR
1	B	384	LEU
1	B	391	LEU
1	B	392	LEU
1	B	396	LEU
1	B	400	LEU
1	B	408	GLN
1	B	425	LEU
1	B	426	ARG
1	B	432	GLU
1	B	444	LEU
1	B	455	VAL
1	B	462	ILE
1	B	469	LYS
1	B	474	LEU
1	B	486	ILE
1	B	492	LEU
1	B	501	GLU
1	B	506	ARG
1	B	516	ASP
1	B	536	LYS
1	B	538	LYS
1	B	539	GLN
1	B	543	LEU
1	B	549	LEU
1	B	555	VAL
1	B	560	ASN
1	B	565	VAL
1	B	574	LYS
1	B	575	ARG
1	B	576	GLN
1	B	579	ASN
1	B	589	ARG
1	B	613	TYR
1	B	640	LEU
1	B	641	ARG
1	B	652	LEU
1	B	662	LEU
1	B	665	GLN
1	B	667	SER

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Mol	Chain	Res	Type
1	B	676	THR
1	B	678	ASN
1	B	683	LEU
1	B	714	ARG
1	B	741	ILE
1	B	760	ASP
1	B	763	ASN
1	B	765	LEU
1	B	766	MET
1	B	786	ARG
1	B	808	SER
1	B	833	ARG
1	C	9	LYS
1	C	12	GLN
1	C	15	VAL
1	C	16	ARG
1	C	18	LEU
1	C	90	TYR
1	C	95	LEU
1	C	128	ASP
1	C	131	LEU
1	C	195	GLU
1	C	209	THR
1	C	230	VAL
1	C	235	ASN
1	C	237	VAL
1	C	242	ARG
1	C	243	LEU
1	C	247	LYS
1	C	250	ASN
1	C	254	LEU
1	C	262	TYR
1	C	264	GLN
1	C	274	ASN
1	C	277	ARG
1	C	279	LEU
1	C	292	ARG
1	C	294	LYS
1	C	304	LEU
1	C	323	ARG
1	C	325	ASN
1	C	332	LYS

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Mol	Chain	Res	Type
1	C	336	GLN
1	C	337	LEU
1	C	339	ASP
1	C	356	LEU
1	C	361	TRP
1	C	378	THR
1	C	379	VAL
1	C	384	LEU
1	C	392	LEU
1	C	395	LEU
1	C	396	LEU
1	C	400	LEU
1	C	425	LEU
1	C	444	LEU
1	C	455	VAL
1	C	469	LYS
1	C	474	LEU
1	C	486	ILE
1	C	509	GLU
1	C	510	GLU
1	C	517	GLN
1	C	522	LEU
1	C	539	GLN
1	C	540	GLU
1	C	543	LEU
1	C	551	ARG
1	C	569	ARG
1	C	576	GLN
1	C	586	LEU
1	C	622	LEU
1	C	646	GLU
1	C	649	ARG
1	C	652	LEU
1	C	662	LEU
1	C	665	GLN
1	C	676	THR
1	C	678	ASN
1	C	683	LEU
1	C	701	GLU
1	C	706	GLU
1	C	714	ARG
1	C	716	GLU

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Mol	Chain	Res	Type
1	C	717	ASP
1	C	720	ARG
1	C	723	GLN
1	C	727	ASN
1	C	760	ASP
1	C	765	LEU
1	C	782	LYS
1	C	783	CYS
1	C	788	SER
1	D	10	ARG
1	D	39	LEU
1	D	45	VAL
1	D	47	THR
1	D	64	VAL
1	D	82	ILE
1	D	90	TYR
1	D	91	MET
1	D	95	LEU
1	D	100	VAL
1	D	102	LEU
1	D	113	TYR
1	D	128	ASP
1	D	131	LEU
1	D	165	ILE
1	D	169	LYS
1	D	177	GLU
1	D	195	GLU
1	D	234	ARG
1	D	235	ASN
1	D	237	VAL
1	D	242	ARG
1	D	245	SER
1	D	264	GLN
1	D	269	ARG
1	D	274	ASN
1	D	280	TYR
1	D	291	LEU
1	D	325	ASN
1	D	337	LEU
1	D	339	ASP
1	D	356	LEU
1	D	358	ARG

