



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID : 2HAV  
Title : Apo-Human Serum Transferrin (Glycosylated)  
Authors : Wally, J.; Everse, S.J.  
Deposited on : 2006-06-13  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

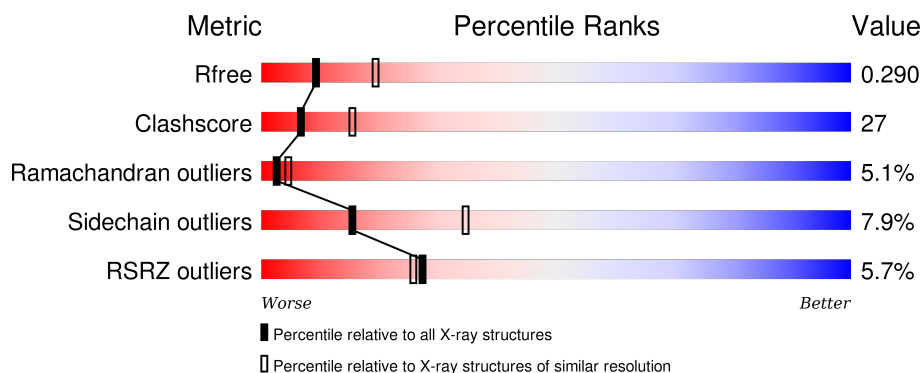
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	676	
1	B	676	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	9202	-	-	X	-
2	CIT	A	9203	-	-	-	X
2	CIT	B	9201	-	-	-	X
2	CIT	B	9204	-	-	-	X
2	CIT	B	9205	-	-	-	X
2	CIT	B	9206	-	-	X	X
3	GOL	A	9103	-	-	X	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10601 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 Serotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5243	3291	909	996	47			
1	B	676	Total	C	N	O	S	0	0	0
			5243	3291	909	996	47			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



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

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

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

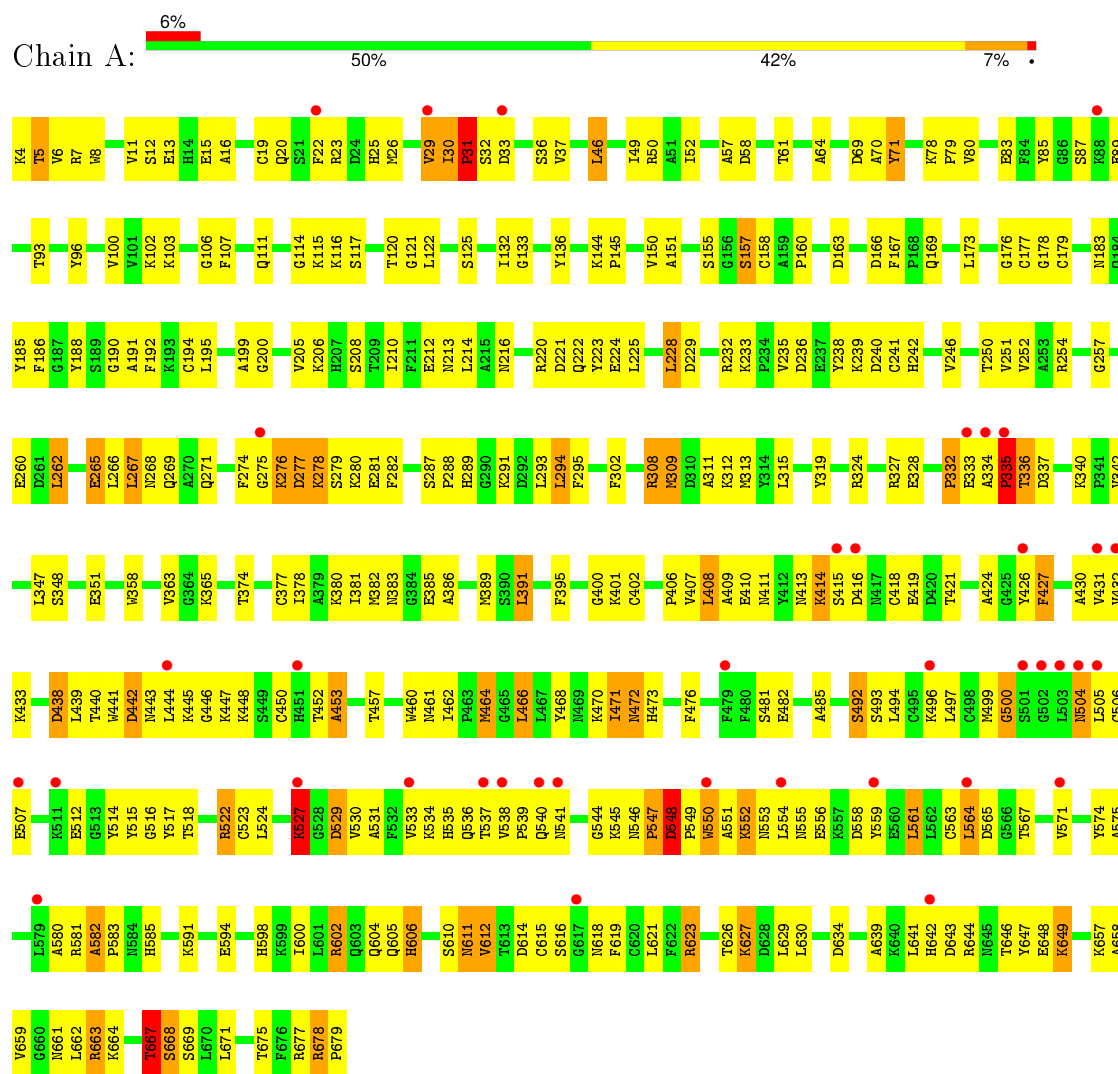


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

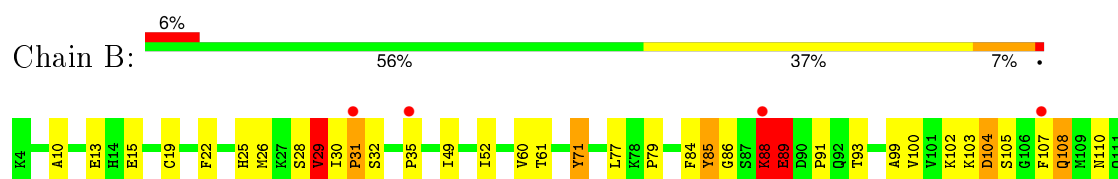
### 3 Residue-property plots

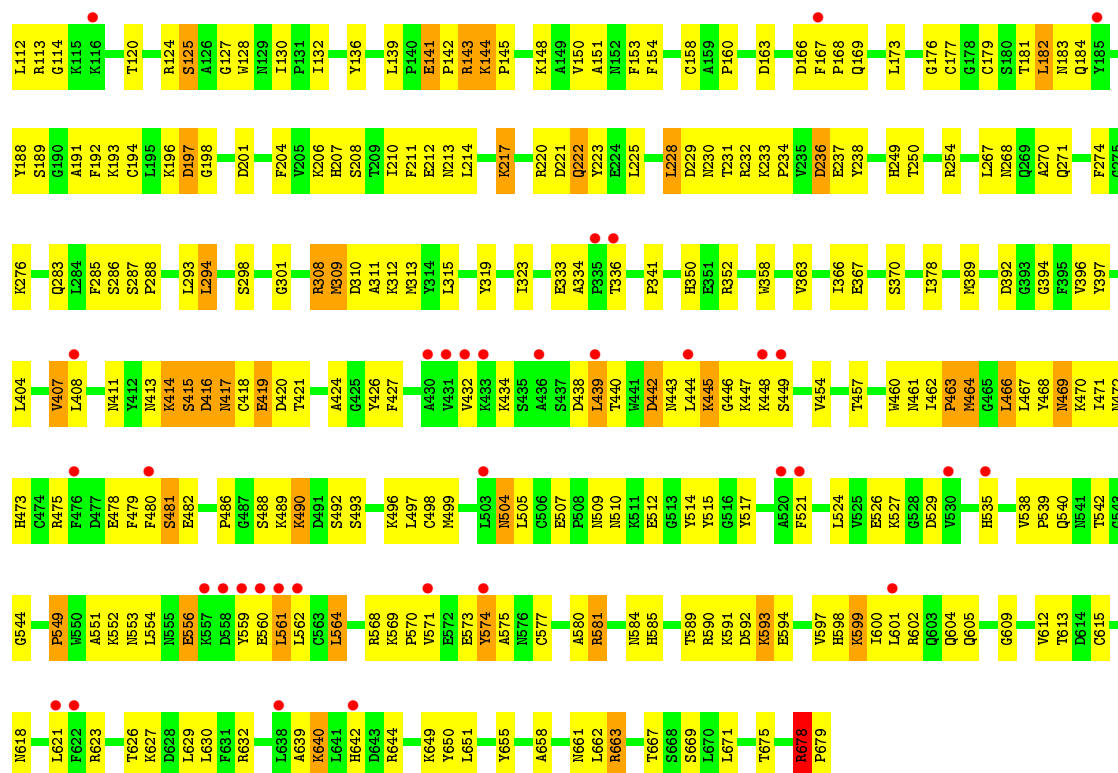
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Serotransferrin



