



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:29 AM GMT

PDB ID : 2HAU  
Title : Apo-Human Serum Transferrin (Non-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

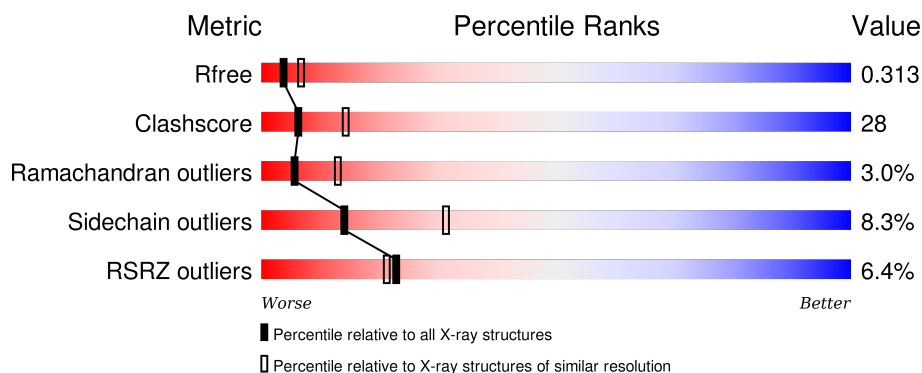
# 1 Overall quality at a glance

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	<div> <div>9%</div> <div>51%</div> <div>44%</div> <div>5%</div> </div>
1	B	676	<div> <div>4%</div> <div>50%</div> <div>44%</div> <div>6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	B	9201	-	-	-	X
2	CIT	B	9204	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10552 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	Se	0	0	0
			5244	3291	907	999	38	9			
1	B	676	Total	C	N	O	S	Se	0	0	0
			5244	3291	907	999	38	9			

There are 22 discrepancies between the modelled and reference sequences:

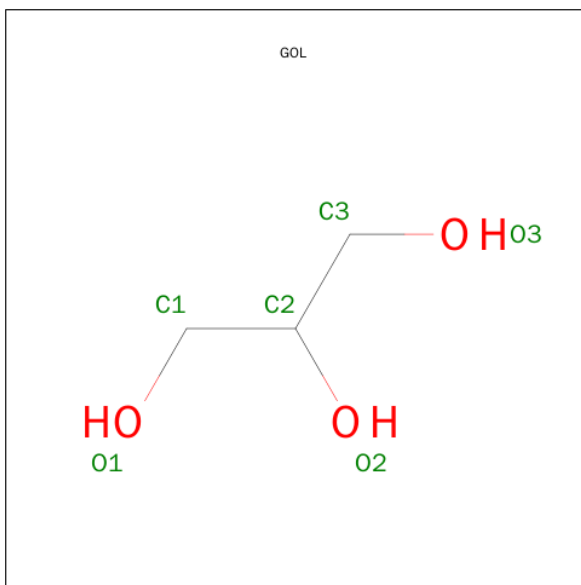
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	109	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	256	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	309	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	313	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	382	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	389	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	413	ASP	ASN	ENGINEERED	UNP P02787
A	464	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	499	MSE	MET	MODIFIED RESIDUE	UNP P02787
A	611	ASP	ASN	ENGINEERED	UNP P02787
B	26	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	109	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	256	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	309	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	313	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	382	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	389	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	413	ASP	ASN	ENGINEERED	UNP P02787
B	464	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	499	MSE	MET	MODIFIED RESIDUE	UNP P02787
B	611	ASP	ASN	ENGINEERED	UNP P02787