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Mol	Chain	Res	Type
1	D	361	TRP
1	D	363	LYS
1	D	382	GLU
1	D	384	LEU
1	D	391	LEU
1	D	392	LEU
1	D	396	LEU
1	D	400	LEU
1	D	426	ARG
1	D	444	LEU
1	D	455	VAL
1	D	457	ARG
1	D	474	LEU
1	D	486	ILE
1	D	489	ARG
1	D	490	ARG
1	D	492	LEU
1	D	499	LEU
1	D	516	ASP
1	D	521	LEU
1	D	522	LEU
1	D	526	ASP
1	D	528	GLU
1	D	530	PHE
1	D	539	GLN
1	D	549	LEU
1	D	555	VAL
1	D	573	TYR
1	D	576	GLN
1	D	579	ASN
1	D	599	VAL
1	D	622	LEU
1	D	649	ARG
1	D	652	LEU
1	D	662	LEU
1	D	665	GLN
1	D	676	THR
1	D	683	LEU
1	D	688	THR
1	D	705	GLU
1	D	706	GLU
1	D	720	ARG

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Mol	Chain	Res	Type
1	D	723	GLN
1	D	724	ARG
1	D	727	ASN
1	D	753	LYS
1	D	756	ASP
1	D	763	ASN
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	779	GLU
1	D	788	SER
1	D	790	LEU
1	D	792	LYS
1	D	795	ARG
1	D	807	THR
1	D	810	LYS
1	D	827	VAL
1	D	833	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	12	GLN
1	A	23	ASN
1	A	34	HIS
1	A	167	ASN
1	A	168	GLN
1	A	235	ASN
1	A	250	ASN
1	A	264	GLN
1	A	270	ASN
1	A	336	GLN
1	A	377	HIS
1	A	399	HIS
1	A	459	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	727	ASN

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Mol	Chain	Res	Type
1	A	744	GLN
1	A	754	GLN
1	B	34	HIS
1	B	97	ASN
1	B	168	GLN
1	B	235	ASN
1	B	274	ASN
1	B	336	GLN
1	B	377	HIS
1	B	399	HIS
1	B	408	GLN
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	560	ASN
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	727	ASN
1	B	744	GLN
1	B	819	GLN
1	C	34	HIS
1	C	97	ASN
1	C	168	GLN
1	C	219	GLN
1	C	235	ASN
1	C	270	ASN
1	C	274	ASN
1	C	336	GLN
1	C	399	HIS
1	C	450	HIS
1	C	453	ASN
1	C	459	HIS
1	C	481	ASN
1	C	541	ASN
1	C	556	HIS
1	C	566	GLN
1	C	576	GLN
1	C	588	ASN
1	C	665	GLN
1	C	727	ASN
1	C	729	GLN

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Mol	Chain	Res	Type
1	C	744	GLN
1	C	763	ASN
1	C	832	GLN
1	D	34	HIS
1	D	62	HIS
1	D	97	ASN
1	D	168	GLN
1	D	211	GLN
1	D	235	ASN
1	D	274	ASN
1	D	336	GLN
1	D	377	HIS
1	D	399	HIS
1	D	453	ASN
1	D	459	HIS
1	D	481	ASN
1	D	539	GLN
1	D	541	ASN
1	D	566	GLN
1	D	579	ASN
1	D	582	HIS
1	D	614	HIS
1	D	665	GLN
1	D	723	GLN
1	D	727	ASN
1	D	744	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	680	1	24,24,25	1.74	4 (16%)	28,32,34	1.27	4 (14%)
1	LLP	B	680	1	24,24,25	1.81	5 (20%)	28,32,34	1.61	6 (21%)
1	LLP	C	680	1	24,24,25	1.77	5 (20%)	28,32,34	1.41	5 (17%)
1	LLP	D	680	1	24,24,25	1.73	5 (20%)	28,32,34	1.33	6 (21%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1
1	LLP	B	680	1	-	0/15/17/19	0/1/1/1
1	LLP	C	680	1	-	0/15/17/19	0/1/1/1
1	LLP	D	680	1	-	0/15/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	680	LLP	O3-C3	-6.17	1.22	1.37
1	A	680	LLP	O3-C3	-5.95	1.23	1.37
1	D	680	LLP	O3-C3	-5.81	1.23	1.37
1	C	680	LLP	O3-C3	-5.61	1.24	1.37
1	D	680	LLP	C2-N1	2.12	1.38	1.33
1	B	680	LLP	CA-C	2.19	1.53	1.50
1	B	680	LLP	C6-N1	2.21	1.39	1.34
1	C	680	LLP	C4'-NZ	2.27	1.34	1.27
1	B	680	LLP	C2-N1	2.32	1.38	1.33
1	D	680	LLP	C4-C4'	2.33	1.50	1.46
1	A	680	LLP	C4'-NZ	2.38	1.34	1.27
1	D	680	LLP	C4'-NZ	2.41	1.34	1.27
1	C	680	LLP	C2-N1	2.42	1.38	1.33
1	A	680	LLP	C2-N1	2.44	1.39	1.33
1	D	680	LLP	CA-C	2.63	1.53	1.50
1	B	680	LLP	C4-C4'	2.64	1.51	1.46
1	C	680	LLP	C4-C4'	2.78	1.51	1.46
1	C	680	LLP	CA-C	2.89	1.54	1.50
1	A	680	LLP	C4-C4'	3.10	1.52	1.46