#### • Molecule 1: Serotransferrin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.32Å 103.26Å 200.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 47.34 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 96.3 (47.34-2.69)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.232 , 0.293 0.235 , 0.290	Depositor DCC
$R_{free}$ test set	2502 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49798 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/5362	0.71	3/7247 (0.0%)
1	B	0.41	0/5362	0.71	2/7247 (0.0%)
All	All	0.41	0/10724	0.71	5/14494 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	SER	N-CA-C	6.01	127.24	111.00
1	A	257	GLY	N-CA-C	-5.81	98.58	113.10
1	B	439	LEU	N-CA-C	-5.61	95.86	111.00
1	B	415	SER	N-CA-C	5.34	125.42	111.00
1	A	46	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	TYR	Sidechain

## 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	5243	0	5068	305	0
1	B	5243	0	5068	248	0
2	A	39	0	15	17	0
2	B	52	0	20	16	0
3	A	18	0	24	9	0
3	B	6	0	8	2	0
All	All	10601	0	10203	563	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (563) 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:108:GLN:HA	1:B:108:GLN:HE21	1.10	1.06
1:A:678:ARG:HB3	1:A:679:PRO:HD3	1.45	0.98
1:A:564:LEU:HD11	3:A:9103:GOL:H12	1.45	0.98
1:B:454:VAL:HG23	1:B:486:PRO:O	1.64	0.95
1:A:411:ASN:HD21	1:A:639:ALA:HB2	1.35	0.90
1:A:15:GLU:HG2	1:A:294:LEU:HD13	1.53	0.89
1:A:275:GLY:H	1:A:278:LYS:HB2	1.37	0.89
1:A:232:ARG:O	1:A:233:LYS:HG3	1.73	0.89
1:A:411:ASN:ND2	1:A:639:ALA:HB2	1.87	0.89
1:B:88:LYS:H	1:B:88:LYS:HE2	1.38	0.88
1:A:461:ASN:HA	1:A:662:LEU:HD11	1.53	0.87
1:B:108:GLN:CA	1:B:108:GLN:HE21	1.91	0.84
1:A:25:HIS:ND1	1:A:282:PHE:HB2	1.92	0.84
2:B:9201:CIT:O1	2:B:9201:CIT:O6	1.98	0.81
1:A:471:ILE:HB	1:A:473:HIS:CD2	2.15	0.81
1:B:108:GLN:NE2	1:B:108:GLN:HA	1.93	0.81
1:B:188:TYR:OH	2:B:9206:CIT:H21	1.81	0.81
1:A:25:HIS:HD1	1:A:282:PHE:HB2	1.47	0.79
1:B:517:TYR:HB2	2:B:9205:CIT:O2	1.82	0.79
1:B:188:TYR:OH	1:B:206:LYS:HD2	1.82	0.78
1:B:538:VAL:HB	1:B:539:PRO:HD3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:ARG:HB3	1:B:679:PRO:CD	2.14	0.78
1:B:424:ALA:O	1:B:581:ARG:HG2	1.85	0.77
1:A:442:ASP:HB3	1:A:470:LYS:NZ	2.00	0.76
1:A:552:LYS:HE3	1:A:553:ASN:ND2	2.00	0.76
1:A:268:ASN:HA	1:A:271:GLN:HE21	1.51	0.76
1:A:626:THR:HG22	1:A:627:LYS:N	1.99	0.76
1:A:482:GLU:HA	1:A:493:SER:OG	1.85	0.76
1:A:114:GLY:O	1:A:155:SER:HB3	1.86	0.76
1:A:365:LYS:HE2	1:A:365:LYS:HA	1.68	0.75
1:A:462:ILE:HD13	1:A:580:ALA:HB3	1.69	0.75
1:A:470:LYS:O	1:A:471:ILE:HG23	1.87	0.75
1:A:667:THR:CG2	1:A:668:SER:N	2.50	0.74
1:B:549:PRO:O	1:B:552:LYS:HG2	1.87	0.74
1:A:561:LEU:HD21	1:A:571:VAL:HA	1.70	0.74
1:A:667:THR:HG23	1:A:668:SER:N	2.03	0.74
1:A:102:LYS:HG2	1:A:223:TYR:CE2	2.23	0.73
1:A:646:THR:OG1	1:A:649:LYS:HD3	1.89	0.73
1:B:144:LYS:HA	1:B:145:PRO:C	2.09	0.73
2:A:9203:CIT:O1	2:A:9203:CIT:O7	2.07	0.73
1:A:432:VAL:HG12	1:A:529:ASP:O	1.88	0.73
1:B:191:ALA:O	1:B:194:CYS:HB3	1.89	0.73
1:A:564:LEU:CD1	3:A:9103:GOL:O3	2.37	0.73
1:A:563:CYS:HB3	3:A:9103:GOL:O2	1.90	0.72
1:A:646:THR:HG23	1:A:649:LYS:HE2	1.70	0.71
1:B:448:LYS:HD3	1:B:497:LEU:HD11	1.71	0.71
1:A:71:TYR:OH	1:A:312:LYS:HD2	1.90	0.71
1:A:288:PRO:HG2	1:A:289:HIS:ND1	2.05	0.71
1:A:342:VAL:HG23	1:A:600:ILE:HD12	1.73	0.71
1:B:504:ASN:HD22	1:B:504:ASN:C	1.94	0.71
1:A:15:GLU:HG2	1:A:294:LEU:CD1	2.21	0.70
1:B:440:THR:H	1:B:443:ASN:HB3	1.54	0.70
1:A:413:ASN:HD22	1:A:414:LYS:HG2	1.55	0.69
1:B:460:TRP:O	1:B:464:MET:HB2	1.92	0.69
1:B:293:LEU:O	1:B:294:LEU:HB2	1.93	0.69
1:A:277:ASP:O	1:A:279:SER:N	2.26	0.69
1:B:471:ILE:O	1:B:473:HIS:HD2	1.75	0.69
1:B:103:LYS:HD3	1:B:221:ASP:O	1.93	0.69
1:B:136:TYR:CE2	1:B:143:ARG:HD2	2.28	0.69
1:B:103:LYS:O	1:B:104:ASP:HB2	1.94	0.68
1:A:678:ARG:CB	1:A:679:PRO:HD3	2.21	0.68
1:B:158:CYS:HB2	1:B:173:LEU:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:C	1:B:183:ASN:H	1.97	0.68
1:A:518:THR:HG22	1:A:541:ASN:OD1	1.92	0.68
1:A:667:THR:CG2	1:A:668:SER:H	2.05	0.68
1:A:268:ASN:O	1:A:271:GLN:HG2	1.92	0.67
1:B:392:ASP:O	1:B:396:VAL:HG23	1.93	0.67
1:A:287:SER:OG	1:A:288:PRO:HD2	1.95	0.67
1:B:478:GLU:O	1:B:478:GLU:HG3	1.94	0.67
1:A:31:PRO:C	1:A:33:ASP:H	1.98	0.67
1:B:468:TYR:HB3	1:B:661:ASN:HD22	1.60	0.67
1:A:332:PRO:C	1:A:334:ALA:H	1.95	0.67
1:B:561:LEU:HD21	1:B:571:VAL:HA	1.75	0.67
1:A:564:LEU:HD11	3:A:9103:GOL:C1	2.22	0.67
1:B:89:GLU:O	1:B:91:PRO:HD3	1.96	0.66
1:A:661:ASN:O	1:A:664:LYS:HB2	1.94	0.66
1:B:49:ILE:HG23	1:B:77:LEU:HD12	1.78	0.66
1:A:407:VAL:HG12	1:A:408:LEU:HG	1.78	0.66
1:B:414:LYS:HA	1:B:414:LYS:HE2	1.77	0.66
1:B:678:ARG:O	1:B:679:PRO:O	2.14	0.65
1:A:334:ALA:HB1	1:A:335:PRO:HD2	1.78	0.65
1:A:25:HIS:HD1	1:A:282:PHE:CB	2.08	0.65
1:B:268:ASN:O	1:B:271:GLN:HG2	1.96	0.65
1:A:214:LEU:HD11	1:A:223:TYR:HE1	1.60	0.65
2:B:9204:CIT:O1	2:B:9204:CIT:C6	2.45	0.65
1:A:442:ASP:HB3	1:A:470:LYS:HZ2	1.59	0.65
1:A:407:VAL:HG13	1:A:598:HIS:NE2	2.12	0.65
1:B:352:ARG:HD3	1:B:370:SER:OG	1.97	0.65
1:A:308:ARG:HG3	1:A:669:SER:OG	1.97	0.65
1:B:447:LYS:HG3	1:B:529:ASP:OD2	1.96	0.64
1:A:102:LYS:HG2	1:A:223:TYR:HE2	1.61	0.64
1:A:504:ASN:HA	1:A:507:GLU:HG3	1.79	0.64
1:A:678:ARG:HB3	1:A:679:PRO:CD	2.25	0.64
1:B:644:ARG:HA	1:B:649:LYS:HD3	1.79	0.64
1:A:514:TYR:HE1	1:A:522:ARG:HG2	1.63	0.64
2:A:9207:CIT:O5	2:A:9207:CIT:O2	2.15	0.63
1:A:107:PHE:H	1:A:232:ARG:HH21	1.46	0.63
1:B:612:VAL:HG13	1:B:612:VAL:O	1.99	0.63
1:A:439:LEU:HD23	1:A:443:ASN:ND2	2.13	0.63
1:B:466:LEU:HD22	1:B:658:ALA:HB2	1.79	0.63
1:B:551:ALA:HA	1:B:554:LEU:CD1	2.28	0.63
1:B:434:LYS:HG3	1:B:560:GLU:OE2	1.99	0.63
1:B:663:ARG:HG2	1:B:671:LEU:CD2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLY:O	1:B:481:SER:HB3	1.98	0.63
1:B:471:ILE:O	1:B:473:HIS:CD2	2.52	0.63
1:B:378:ILE:CG1	1:B:389:MET:HE1	2.28	0.63
1:A:667:THR:O	1:A:668:SER:HB3	1.99	0.62
1:B:232:ARG:O	1:B:233:LYS:HG3	1.99	0.62
1:A:552:LYS:HE3	1:A:553:ASN:HD21	1.64	0.62
1:B:309:MET:HE3	1:B:313:MET:SD	2.39	0.62
1:A:413:ASN:ND2	1:A:414:LYS:HG2	2.15	0.62
1:A:46:LEU:HB3	1:A:50:ARG:HH21	1.65	0.62
1:A:471:ILE:HB	1:A:473:HIS:HD2	1.59	0.62
1:A:116:LYS:HG2	1:A:155:SER:OG	1.97	0.62
1:B:591:LYS:C	1:B:593:LYS:H	2.01	0.62
1:B:438:ASP:O	1:B:440:THR:HG23	1.99	0.62
1:A:16:ALA:O	1:A:20:GLN:HG3	1.99	0.61
1:A:401:LYS:HE3	1:A:679:PRO:HG2	1.83	0.61
1:B:158:CYS:O	1:B:160:PRO:HD3	2.00	0.61
1:A:103:LYS:HB2	1:A:222:GLN:O	1.99	0.61
1:A:452:THR:O	1:A:453:ALA:HB2	2.00	0.61