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

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

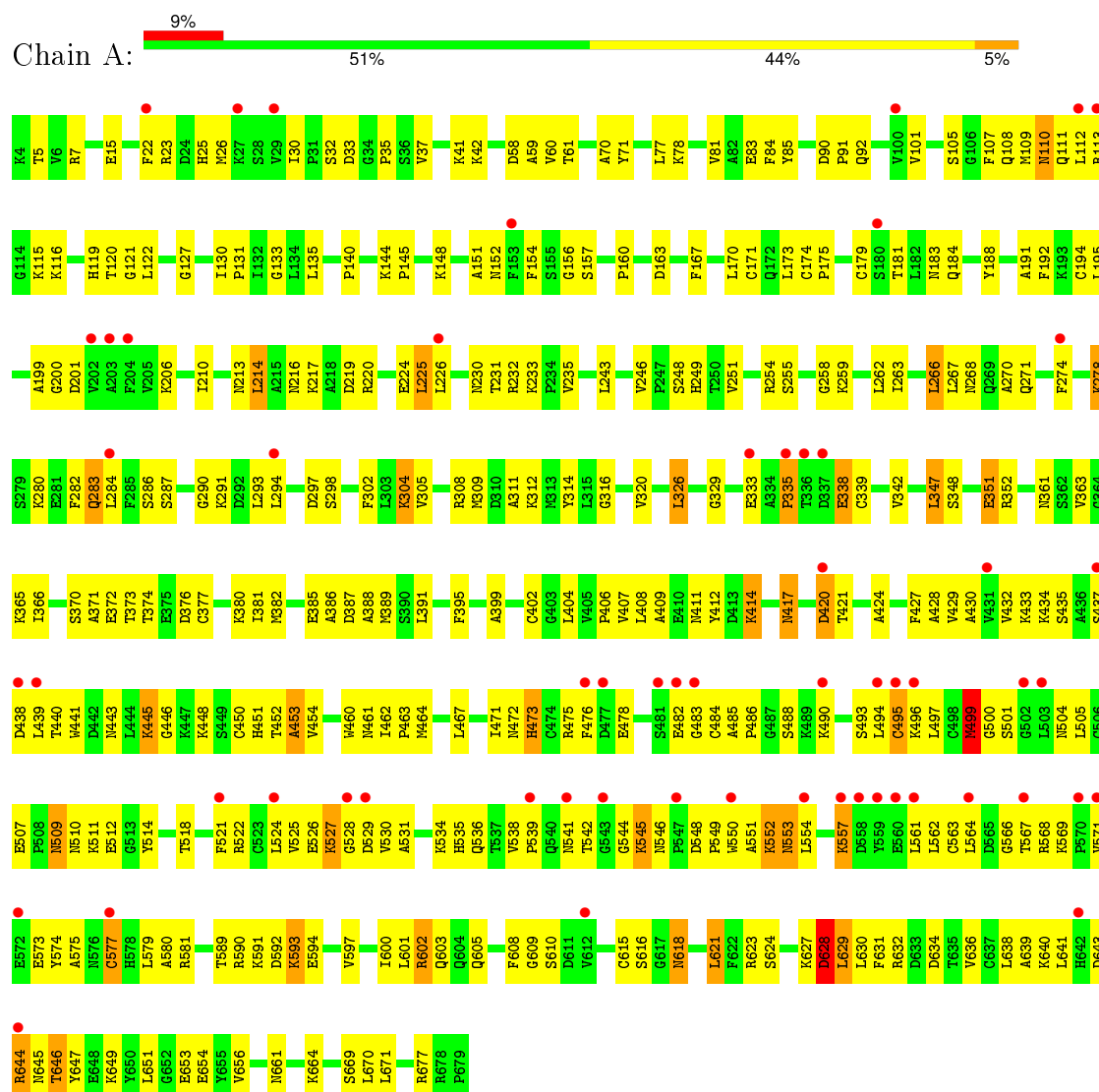


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

### 3 Residue-property plots

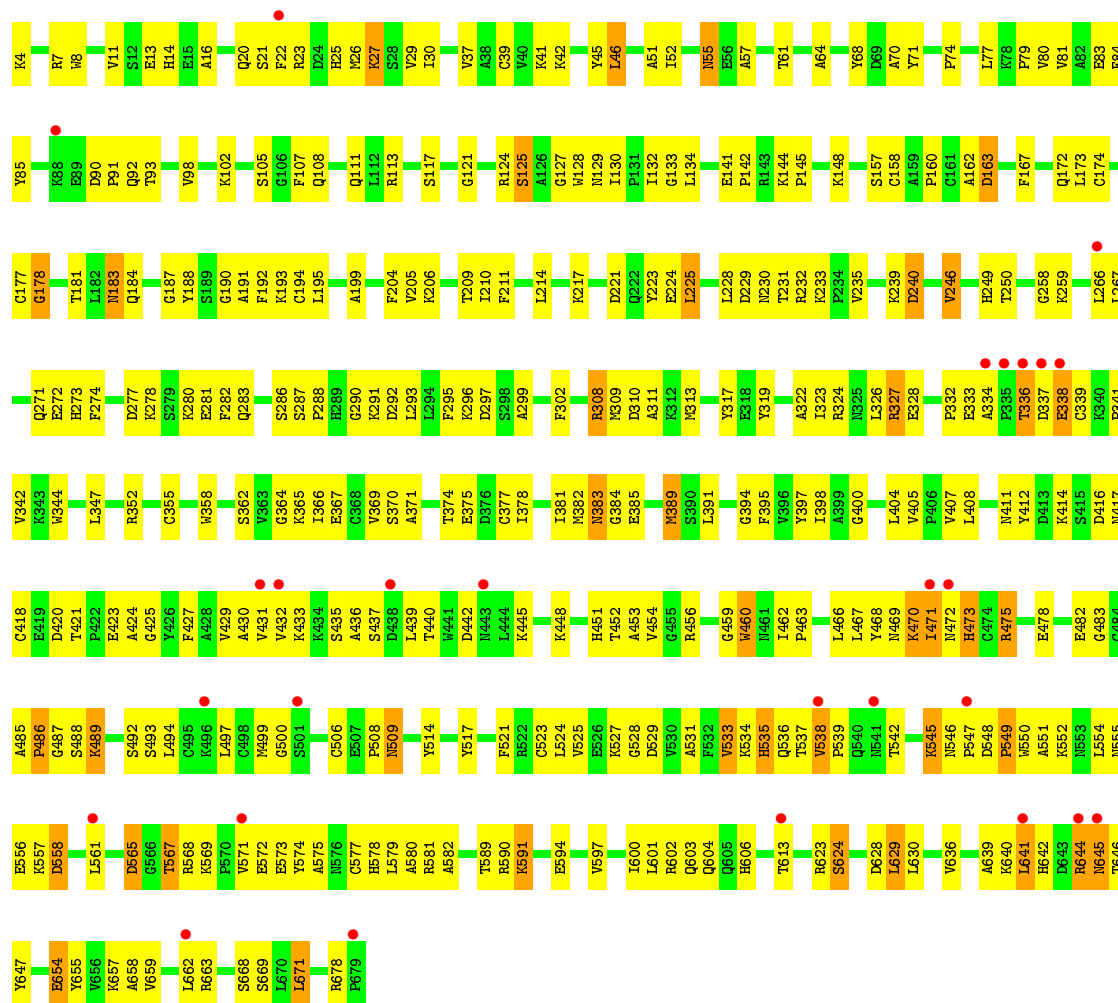
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	88.00Å 102.16Å 197.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 55.25 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 89.8 (55.25-2.57)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.273 , 0.324 0.279 , 0.313	Depositor DCC
$R_{free}$ test set	2307 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51224 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/5354	0.66	1/7220 (0.0%)
1	B	0.48	0/5354	0.65	0/7220
All	All	0.48	0/10708	0.65	1/14440 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	LEU	CA-CB-CG	5.62	128.23	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5244	0	5064	296	0
1	B	5244	0	5064	283	0
2	A	13	0	5	1	0
2	B	39	0	15	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
All	All	10552	0	10164	577	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 28.