All (21) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	680	LLP	CE-NZ-C4'	-3.33	109.37	119.03
1	B	680	LLP	OP2-P-OP4	-3.03	98.68	106.73
1	C	680	LLP	C5-C6-N1	-2.88	118.99	123.87
1	D	680	LLP	CE-NZ-C4'	-2.84	110.79	119.03
1	C	680	LLP	C4-C4'-NZ	-2.76	111.25	124.66
1	D	680	LLP	C5-C6-N1	-2.41	119.79	123.87
1	D	680	LLP	C4-C4'-NZ	-2.35	113.26	124.66
1	B	680	LLP	C4-C4'-NZ	-2.34	113.30	124.66
1	C	680	LLP	OP3-P-OP4	-2.32	100.55	106.73
1	A	680	LLP	C4-C4'-NZ	-2.29	113.53	124.66
1	D	680	LLP	C5'-C5-C6	-2.28	115.41	119.33
1	A	680	LLP	CE-NZ-C4'	-2.27	112.44	119.03
1	A	680	LLP	C5-C6-N1	-2.25	120.06	123.87
1	D	680	LLP	OP2-P-OP4	-2.21	100.85	106.73
1	B	680	LLP	C5-C6-N1	-2.21	120.13	123.87
1	B	680	LLP	C5-C4-C4'	-2.06	118.28	121.36
1	D	680	LLP	OP3-P-OP2	2.19	116.44	107.61
1	C	680	LLP	OP4-C5'-C5	2.47	114.28	109.32
1	C	680	LLP	OP3-P-OP2	2.59	118.05	107.61
1	A	680	LLP	OP4-C5'-C5	3.26	115.87	109.32
1	B	680	LLP	OP4-C5'-C5	4.04	117.44	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	2	0
1	B	680	LLP	2	0
1	C	680	LLP	2	0
1	D	680	LLP	6	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SO4	A	901	-	4,4,4	0.19	0	6,6,6	0.25	0
3	IMP	A	920	-	21,25,25	1.45	3 (14%)	22,38,38	2.28	3 (13%)
2	SO4	B	900	-	4,4,4	0.15	0	6,6,6	0.41	0
2	SO4	B	901	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	B	902	-	4,4,4	0.19	0	6,6,6	0.47	0
3	IMP	B	920	-	21,25,25	1.42	3 (14%)	22,38,38	2.66	3 (13%)
2	SO4	C	900	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	C	901	-	4,4,4	0.16	0	6,6,6	0.29	0
3	IMP	C	920	-	21,25,25	1.53	3 (14%)	22,38,38	2.58	4 (18%)
2	SO4	D	900	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	D	901	-	4,4,4	0.16	0	6,6,6	0.14	0
3	IMP	D	920	-	21,25,25	1.40	3 (14%)	22,38,38	2.39	2 (9%)