1:B:552:LYS:HG3	1:B:553:ASN:N	2.16	0.61
1:B:640:LYS:HE2	1:B:642:HIS:CE1	2.36	0.61
1:A:107:PHE:HA	1:A:111:GLN:OE1	1.99	0.61
1:A:13:GLU:HG2	1:B:179:CYS:SG	2.41	0.61
1:A:433:LYS:HG2	1:A:559:TYR:CE2	2.34	0.61
1:A:391:LEU:HG	1:A:395:PHE:HB3	1.82	0.61
1:B:192:PHE:CZ	1:B:210:ILE:HG13	2.36	0.60
1:A:407:VAL:HG22	1:A:594:GLU:HG3	1.82	0.60
1:A:383:ASN:OD1	1:A:385:GLU:HG3	2.02	0.60
1:B:678:ARG:HB3	1:B:679:PRO:HD3	1.84	0.60
1:B:105:SER:HB2	1:B:107:PHE:HE2	1.67	0.60
1:A:602:ARG:HA	1:A:605:GLN:HE21	1.67	0.60
1:B:315:LEU:HB3	1:B:319:TYR:HD2	1.68	0.59
1:A:551:ALA:HA	1:A:554:LEU:HG	1.83	0.59
1:A:381:ILE:HA	1:A:386:ALA:O	2.02	0.59
2:A:9202:CIT:C6	2:A:9202:CIT:O1	2.50	0.59
1:A:471:ILE:HG13	1:A:472:ASN:H	1.67	0.59
1:B:196:LYS:C	1:B:198:GLY:H	2.04	0.59
1:B:468:TYR:O	1:B:470:LYS:N	2.36	0.59
2:B:9201:CIT:C1	2:B:9201:CIT:O6	2.50	0.59
1:B:49:ILE:HG23	1:B:77:LEU:CD1	2.33	0.59
1:A:574:TYR:CD1	1:A:575:ALA:N	2.71	0.59
1:A:262:LEU:HD12	1:A:262:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:THR:HG23	1:B:679:PRO:HG2	1.83	0.58
1:B:551:ALA:HA	1:B:554:LEU:HD12	1.85	0.58
1:B:181:THR:O	1:B:183:ASN:N	2.36	0.58
1:B:378:ILE:HG13	1:B:389:MET:HE1	1.85	0.58
1:A:179:CYS:SG	1:B:13:GLU:HG2	2.43	0.58
1:B:168:PRO:HG2	1:B:169:GLN:NE2	2.19	0.58
1:B:517:TYR:N	2:B:9205:CIT:O1	2.36	0.58
1:A:315:LEU:HD22	1:A:319:TYR:CE2	2.38	0.58
1:A:457:THR:OG1	2:A:9202:CIT:H22	2.03	0.58
1:A:334:ALA:O	1:A:335:PRO:C	2.42	0.58
1:B:424:ALA:HB3	1:B:581:ARG:CZ	2.34	0.58
1:A:188:TYR:CE2	1:A:206:LYS:HG3	2.39	0.58
1:A:581:ARG:O	1:A:582:ALA:HB3	2.04	0.58
1:B:678:ARG:CB	1:B:679:PRO:CD	2.82	0.57
1:B:71:TYR:CZ	1:B:312:LYS:HD3	2.38	0.57
1:A:214:LEU:HD11	1:A:223:TYR:CE1	2.37	0.57
2:A:9207:CIT:C5	2:A:9207:CIT:O6	2.53	0.57
1:A:561:LEU:CD2	1:A:571:VAL:HA	2.35	0.57
1:B:585:HIS:CE1	1:B:632:ARG:HD3	2.38	0.57
1:A:409:ALA:HB2	1:A:641:LEU:HD21	1.85	0.57
1:A:444:LEU:O	1:A:447:LYS:HB2	2.04	0.57
1:A:267:LEU:HB3	1:A:302:PHE:CD2	2.39	0.57
1:A:413:ASN:ND2	1:A:414:LYS:H	2.03	0.57
1:A:466:LEU:HD13	1:A:658:ALA:HB2	1.85	0.57
1:A:667:THR:HG22	1:A:668:SER:H	1.69	0.57
1:A:205:VAL:HG23	1:A:206:LYS:O	2.04	0.57
1:A:413:ASN:CG	1:A:414:LYS:H	2.06	0.56
1:B:105:SER:HB2	1:B:107:PHE:CE2	2.39	0.56
1:A:363:VAL:O	1:A:363:VAL:HG12	2.05	0.56
1:A:158:CYS:HB2	1:A:173:LEU:HB2	1.86	0.56
1:A:439:LEU:HD23	1:A:443:ASN:HD22	1.71	0.56
2:A:9202:CIT:O5	2:A:9202:CIT:O1	2.23	0.56
1:B:26:MET:HE1	1:B:270:ALA:HA	1.86	0.56
1:A:117:SER:OG	1:A:157:SER:HB3	2.05	0.56
1:B:568:ARG:O	1:B:569:LYS:HG3	2.05	0.56
1:A:517:TYR:HD1	2:A:9203:CIT:O6	1.89	0.56
1:B:475:ARG:HE	1:B:478:GLU:CD	2.08	0.56
1:A:389:MET:HG3	1:A:391:LEU:HD13	1.87	0.56
1:A:232:ARG:O	1:A:233:LYS:CG	2.50	0.56
1:B:189:SER:HA	1:B:213:ASN:HD21	1.70	0.56
1:A:107:PHE:N	1:A:232:ARG:HH21	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TYR:CZ	1:B:206:LYS:HD2	2.40	0.55
1:B:19:CYS:O	1:B:22:PHE:HB3	2.05	0.55
1:B:89:GLU:H	1:B:89:GLU:CD	2.07	0.55
1:B:214:LEU:HD11	1:B:223:TYR:HE1	1.71	0.55
1:A:564:LEU:HD11	3:A:9103:GOL:O3	2.04	0.55
1:B:30:ILE:HD13	1:B:35:PRO:HG2	1.88	0.55
1:B:229:ASP:OD1	1:B:231:THR:HG23	2.06	0.55
1:A:439:LEU:HA	1:A:443:ASN:HD22	1.71	0.55
1:B:188:TYR:HD1	3:B:9102:GOL:O2	1.90	0.55
1:A:438:ASP:O	1:A:440:THR:HG23	2.07	0.55
1:A:565:ASP:OD1	1:A:567:THR:HG23	2.06	0.55
2:B:9204:CIT:O7	2:B:9204:CIT:O3	2.24	0.55
1:B:600:ILE:O	1:B:604:GLN:HG2	2.06	0.55
1:A:460:TRP:O	1:A:464:MET:HB2	2.07	0.54
1:A:517:TYR:CZ	1:A:534:LYS:HD3	2.42	0.54
1:B:473:HIS:CE1	1:B:475:ARG:HB2	2.42	0.54
1:B:413:ASN:O	1:B:414:LYS:C	2.46	0.54
1:B:514:TYR:HE1	1:B:527:LYS:HD3	1.72	0.54
1:A:514:TYR:CE1	1:A:522:ARG:HG2	2.42	0.54
1:A:275:GLY:H	1:A:278:LYS:CB	2.16	0.54
1:A:100:VAL:HG22	1:A:225:LEU:CD2	2.37	0.54
1:B:132:ILE:HD12	1:B:150:VAL:HG22	1.90	0.54
1:A:358:TRP:HE1	1:A:604:GLN:NE2	2.06	0.54
1:B:408:LEU:HD23	1:B:640:LYS:HA	1.90	0.53
1:A:426:TYR:OH	2:A:9202:CIT:O5	2.23	0.53
1:B:521:PHE:O	1:B:524:LEU:HB3	2.08	0.53
1:B:192:PHE:HD2	1:B:213:ASN:HD22	1.56	0.53
1:A:324:ARG:HD2	1:A:328:GLU:OE2	2.07	0.53
1:A:471:ILE:O	1:A:472:ASN:HB2	2.07	0.53
1:A:413:ASN:O	1:A:414:LYS:C	2.46	0.53
1:A:536:GLN:CB	1:A:540:GLN:HE21	2.21	0.53
1:A:265:GLU:O	1:A:269:GLN:HG3	2.09	0.53
1:B:79:PRO:HB3	1:B:250:THR:HG21	1.91	0.53
1:B:605:GLN:O	1:B:609:GLY:HA3	2.09	0.53
1:A:657:LYS:O	1:A:661:ASN:ND2	2.42	0.53
1:B:125:SER:HB2	2:B:9206:CIT:O2	2.09	0.53
1:A:20:GLN:HB3	1:A:23:ARG:HH21	1.72	0.53
1:A:424:ALA:HB3	1:A:581:ARG:NH1	2.23	0.53
1:A:37:VAL:HG22	1:A:266:LEU:HD21	1.91	0.53
1:A:57:ALA:O	1:A:254:ARG:NH2	2.42	0.53
1:A:518:THR:N	2:A:9203:CIT:O4	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:HB2	1:A:531:ALA:HB2	1.90	0.53
1:B:208:SER:O	1:B:212:GLU:HG3	2.09	0.53
1:B:287:SER:OG	1:B:288:PRO:HD2	2.08	0.52
1:A:564:LEU:CD1	3:A:9103:GOL:H12	2.31	0.52
1:B:591:LYS:O	1:B:593:LYS:N	2.41	0.52
1:B:26:MET:CE	1:B:270:ALA:HA	2.39	0.52
1:A:26:MET:O	1:A:30:ILE:HD12	2.09	0.52
1:A:466:LEU:CD1	1:A:658:ALA:HB2	2.40	0.52
1:A:564:LEU:HD12	3:A:9103:GOL:O3	2.09	0.52
1:A:516:GLY:HA3	2:A:9203:CIT:C5	2.40	0.52
1:B:333:GLU:OE2	1:B:333:GLU:N	2.32	0.52
1:A:482:GLU:HG2	1:A:497:LEU:HG	1.92	0.52
1:B:341:PRO:HB2	1:B:367:GLU:HG3	1.91	0.52
1:A:87:SER:OG	1:A:89:GLU:HB2	2.09	0.52
1:A:315:LEU:HD22	1:A:319:TYR:CD2	2.45	0.52
1:A:505:LEU:O	1:A:506:CYS:HB3	2.10	0.52
1:B:561:LEU:HD12	1:B:577:CYS:SG	2.50	0.52
1:A:517:TYR:N	2:A:9203:CIT:O4	2.43	0.52
1:A:185:TYR:HA	1:A:190:GLY:O	2.09	0.51
1:A:555:ASN:HB2	1:A:558:ASP:OD2	2.09	0.51
1:B:504:ASN:HA	1:B:507:GLU:HG2	1.92	0.51
1:A:535:HIS:HB2	1:A:574:TYR:CG	2.44	0.51
1:A:407:VAL:HG12	1:A:408:LEU:CD1	2.41	0.51
1:B:378:ILE:HG12	1:B:389:MET:CE	2.41	0.51
1:A:11:VAL:O	1:A:12:SER:HB3	2.10	0.51
1:B:350:HIS:HD2	2:B:9201:CIT:O3	1.93	0.51
1:A:374:THR:HG21	1:A:395:PHE:CD1	2.46	0.51
1:B:308:ARG:HB2	1:B:669:SER:HB3	1.92	0.51
1:A:629:LEU:O	1:A:630:LEU:HB2	2.10	0.51
1:B:574:TYR:CD1	1:B:575:ALA:N	2.79	0.51
1:B:378:ILE:HG12	1:B:389:MET:HE1	1.91	0.51
1:B:526:GLU:O	1:B:527:LYS:HG3	2.11	0.51
1:A:5:THR:HB	1:A:36:SER:OG	2.11	0.51
1:B:418:CYS:O	1:B:420:ASP:N	2.44	0.51
1:B:526:GLU:C	1:B:527:LYS:HG3	2.32	0.51
1:B:597:VAL:HG12	1:B:601:LEU:HD12	1.93	0.51
1:A:535:HIS:CD2	1:A:536:GLN:HG3	2.45	0.50
1:B:234:PRO:HD2	1:B:237:GLU:OE1	2.11	0.50
1:B:538:VAL:HB	1:B:571:VAL:HG11	1.93	0.50
1:A:426:TYR:O	1:A:426:TYR:HD1	1.94	0.50
1:A:426:TYR:OH	2:A:9202:CIT:O1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ALA:HB3	1:A:494:LEU:HB3	1.92	0.50
1:A:220:ARG:C	1:A:222:GLN:H	2.15	0.50
1:B:598:HIS:O	1:B:602:ARG:CG	2.59	0.50
1:A:158:CYS:O	1:A:160:PRO:HD3	2.11	0.50
1:B:222:GLN:HE21	1:B:222:GLN:CA	2.24	0.50
1:B:651:LEU:HD22	1:B:655:TYR:CD2	2.47	0.50
1:A:333:GLU:H	1:A:333:GLU:CD	2.15	0.50
1:B:214:LEU:HD11	1:B:223:TYR:CE1	2.46	0.50
1:B:30:ILE:O	1:B:32:SER:N	2.39	0.50
1:B:420:ASP:O	1:B:421:THR:HG23	2.12	0.50
1:A:380:LYS:HG2	1:A:385:GLU:HB2	1.94	0.50
1:B:283:GLN:N	1:B:283:GLN:CD	2.64	0.50
1:A:151:ALA:HB1	1:A:169:GLN:CG	2.42	0.50
1:B:626:THR:HG22	1:B:627:LYS:N	2.27	0.49
1:A:675:THR:HA	1:A:679:PRO:HD2	1.93	0.49
1:A:228:LEU:HD22	3:A:9104:GOL:H2	1.95	0.49
1:A:176:GLY:O	1:A:177:CYS:HB2	2.12	0.49
1:B:113:ARG:HG3	1:B:114:GLY:N	2.28	0.49
1:A:29:VAL:O	1:A:30:ILE:HG13	2.11	0.49
1:B:103:LYS:O	1:B:104:ASP:CB	2.60	0.49
1:B:148:LYS:HB2	1:B:167:PHE:CE2	2.48	0.49
1:A:441:TRP:O	1:A:444:LEU:HD13	2.11	0.49
1:A:107:PHE:O	1:A:232:ARG:NH2	2.44	0.49
1:B:538:VAL:O	1:B:540:GLN:N	2.41	0.49
1:B:188:TYR:OH	2:B:9206:CIT:C2	2.58	0.49
1:B:142:PRO:O	1:B:144:LYS:N	2.44	0.49
1:B:471:ILE:HG21	1:B:479:PHE:HD1	1.77	0.49
1:A:335:PRO:O	1:A:336:THR:HB	2.13	0.49
1:B:413:ASN:HD22	1:B:414:LYS:HD2	1.78	0.49
1:B:319:TYR:O	1:B:323:ILE:HG12	2.12	0.49
1:B:181:THR:C	1:B:183:ASN:N	2.64	0.49
1:B:30:ILE:CD1	1:B:35:PRO:HG2	2.43	0.49
1:A:151:ALA:HB1	1:A:169:GLN:HG2	1.93	0.49
1:A:191:ALA:O	1:A:194:CYS:HB3	2.12	0.49
1:A:678:ARG:CB	1:A:679:PRO:CD	2.87	0.49
1:B:591:LYS:C	1:B:593:LYS:N	2.66	0.49
1:A:677:ARG:HB3	1:A:677:ARG:NH1	2.27	0.49
1:B:120:THR:HG23	1:B:204:PHE:O	2.13	0.49
1:B:217:LYS:HG2	1:B:220:ARG:NH2	2.28	0.49
1:A:332:PRO:C	1:A:334:ALA:N	2.65	0.49
1:B:285:PHE:O	1:B:286:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:GLU:OE2	1:A:496:LYS:HB3	2.13	0.48
1:A:31:PRO:C	1:A:33:ASP:N	2.66	0.48
1:B:598:HIS:CD2	1:B:640:LYS:HG2	2.48	0.48
1:B:358:TRP:CE2	1:B:366:ILE:HG13	2.48	0.48
1:A:64:ALA:CB	1:A:246:VAL:HG13	2.43	0.48
2:B:9204:CIT:O1	2:B:9204:CIT:O5	2.31	0.48
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.95	0.48
1:B:462:ILE:HB	1:B:463:PRO:CD	2.43	0.48
1:A:220:ARG:O	1:A:222:GLN:N	2.46	0.48
1:A:544:GLY:C	1:A:546:ASN:H	2.16	0.48
1:B:629:LEU:O	1:B:630:LEU:HB2	2.13	0.48
1:A:564:LEU:HD12	1:A:565:ASP:N	2.28	0.48
1:A:547:PRO:O	1:A:548:ASP:O	2.31	0.48
1:B:658:ALA:O	1:B:662:LEU:HB2	2.13	0.48
1:B:196:LYS:C	1:B:198:GLY:N	2.67	0.48
1:A:22:PHE:CE2	1:A:37:VAL:HG21	2.48	0.48
1:B:471:ILE:CG2	1:B:479:PHE:HD1	2.27	0.48
1:B:471:ILE:HG21	1:B:479:PHE:CD1	2.48	0.48
1:B:89:GLU:CD	1:B:89:GLU:N	2.67	0.48
1:B:552:LYS:HG3	1:B:553:ASN:H	1.78	0.48
1:B:413:ASN:O	1:B:414:LYS:O	2.31	0.48
1:A:536:GLN:HB2	1:A:540:GLN:HE21	1.79	0.48
1:A:564:LEU:N	1:A:564:LEU:HD12	2.29	0.48
1:A:544:GLY:C	1:A:546:ASN:N	2.66	0.48
1:A:646:THR:CG2	1:A:649:LYS:HE2	2.42	0.48
1:A:530:VAL:O	1:A:530:VAL:HG13	2.13	0.48
1:B:426:TYR:O	1:B:535:HIS:ND1	2.44	0.48
1:B:489:LYS:O	1:B:492:SER:N	2.47	0.47
1:A:102:LYS:CG	1:A:223:TYR:HE2	2.27	0.47
1:B:211:PHE:HZ	1:B:236:ASP:HB3	1.79	0.47
1:A:242:HIS:N	3:A:9104:GOL:O3	2.46	0.47
1:B:85:TYR:CD1	1:B:85:TYR:N	2.82	0.47
1:B:411:ASN:ND2	1:B:639:ALA:HB2	2.30	0.47
1:A:114:GLY:O	1:A:155:SER:CB	2.61	0.47
1:A:279:SER:OG	1:A:281:GLU:HB3	2.14	0.47
1:A:407:VAL:HG12	1:A:408:LEU:CG	2.42	0.47
1:A:539:PRO:O	1:A:545:LYS:HD2	2.13	0.47
1:A:547:PRO:O	1:A:552:LYS:HB3	2.13	0.47
1:B:468:TYR:HD2	1:B:661:ASN:ND2	2.13	0.47
1:A:347:LEU:HD21	1:A:374:THR:HA	1.96	0.47
1:B:234:PRO:HB2	1:B:237:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:GLU:HB3	1:B:497:LEU:HG	1.95	0.47
1:A:426:TYR:O	1:A:427:PHE:O	2.32	0.47
1:B:509:ASN:HA	1:B:515:TYR:CE2	2.50	0.47
1:A:107:PHE:H	1:A:232:ARG:NH2	2.11	0.47
1:A:25:HIS:CE1	1:A:282:PHE:HB2	2.49	0.47
1:A:100:VAL:HG22	1:A:225:LEU:HD21	1.96	0.47
1:A:206:LYS:NZ	2:A:9207:CIT:O6	2.48	0.47
1:A:52:ILE:O	1:A:254:ARG:NE	2.48	0.47
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.50	0.47
1:A:240:ASP:CG	1:A:678:ARG:HH22	2.18	0.47
1:B:416:ASP:O	1:B:417:ASN:CB	2.62	0.47
2:A:9207:CIT:O2	2:A:9207:CIT:C6	2.62	0.46
1:B:434:LYS:HG3	1:B:560:GLU:CD	2.35	0.46
1:B:432:VAL:HG21	1:B:562:LEU:HD21	1.96	0.46
1:A:407:VAL:HG13	1:A:598:HIS:CD2	2.50	0.46
1:B:100:VAL:HG22	1:B:225:LEU:CD2	2.45	0.46
1:B:449:SER:HB3	1:B:480:PHE:CE1	2.50	0.46
1:B:169:GLN:CD	1:B:169:GLN:H	2.19	0.46
1:B:514:TYR:CE1	1:B:527:LYS:HD3	2.50	0.46
1:A:410:GLU:CD	1:A:585:HIS:HB2	2.36	0.46
1:A:457:THR:N	2:A:9202:CIT:O2	2.46	0.46
1:B:600:ILE:H	1:B:600:ILE:HD12	1.81	0.46
1:B:471:ILE:CG2	1:B:479:PHE:CD1	2.99	0.46
1:B:210:ILE:HD11	1:B:223:TYR:CD1	2.50	0.46
1:B:163:ASP:OD2	1:B:166:ASP:OD2	2.33	0.46
1:A:333:GLU:N	1:A:333:GLU:OE2	2.46	0.46
1:B:499:MET:O	1:B:505:LEU:HG	2.15	0.46
1:A:493:SER:HA	1:A:496:LYS:HE3	1.97	0.46
1:A:659:VAL:O	1:A:663:ARG:HG2	2.15	0.46
1:A:400:GLY:HA3	1:A:647:TYR:CD2	2.51	0.46
1:B:504:ASN:ND2	1:B:504:ASN:C	2.67	0.45
1:B:613:THR:O	1:B:615:CYS:N	2.45	0.45
1:B:28:SER:O	1:B:29:VAL:HG23	2.16	0.45
1:A:144:LYS:HA	1:A:145:PRO:C	2.36	0.45
1:A:31:PRO:O	1:A:33:ASP:N	2.49	0.45
1:A:536:GLN:O	1:A:539:PRO:HD2	2.16	0.45
1:A:452:THR:O	1:A:453:ALA:CB	2.63	0.45
1:B:102:LYS:HG3	1:B:223:TYR:HE2	1.81	0.45
1:B:84:PHE:CZ	1:B:301:GLY:HA3	2.51	0.45
1:A:602:ARG:O	1:A:606:HIS:ND1	2.49	0.45
1:B:151:ALA:O	1:B:154:PHE:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CZ	1:A:210:ILE:HG13	2.51	0.45
1:A:116:LYS:HE2	1:A:199:ALA:O	2.16	0.45
1:A:213:ASN:O	1:A:214:LEU:HD23	2.17	0.45
1:B:591:LYS:NZ	1:B:594:GLU:OE1	2.33	0.45
1:A:377:CYS:HB3	1:A:389:MET:SD	2.57	0.45
1:B:542:THR:OG1	1:B:556:GLU:HB2	2.16	0.45
1:B:538:VAL:HG11	1:B:571:VAL:HG21	1.99	0.45
1:A:539:PRO:HG3	1:A:556:GLU:OE1	2.16	0.45
1:A:71:TYR:HB2	1:A:311:ALA:CB	2.47	0.45
1:B:30:ILE:HA	1:B:31:PRO:HD2	1.68	0.45
1:B:416:ASP:O	1:B:417:ASN:HB2	2.17	0.45
1:A:431:VAL:HG12	1:A:432:VAL:N	2.32	0.45
1:B:462:ILE:HG21	1:B:580:ALA:HB3	1.99	0.45
1:B:598:HIS:O	1:B:602:ARG:HG2	2.17	0.44
1:B:512:GLU:OE2	1:B:514:TYR:HB2	2.18	0.44
1:A:662:LEU:C	1:A:664:LYS:H	2.19	0.44
1:A:468:TYR:C	1:A:470:LYS:H	2.20	0.44
1:B:125:SER:C	1:B:130:ILE:HD12	2.37	0.44
1:B:196:LYS:O	1:B:198:GLY:N	2.51	0.44
1:A:186:PHE:O	1:A:190:GLY:HA3	2.17	0.44
1:A:522:ARG:HB2	1:A:550:TRP:CH2	2.53	0.44
1:A:634:ASP:N	1:A:634:ASP:OD1	2.44	0.44
1:A:132:ILE:HD12	1:A:150:VAL:CG2	2.47	0.44
1:A:527:LYS:HE2	1:A:527:LYS:O	2.17	0.44
1:B:188:TYR:CE2	1:B:206:LYS:HG3	2.52	0.44
1:A:177:CYS:O	1:A:178:GLY:C	2.56	0.44
1:A:83:GLU:OE2	1:A:295:PHE:HB3	2.17	0.44
1:B:440:THR:H	1:B:443:ASN:CB	2.27	0.44