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	901	-	-	0/0/0/0	0/0/0/0
3	IMP	A	920	-	-	0/6/26/26	0/3/3/3
2	SO4	B	900	-	-	0/0/0/0	0/0/0/0
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	902	-	-	0/0/0/0	0/0/0/0
3	IMP	B	920	-	-	0/6/26/26	0/3/3/3
2	SO4	C	900	-	-	0/0/0/0	0/0/0/0
2	SO4	C	901	-	-	0/0/0/0	0/0/0/0
3	IMP	C	920	-	-	0/6/26/26	0/3/3/3
2	SO4	D	900	-	-	0/0/0/0	0/0/0/0
2	SO4	D	901	-	-	0/0/0/0	0/0/0/0
3	IMP	D	920	-	-	0/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	920	IMP	C2-N1	2.64	1.38	1.33
3	A	920	IMP	C2-N1	2.74	1.39	1.33
3	B	920	IMP	C2-N1	2.81	1.39	1.33
3	C	920	IMP	C2-N1	3.02	1.39	1.33
3	D	920	IMP	C6-N1	3.04	1.38	1.33
3	A	920	IMP	C6-N1	3.07	1.38	1.33
3	C	920	IMP	C6-N1	3.21	1.38	1.33
3	B	920	IMP	C6-N1	3.51	1.39	1.33
3	B	920	IMP	C2-N3	3.74	1.38	1.32
3	C	920	IMP	C2-N3	3.94	1.38	1.32
3	A	920	IMP	C2-N3	4.26	1.39	1.32
3	D	920	IMP	C2-N3	4.27	1.39	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	920	IMP	N3-C2-N1	-11.31	119.01	128.86
3	C	920	IMP	N3-C2-N1	-10.89	119.37	128.86
3	D	920	IMP	N3-C2-N1	-10.21	119.97	128.86
3	A	920	IMP	N3-C2-N1	-9.49	120.59	128.86
3	C	920	IMP	C6-C5-C4	-2.44	118.42	120.84
3	A	920	IMP	O2P-P-O5'	2.04	112.16	106.73
3	A	920	IMP	C2-N1-C6	2.09	119.39	115.91
3	C	920	IMP	O2P-P-O5'	2.23	112.67	106.73
3	D	920	IMP	C2-N1-C6	2.34	119.81	115.91
3	B	920	IMP	O3P-P-O5'	2.37	113.05	106.73
3	B	920	IMP	C2-N1-C6	2.72	120.45	115.91
3	C	920	IMP	C2-N1-C6	2.83	120.64	115.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	920	IMP	1	0
3	D	920	IMP	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	809/842 (96%)	-0.01	23 (2%)	53	46	23, 38, 53, 73	0
1	B	811/842 (96%)	0.11	46 (5%)	24	18	18, 43, 64, 70	0
1	C	807/842 (95%)	0.11	40 (4%)	30	23	21, 44, 66, 72	0
1	D	805/842 (95%)	0.29	63 (7%)	14	9	27, 47, 70, 75	0
All	All	3232/3368 (95%)	0.13	172 (5%)	27	20	18, 43, 66, 75	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	THR	7.6
1	B	259	VAL	6.8
1	A	281	PRO	6.6
1	D	22	GLU	6.6
1	D	288	GLY	5.7
1	B	288	GLY	5.2
1	A	165	ILE	4.9
1	D	595	ASN	4.7
1	C	555	VAL	4.3
1	B	22	GLU	4.3
1	B	287	GLU	4.3
1	B	176	MET	4.2
1	D	530	PHE	4.1
1	D	324	THR	4.1
1	B	16	ARG	4.1
1	B	165	ILE	4.1
1	B	551	ARG	4.0
1	B	21	VAL	4.0
1	C	165	ILE	3.9
1	B	211	GLN	3.8
1	D	210	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	580	CYS	3.8
1	C	556	HIS	3.8
1	C	565	VAL	3.8
1	D	598	VAL	3.8
1	C	252	PHE	3.8
1	B	208	HIS	3.7
1	C	22	GLU	3.7
1	D	592	LYS	3.7
1	A	22	GLU	3.7
1	D	635	VAL	3.7
1	D	594	PRO	3.6
1	A	554	LYS	3.6
1	C	720	ARG	3.6
1	B	598	VAL	3.5
1	C	605	ILE	3.4
1	D	789	ALA	3.4
1	B	553	TYR	3.4
1	B	343	SER	3.4
1	A	288	GLY	3.3
1	B	210	SER	3.3
1	C	581	LEU	3.3
1	B	209	THR	3.3
1	D	583	VAL	3.3
1	C	597	PHE	3.3
1	D	113	TYR	3.2
1	D	596	LYS	3.2
1	C	833	ARG	3.2
1	D	76	GLU	3.1
1	D	728	ALA	3.1
1	D	733	ASP	3.1
1	A	252	PHE	3.1
1	B	344	LEU	3.1
1	D	543	LEU	3.1
1	B	345	ALA	3.0
1	C	262	TYR	3.0
1	D	540	GLU	3.0
1	D	632	HIS	3.0
1	D	597	PHE	3.0
1	B	723	GLN	2.9
1	C	593	GLU	2.9
1	D	792	LYS	2.9
1	C	635	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	663	SER	2.9
1	C	250	ASN	2.8
1	D	579	ASN	2.8
1	B	327	ASP	2.8
1	D	591	LYS	2.8
1	B	280	TYR	2.8
1	B	281	PRO	2.8
1	D	527	ASP	2.8
1	D	565	VAL	2.8
1	D	639	ARG	2.8
1	B	337	LEU	2.8
1	D	730	GLU	2.7
1	C	594	PRO	2.7
1	A	260	GLY	2.7
1	D	252	PHE	2.7
1	C	564	ASP	2.7
1	D	582	HIS	2.7
1	C	623	ILE	2.7
1	D	564	ASP	2.7
1	D	791	TYR	2.7
1	A	612	GLY	2.7
1	B	380	ILE	2.7
1	A	381	PRO	2.6
1	C	579	ASN	2.6
1	D	457	ARG	2.6
1	B	20	GLY	2.6
1	A	342	PRO	2.6
1	B	611	PRO	2.6
1	C	598	VAL	2.6
1	D	536	LYS	2.6
1	D	209	THR	2.6
1	C	10	ARG	2.6
1	D	681	PHE	2.6
1	D	533	ASP	2.5
1	D	677	GLY	2.5
1	C	592	LYS	2.5
1	D	605	ILE	2.5
1	B	565	VAL	2.5
1	B	720	ARG	2.5
1	C	753	LYS	2.5
1	D	287	GLU	2.5
1	D	537	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	603	VAL	2.5
1	C	595	ASN	2.5
1	C	577	LEU	2.5
1	D	165	ILE	2.5
1	D	686	ALA	2.5
1	D	833	ARG	2.5
1	A	435	ALA	2.4
1	B	435	ALA	2.4
1	D	85	LEU	2.4
1	A	372	CYS	2.4
1	C	253	ASN	2.4
1	C	604	MET	2.4
1	A	11	LYS	2.4
1	C	566	GLN	2.4
1	B	580	CYS	2.4
1	D	534	VAL	2.4
1	D	211	GLN	2.4
1	B	85	LEU	2.4
1	B	269	ARG	2.3
1	A	335	ILE	2.3
1	B	252	PHE	2.3
1	B	566	GLN	2.3
1	B	552	GLU	2.3
1	A	85	LEU	2.3
1	C	795	ARG	2.3
1	D	212	GLY	2.3
1	C	532	ARG	2.3
1	B	612	GLY	2.3
1	D	164	GLY	2.3
1	D	634	PRO	2.3
1	D	566	GLN	2.3
1	B	557	ILE	2.3
1	B	554	LYS	2.3
1	B	346	ILE	2.3
1	B	379	VAL	2.3
1	B	342	PRO	2.2
1	C	323	ARG	2.2
1	D	554	LYS	2.2
1	D	832	GLN	2.2
1	D	689	ILE	2.2
1	D	580	CYS	2.2
1	A	210	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	380	ILE	2.2
1	A	337	LEU	2.2
1	C	832	GLN	2.2
1	C	642	VAL	2.1
1	A	20	GLY	2.1
1	B	548	TYR	2.1
1	D	662	LEU	2.1
1	B	579	ASN	2.1
1	A	21	VAL	2.1
1	D	21	VAL	2.1
1	C	611	PRO	2.1
1	D	795	ARG	2.1
1	D	509	GLU	2.1
1	D	664	GLU	2.1
1	A	75	TYR	2.1
1	B	596	LYS	2.1
1	C	164	GLY	2.1
1	A	837	PRO	2.0
1	C	603	VAL	2.0
1	C	768	HIS	2.0
1	A	611	PRO	2.0
1	B	567	VAL	2.0
1	D	524	TYR	2.0
1	B	434	GLY	2.0
1	A	426	ARG	2.0