1:A:46:LEU:CB	1:A:50:ARG:HH21	2.28	0.44
1:B:85:TYR:HD2	1:B:298:SER:HG	1.66	0.44
1:B:469:ASN:ND2	1:B:661:ASN:HD21	2.16	0.44
1:A:8:TRP:CH2	1:A:267:LEU:HD21	2.53	0.44
1:A:206:LYS:HZ1	2:A:9207:CIT:C6	2.31	0.43
1:A:401:LYS:HG3	1:A:671:LEU:HD11	2.01	0.43
1:B:188:TYR:CD1	3:B:9102:GOL:O2	2.71	0.43
1:A:183:ASN:HD22	1:A:186:PHE:HB2	1.83	0.43
1:A:163:ASP:OD2	1:A:166:ASP:OD2	2.36	0.43
1:B:473:HIS:HE1	1:B:478:GLU:OE1	2.01	0.43
1:B:136:TYR:O	1:B:139:LEU:HB2	2.18	0.43
1:A:208:SER:O	1:A:212:GLU:HG3	2.18	0.43
1:A:133:GLY:O	1:A:136:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:THR:O	1:A:443:ASN:HB3	2.17	0.43
1:B:602:ARG:NH1	1:B:602:ARG:HB3	2.32	0.43
1:A:8:TRP:HH2	1:A:267:LEU:HD21	1.83	0.43
1:B:589:THR:OG1	1:B:590:ARG:N	2.51	0.43
1:B:124:ARG:CB	2:B:9206:CIT:O5	2.66	0.43
1:B:192:PHE:CE1	1:B:210:ILE:HG13	2.53	0.43
1:A:183:ASN:ND2	1:A:186:PHE:HB2	2.33	0.43
1:B:120:THR:OG1	1:B:127:GLY:HA3	2.18	0.43
1:A:450:CYS:SG	1:A:523:CYS:C	2.97	0.43
1:A:85:TYR:CD1	1:A:85:TYR:N	2.87	0.43
1:A:238:TYR:CD1	1:A:239:LYS:N	2.87	0.43
1:B:552:LYS:HE3	1:B:553:ASN:HD22	1.83	0.43
1:A:533:VAL:HG23	1:A:534:LYS:N	2.33	0.43
1:A:378:ILE:CG1	1:A:389:MET:HE1	2.48	0.43
1:B:315:LEU:HB3	1:B:319:TYR:CD2	2.52	0.43
1:A:647:TYR:CE1	1:A:648:GLU:HG3	2.54	0.43
1:B:52:ILE:O	1:B:254:ARG:HD3	2.19	0.43
1:B:493:SER:HA	1:B:496:LYS:HG3	1.99	0.43
1:B:124:ARG:HA	2:B:9206:CIT:O5	2.19	0.43
1:A:220:ARG:C	1:A:222:GLN:N	2.71	0.43
1:B:613:THR:C	1:B:615:CYS:N	2.72	0.43
1:A:614:ASP:C	1:A:616:SER:N	2.72	0.43
1:B:407:VAL:HG13	1:B:408:LEU:HG	2.01	0.43
1:A:309:MET:HE3	1:A:313:MET:SD	2.59	0.43
1:A:61:THR:HA	1:A:250:THR:O	2.18	0.43
1:A:274:PHE:HB3	1:A:282:PHE:O	2.18	0.43
1:B:598:HIS:HD2	1:B:640:LYS:HG2	1.84	0.43
1:A:504:ASN:HA	1:A:507:GLU:CG	2.46	0.43
1:A:120:THR:O	1:A:160:PRO:HG2	2.18	0.43
1:B:193:LYS:HD3	1:B:197:ASP:OD2	2.19	0.43
1:A:497:LEU:HD22	1:A:527:LYS:HD3	2.00	0.42
1:A:407:VAL:CG2	1:A:594:GLU:HG3	2.47	0.42
1:A:615:CYS:SG	1:A:623:ARG:NH1	2.92	0.42
1:B:232:ARG:O	1:B:233:LYS:CG	2.66	0.42
1:B:110:ASN:ND2	1:B:230:ASN:CG	2.72	0.42
1:A:340:LYS:HA	1:A:340:LYS:HD2	1.91	0.42
1:B:584:ASN:O	1:B:650:TYR:OH	2.32	0.42
1:A:446:GLY:O	1:A:481:SER:HB3	2.19	0.42
1:A:275:GLY:N	1:A:278:LYS:HB2	2.19	0.42
1:A:461:ASN:HA	1:A:662:LEU:CD1	2.36	0.42
1:A:79:PRO:HB3	1:A:250:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD13	1:A:70:ALA:HB2	2.00	0.42
1:A:441:TRP:CD1	1:A:564:LEU:HA	2.55	0.42
1:A:19:CYS:O	1:A:22:PHE:HB3	2.19	0.42
1:B:283:GLN:N	1:B:283:GLN:OE1	2.53	0.42
1:A:544:GLY:O	1:A:546:ASN:N	2.52	0.42
1:A:96:TYR:N	1:A:96:TYR:CD1	2.87	0.42
1:B:207:HIS:HB2	1:B:238:TYR:CD2	2.54	0.42
1:A:107:PHE:N	1:A:232:ARG:NH2	2.66	0.42
1:B:490:LYS:NZ	1:B:507:GLU:OE2	2.43	0.42
1:A:406:PRO:HB2	1:A:641:LEU:CD1	2.49	0.42
1:A:71:TYR:CD1	1:A:71:TYR:O	2.73	0.42
1:A:457:THR:HB	2:A:9202:CIT:C1	2.49	0.42
1:A:505:LEU:O	1:A:506:CYS:CB	2.68	0.42
1:B:60:VAL:HG22	1:B:61:THR:N	2.35	0.42
1:A:7:ARG:HB2	1:A:58:ASP:OD2	2.20	0.42
1:A:612:VAL:O	1:A:612:VAL:CG1	2.67	0.42
2:B:9201:CIT:O7	2:B:9201:CIT:O4	2.28	0.42
1:B:468:TYR:CD2	1:B:661:ASN:ND2	2.88	0.42
1:A:358:TRP:HB2	1:A:619:PHE:CZ	2.54	0.42
1:B:461:ASN:HA	1:B:662:LEU:HD21	2.01	0.42
1:A:6:VAL:HG22	1:A:262:LEU:HG	2.02	0.42
1:A:169:GLN:H	1:A:169:GLN:CD	2.17	0.42
1:B:542:THR:HB	1:B:556:GLU:N	2.35	0.42
1:A:464:MET:HE3	1:A:476:PHE:HD1	1.85	0.42
1:A:4:LYS:O	1:A:4:LYS:HG3	2.19	0.42
1:B:570:PRO:HD2	1:B:573:GLU:CD	2.39	0.42
1:A:527:LYS:CE	1:A:527:LYS:HA	2.49	0.42
1:B:457:THR:N	2:B:9204:CIT:O4	2.32	0.42
1:A:448:LYS:O	1:A:530:VAL:HG12	2.20	0.42
1:A:441:TRP:C	1:A:443:ASN:H	2.23	0.41
1:A:426:TYR:O	1:A:426:TYR:CD1	2.72	0.41
1:A:512:GLU:O	1:A:515:TYR:HB3	2.20	0.41
1:A:644:ARG:HD2	1:A:649:LYS:O	2.19	0.41
1:B:415:SER:HB3	1:B:416:ASP:H	1.64	0.41
1:A:132:ILE:HD12	1:A:150:VAL:HG22	2.01	0.41
1:A:499:MET:O	1:A:500:GLY:O	2.37	0.41
1:A:224:GLU:OE1	1:A:232:ARG:HD2	2.20	0.41
1:B:418:CYS:O	1:B:419:GLU:C	2.57	0.41
1:A:293:LEU:O	1:A:294:LEU:HB2	2.18	0.41
1:A:612:VAL:HG13	1:A:612:VAL:O	2.20	0.41
1:B:176:GLY:O	1:B:177:CYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:LEU:HD13	1:B:479:PHE:CE2	2.56	0.41
1:B:394:GLY:O	1:B:397:TYR:HB3	2.20	0.41
1:B:623:ARG:HA	1:B:623:ARG:HD3	1.81	0.41
1:A:210:ILE:HD11	1:A:223:TYR:CD1	2.56	0.41
1:B:504:ASN:HA	1:B:507:GLU:CG	2.50	0.41
1:B:71:TYR:HB2	1:B:311:ALA:CB	2.51	0.41
1:B:10:ALA:HB1	1:B:15:GLU:HB2	2.02	0.41
1:A:439:LEU:HD11	1:A:529:ASP:HB2	2.03	0.41
1:A:445:LYS:HG3	1:A:446:GLY:N	2.35	0.41
1:A:662:LEU:HD23	1:A:662:LEU:HA	1.90	0.41
1:B:574:TYR:HD1	1:B:575:ALA:N	2.18	0.41
1:A:195:LEU:HD12	1:A:200:GLY:O	2.20	0.41
1:B:457:THR:HA	1:B:461:ASN:HB2	2.03	0.41
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.84	0.41
1:A:276:LYS:HD3	1:A:276:LYS:O	2.20	0.41
1:B:468:TYR:C	1:B:470:LYS:N	2.75	0.41
1:A:262:LEU:HD12	1:A:262:LEU:C	2.42	0.41
1:A:229:ASP:OD1	1:A:229:ASP:C	2.59	0.41
1:A:591:LYS:HD2	1:A:591:LYS:HA	1.90	0.41
1:A:348:SER:H	1:A:351:GLU:HB2	1.86	0.41
1:A:662:LEU:C	1:A:664:LYS:N	2.75	0.41
1:B:124:ARG:HB3	2:B:9206:CIT:O5	2.21	0.41
1:B:142:PRO:C	1:B:144:LYS:H	2.23	0.41
1:B:128:TRP:CH2	1:B:150:VAL:HG21	2.56	0.41
1:B:442:ASP:N	1:B:442:ASP:OD1	2.53	0.41
1:B:481:SER:OG	1:B:482:GLU:N	2.52	0.40
1:B:439:LEU:HD23	1:B:443:ASN:HD22	1.85	0.40
1:B:444:LEU:O	1:B:445:LYS:C	2.59	0.40
1:A:382:MET:SD	1:A:402:CYS:HB3	2.60	0.40
1:B:228:LEU:HA	1:B:228:LEU:HD12	1.85	0.40
1:A:78:LYS:O	1:A:252:VAL:HA	2.20	0.40
1:A:102:LYS:HG2	1:A:223:TYR:CD2	2.56	0.40
1:A:30:ILE:O	1:A:31:PRO:C	2.59	0.40
1:B:498:CYS:HA	1:B:514:TYR:CD1	2.56	0.40
1:A:444:LEU:O	1:A:445:LYS:C	2.59	0.40
1:A:430:ALA:O	1:A:561:LEU:HA	2.21	0.40
1:B:378:ILE:HG23	1:B:404:LEU:HD12	2.02	0.40
1:A:121:GLY:HA2	1:A:160:PRO:HB2	2.02	0.40
1:B:99:ALA:O	1:B:225:LEU:HA	2.22	0.40
1:A:614:ASP:C	1:A:616:SER:H	2.24	0.40
1:B:623:ARG:NH1	1:B:623:ARG:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:H	1:B:141:GLU:HG2	1.53	0.40
1:A:80:VAL:HG22	1:A:251:VAL:O	2.22	0.40
1:A:533:VAL:HG11	1:A:537:THR:HG21	2.03	0.40
1:B:139:LEU:HD23	1:B:153:PHE:HB2	2.03	0.40
1:B:85:TYR:OH	1:B:249:HIS:HB2	2.21	0.40
1:A:69:ASP:OD1	1:A:327:ARG:NH2	2.46	0.40
1:B:144:LYS:NZ	1:B:144:LYS:CB	2.85	0.40
1:B:599:LYS:C	1:B:599:LYS:HD3	2.40	0.40
1:B:559:TYR:CD1	1:B:559:TYR:N	2.89	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	674/676 (100%)	552 (82%)	85 (13%)	37 (6%)	2	4
1	B	674/676 (100%)	554 (82%)	88 (13%)	32 (5%)	3	5
All	All	1348/1352 (100%)	1106 (82%)	173 (13%)	69 (5%)	2	4

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	LYS
1	A	335	PRO
1	A	336	THR
1	A	418	CYS
1	A	427	PHE
1	A	453	ALA
1	A	471	ILE
1	A	548	ASP
1	A	678	ARG

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Mol	Chain	Res	Type
1	B	31	PRO
1	B	143	ARG
1	B	182	LEU
1	B	414	LYS
1	B	416	ASP
1	B	417	ASN
1	B	419	GLU
1	B	469	ASN
1	B	678	ARG
1	A	32	SER
1	A	276	LYS
1	A	414	LYS
1	A	419	GLU
1	A	438	ASP
1	A	492	SER
1	A	500	GLY
1	A	527	LYS
1	A	549	PRO
1	A	550	TRP
1	A	611	ASN
1	A	667	THR
1	B	29	VAL
1	B	112	LEU
1	B	445	LYS
1	B	490	LYS
1	B	556	GLU
1	B	574	TYR
1	B	592	ASP
1	B	599	LYS
1	A	221	ASP
1	A	241	CYS
1	A	442	ASP
1	A	642	HIS
1	B	104	ASP
1	B	197	ASP
1	B	564	LEU
1	A	29	VAL
1	A	106	GLY
1	A	125	SER
1	B	86	GLY
1	B	125	SER
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	427	PHE
1	B	472	ASN
1	B	544	GLY
1	A	582	ALA
1	A	627	LYS
1	B	88	LYS
1	B	549	PRO
1	A	472	ASN
1	A	668	SER
1	B	89	GLU
1	B	334	ALA
1	B	363	VAL
1	A	30	ILE
1	A	235	VAL
1	A	332	PRO
1	A	547	PRO
1	B	463	PRO
1	A	31	PRO