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

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
1	LLP	C	680	24/25	0.96	0.16	-	38,41,45,45	0
1	LLP	D	680	24/25	0.98	0.25	-	42,44,46,47	0
1	LLP	A	680	24/25	0.96	0.19	-	22,24,34,36	0
1	LLP	B	680	24/25	0.93	0.21	-	37,39,42,43	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	IMP	B	920	23/23	0.97	0.23	4.11	44,58,58,59	0
3	IMP	A	920	23/23	0.92	0.32	2.93	73,80,82,82	0
3	IMP	D	920	23/23	0.94	0.26	1.49	51,70,72,73	0
2	SO4	C	901	5/5	0.86	0.22	1.15	100,101,101,101	0
2	SO4	A	901	5/5	0.89	0.19	0.14	98,99,99,100	0
2	SO4	B	902	5/5	0.93	0.20	0.01	83,84,85,85	0
3	IMP	C	920	23/23	0.97	0.15	-0.22	44,54,56,56	0
2	SO4	D	900	5/5	0.88	0.18	-0.54	94,94,95,96	0
2	SO4	B	901	5/5	0.95	0.14	-0.72	81,81,82,82	0
2	SO4	C	900	5/5	0.95	0.15	-0.76	97,98,98,98	0
2	SO4	B	900	5/5	0.93	0.13	-1.12	83,84,84,85	0
2	SO4	D	901	5/5	0.94	0.11	-	104,104,104,104	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.