### 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	569/569 (100%)	518 (91%)	51 (9%)	12	27
1	B	569/569 (100%)	530 (93%)	39 (7%)	19	43
All	All	1138/1138 (100%)	1048 (92%)	90 (8%)	15	34

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	31	PRO
1	A	71	TYR
1	A	93	THR
1	A	115	LYS

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	157	SER
1	A	167	PHE
1	A	216	ASN
1	A	228	LEU
1	A	236	ASP
1	A	260	GLU
1	A	262	LEU
1	A	265	GLU
1	A	267	LEU
1	A	277	ASP
1	A	280	LYS
1	A	291	LYS
1	A	294	LEU
1	A	308	ARG
1	A	309	MET
1	A	335	PRO
1	A	337	ASP
1	A	391	LEU
1	A	408	LEU
1	A	416	ASP
1	A	421	THR
1	A	464	MET
1	A	466	LEU
1	A	492	SER
1	A	504	ASN
1	A	522	ARG
1	A	527	LYS
1	A	529	ASP
1	A	548	ASP
1	A	552	LYS
1	A	561	LEU
1	A	564	LEU
1	A	583	PRO
1	A	602	ARG
1	A	606	HIS
1	A	610	SER
1	A	611	ASN
1	A	612	VAL
1	A	618	ASN
1	A	621	LEU
1	A	623	ARG

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Mol	Chain	Res	Type
1	A	643	ASP
1	A	649	LYS
1	A	663	ARG
1	A	667	THR
1	B	29	VAL
1	B	71	TYR
1	B	88	LYS
1	B	89	GLU
1	B	93	THR
1	B	108	GLN
1	B	141	GLU
1	B	144	LYS
1	B	182	LEU
1	B	201	ASP
1	B	217	LYS
1	B	222	GLN
1	B	228	LEU
1	B	236	ASP
1	B	267	LEU
1	B	276	LYS
1	B	294	LEU
1	B	308	ARG
1	B	309	MET
1	B	310	ASP
1	B	336	THR
1	B	407	VAL
1	B	442	ASP
1	B	464	MET
1	B	466	LEU
1	B	481	SER
1	B	488	SER
1	B	504	ASN
1	B	510	ASN
1	B	561	LEU
1	B	564	LEU
1	B	581	ARG
1	B	593	LYS
1	B	618	ASN
1	B	621	LEU
1	B	640	LYS
1	B	663	ARG
1	B	667	THR

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Mol	Chain	Res	Type
1	B	678	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	216	ASN
1	A	230	ASN
1	A	268	ASN
1	A	271	GLN
1	A	283	GLN
1	A	411	ASN
1	A	413	ASN
1	A	417	ASN
1	A	443	ASN
1	A	540	GLN
1	A	604	GLN
1	A	611	ASN
1	A	661	ASN
1	B	108	GLN
1	B	110	ASN
1	B	152	ASN
1	B	213	ASN
1	B	222	GLN
1	B	350	HIS
1	B	413	ASN
1	B	443	ASN
1	B	469	ASN
1	B	472	ASN
1	B	473	HIS
1	B	504	ASN
1	B	553	ASN
1	B	585	HIS
1	B	598	HIS
1	B	603	GLN
1	B	604	GLN
1	B	642	HIS
1	B	661	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	GOL	A	9101	-	5,5,5	0.61	0	5,5,5	0.43	0
3	GOL	A	9103	-	5,5,5	0.53	0	5,5,5	0.72	0
3	GOL	A	9104	-	5,5,5	0.41	0	5,5,5	1.04	0
2	CIT	A	9202	-	3,12,12	1.58	1 (33%)	3,17,17	1.77	1 (33%)
2	CIT	A	9203	-	3,12,12	2.01	2 (66%)	3,17,17	3.53	1 (33%)
2	CIT	A	9207	-	3,12,12	2.07	1 (33%)	3,17,17	1.02	0
3	GOL	B	9102	-	5,5,5	0.47	0	5,5,5	0.27	0
2	CIT	B	9201	-	3,12,12	3.07	2 (66%)	3,17,17	1.40	1 (33%)
2	CIT	B	9204	-	3,12,12	2.53	1 (33%)	3,17,17	1.86	1 (33%)
2	CIT	B	9205	-	3,12,12	2.64	1 (33%)	3,17,17	2.59	1 (33%)
2	CIT	B	9206	-	3,12,12	2.78	1 (33%)	3,17,17	1.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	9101	-	-	0/4/4/4	0/0/0/0
3	GOL	A	9103	-	-	0/4/4/4	0/0/0/0
3	GOL	A	9104	-	-	0/4/4/4	0/0/0/0
2	CIT	A	9202	-	-	0/6/16/16	0/0/0/0
2	CIT	A	9203	-	-	0/6/16/16	0/0/0/0
2	CIT	A	9207	-	-	0/6/16/16	0/0/0/0
3	GOL	B	9102	-	-	0/4/4/4	0/0/0/0
2	CIT	B	9201	-	-	0/6/16/16	0/0/0/0
2	CIT	B	9204	-	-	0/6/16/16	0/0/0/0
2	CIT	B	9205	-	-	0/6/16/16	0/0/0/0
2	CIT	B	9206	-	-	0/6/16/16	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9203	CIT	C4-C3	2.22	1.58	1.54
2	A	9203	CIT	O7-C3	2.34	1.46	1.43
2	A	9202	CIT	O7-C3	2.58	1.47	1.43
2	A	9207	CIT	O7-C3	2.70	1.47	1.43
2	B	9201	CIT	C2-C3	2.79	1.59	1.54
2	B	9204	CIT	O7-C3	4.11	1.49	1.43
2	B	9205	CIT	O7-C3	4.48	1.50	1.43
2	B	9201	CIT	O7-C3	4.52	1.50	1.43
2	B	9206	CIT	O7-C3	4.52	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9203	CIT	C3-C2-C1	-6.09	105.23	114.96
2	B	9205	CIT	C3-C4-C5	-4.32	108.06	114.96
2	A	9202	CIT	C4-C3-C2	-3.07	102.47	109.81
2	B	9204	CIT	C3-C4-C5	-2.83	110.43	114.96
2	B	9201	CIT	C3-C4-C5	-2.41	111.10	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9103	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9104	GOL	2	0
2	A	9202	CIT	7	0
2	A	9203	CIT	5	0
2	A	9207	CIT	5	0
3	B	9102	GOL	2	0
2	B	9201	CIT	4	0
2	B	9204	CIT	4	0
2	B	9205	CIT	2	0
2	B	9206	CIT	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	676/676 (100%)	0.38	38 (5%)	28 26	38, 74, 105, 123	0
1	B	676/676 (100%)	0.44	39 (5%)	26 25	38, 75, 107, 124	0
All	All	1352/1352 (100%)	0.41	77 (5%)	27 26	38, 75, 106, 124	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	TYR	6.1
1	B	431	VAL	5.1
1	B	571	VAL	4.8
1	A	541	ASN	4.4
1	B	439	LEU	4.3
1	A	503	LEU	4.1
1	B	433	LYS	4.0
1	A	505	LEU	3.8
1	B	621	LEU	3.7
1	B	448	LYS	3.7
1	B	432	VAL	3.6
1	A	335	PRO	3.5
1	A	504	ASN	3.4
1	B	430	ALA	3.4
1	B	335	PRO	3.3
1	B	503	LEU	3.3
1	B	521	PHE	3.3
1	B	167	PHE	3.1
1	A	479	PHE	3.0
1	A	527	LYS	2.9
1	B	476	PHE	2.9
1	A	431	VAL	2.9
1	B	436	ALA	2.9
1	B	520	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	537	THR	2.8
1	A	334	ALA	2.8
1	B	535	HIS	2.8
1	A	571	VAL	2.8
1	A	444	LEU	2.6
1	A	540	GLN	2.6
1	A	502	GLY	2.6
1	A	22	PHE	2.6
1	B	107	PHE	2.6
1	A	496	LYS	2.5
1	B	557	LYS	2.5
1	B	560	GLU	2.5
1	B	574	TYR	2.5
1	A	333	GLU	2.5
1	A	533	VAL	2.5
1	B	562	LEU	2.5
1	B	185	TYR	2.4
1	B	408	LEU	2.4
1	A	415	SER	2.4
1	A	416	ASP	2.4
1	A	33	ASP	2.4
1	A	29	VAL	2.4
1	A	559	TYR	2.4
1	A	432	VAL	2.4
1	A	579	LEU	2.3
1	B	561	LEU	2.3
1	B	622	PHE	2.3
1	A	501	SER	2.3
1	B	638	LEU	2.3
1	B	336	THR	2.3
1	A	88	LYS	2.3
1	A	554	LEU	2.2
1	B	601	LEU	2.2
1	A	426	TYR	2.2
1	B	480	PHE	2.2
1	B	558	ASP	2.2
1	A	511	LYS	2.2
1	B	35	PRO	2.2
1	B	444	LEU	2.2
1	B	88	LYS	2.1
1	A	275	GLY	2.1
1	A	550	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	449	SER	2.1
1	B	31	PRO	2.1
1	A	451	HIS	2.1
1	A	564	LEU	2.0
1	A	538	VAL	2.0
1	B	642	HIS	2.0
1	A	507	GLU	2.0
1	A	642	HIS	2.0
1	B	530	VAL	2.0
1	A	617	GLY	2.0
1	B	116	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CIT	B	9201	13/13	0.77	0.32	9.09	68,71,82,84	0
2	CIT	B	9204	13/13	0.81	0.33	6.36	73,77,84,86	0
2	CIT	B	9206	13/13	0.59	0.34	6.30	76,78,81,81	0
2	CIT	A	9203	13/13	0.76	0.43	5.66	77,81,88,89	0
2	CIT	B	9205	13/13	0.67	0.37	4.19	81,87,91,94	0
3	GOL	A	9103	6/6	0.80	0.38	2.73	79,83,85,86	0
3	GOL	A	9104	6/6	0.86	0.21	0.75	73,75,78,80	0
2	CIT	A	9202	13/13	0.78	0.24	0.71	76,81,87,90	0
2	CIT	A	9207	13/13	0.82	0.22	0.36	80,85,89,90	0
3	GOL	B	9102	6/6	0.69	0.40	-	78,82,86,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	9101	6/6	0.88	0.26	-	82,86,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.