All (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:THR:HG21	1:A:597:VAL:HG21	1.29	1.12
1:B:105:SER:HB2	1:B:232:ARG:HH22	1.19	1.04
1:B:624:SER:HB3	1:B:629:LEU:HG	1.40	1.03
1:A:602:ARG:HH11	1:A:602:ARG:HB2	1.19	1.02
1:A:538:VAL:HB	1:A:539:PRO:HD3	1.42	1.00
1:B:641:LEU:HB2	1:B:644:ARG:HB3	1.41	0.99
1:A:351:GLU:HG2	1:A:630:LEU:HD23	1.46	0.98
1:A:546:ASN:HD22	1:A:551:ALA:HB3	1.25	0.96
1:A:628:ASP:HB3	1:A:632:ARG:HA	1.52	0.89
1:A:551:ALA:HA	1:A:554:LEU:HD23	1.55	0.88
1:B:124:ARG:HH12	1:B:187:GLY:HA2	1.39	0.88
1:A:105:SER:HB2	1:A:232:ARG:HH22	1.39	0.88
1:B:383:ASN:C	1:B:383:ASN:HD22	1.75	0.87
1:A:351:GLU:HG2	1:A:630:LEU:CD2	2.04	0.87
1:B:309:MSE:HA	1:B:313:MSE:CE	2.05	0.87
1:A:15:GLU:HG2	1:A:294:LEU:CD1	2.05	0.86
1:B:668:SER:OG	1:B:671:LEU:HB2	1.73	0.86
1:A:15:GLU:HG2	1:A:294:LEU:HD13	1.58	0.85
1:A:23:ARG:HA	1:A:37:VAL:HG13	1.58	0.84
1:B:473:HIS:HB2	1:B:475:ARG:NE	1.92	0.84
1:A:420:ASP:HA	1:A:640:LYS:HE2	1.59	0.83
1:A:646:THR:OG1	1:A:649:LYS:HG2	1.79	0.83
1:B:108:GLN:H	1:B:111:GLN:HE21	1.27	0.82
1:B:538:VAL:HG13	1:B:539:PRO:HD3	1.61	0.82
1:B:27:LYS:HA	1:B:27:LYS:HE3	1.62	0.82
1:A:387:ASP:O	1:A:589:THR:HG22	1.81	0.81
1:B:29:VAL:HB	1:B:273:HIS:ND1	1.94	0.81
1:A:514:TYR:HE1	1:A:522:ARG:HG2	1.47	0.80
1:A:266:LEU:HD23	1:A:267:LEU:N	1.97	0.79
1:B:471:ILE:HB	1:B:473:HIS:CD2	2.18	0.79
1:A:464:MSE:HE3	1:A:476:PHE:HB3	1.63	0.79
1:A:308:ARG:HB2	1:A:669:SER:HB3	1.65	0.79
1:A:283:GLN:HB2	1:A:286:SER:HB3	1.64	0.79
1:B:475:ARG:N	1:B:475:ARG:HD3	1.98	0.78
1:A:484:CYS:HA	1:A:494:LEU:O	1.83	0.78
1:B:85:TYR:OH	1:B:296:LYS:HD2	1.84	0.77
1:A:602:ARG:HB2	1:A:602:ARG:NH1	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASN:ND2	1:B:385:GLU:H	1.83	0.77
1:A:70:ALA:HB1	1:A:77:LEU:HD12	1.65	0.77
1:A:434:LYS:HA	1:A:568:ARG:HH22	1.50	0.76
1:A:493:SER:HA	1:A:496:LYS:HE3	1.66	0.76
1:A:342:VAL:HG23	1:A:600:ILE:HD12	1.66	0.76
1:A:497:LEU:O	1:A:497:LEU:HD23	1.88	0.74
1:B:324:ARG:HD2	1:B:328:GLU:OE1	1.86	0.73
1:A:105:SER:HB2	1:A:232:ARG:NH2	2.04	0.73
1:B:488:SER:HB3	1:B:489:LYS:HE2	1.70	0.73
1:B:383:ASN:C	1:B:383:ASN:ND2	2.39	0.73
1:B:391:LEU:HD22	1:B:395:PHE:HB3	1.70	0.73
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.24	0.73
1:A:267:LEU:HD22	1:A:302:PHE:CE2	2.23	0.73
1:B:105:SER:HB2	1:B:232:ARG:NH2	2.01	0.72
1:A:7:ARG:NE	1:A:58:ASP:OD1	2.19	0.72
1:B:668:SER:HG	1:B:671:LEU:HB2	1.55	0.71
1:A:432:VAL:HG12	1:A:530:VAL:HA	1.72	0.71
1:A:661:ASN:HA	1:A:664:LYS:HE3	1.72	0.71
1:B:124:ARG:NH1	1:B:187:GLY:HA2	2.05	0.71
1:B:362:SER:HB2	1:B:365:LYS:HB2	1.71	0.71
1:B:466:LEU:HD22	1:B:658:ALA:HB2	1.73	0.71
1:A:427:PHE:H	1:A:535:HIS:HD2	1.39	0.71
1:A:232:ARG:O	1:A:233:LYS:HG3	1.91	0.70
1:B:654:GLU:OE1	1:B:655:TYR:N	2.23	0.70
1:A:441:TRP:CZ2	1:A:467:LEU:HD13	2.27	0.70
1:B:287:SER:HB2	1:B:290:GLY:O	1.91	0.70
1:A:451:HIS:HD2	1:A:485:ALA:HB2	1.57	0.69
1:A:475:ARG:HD3	1:A:478:GLU:OE2	1.93	0.69
1:B:489:LYS:H	1:B:489:LYS:CE	2.06	0.69
1:B:561:LEU:HD12	1:B:571:VAL:HA	1.75	0.68
1:B:489:LYS:H	1:B:489:LYS:CD	2.06	0.68
1:A:557:LYS:HE2	1:A:557:LYS:HA	1.74	0.68
1:A:188:TYR:CZ	1:A:206:LYS:HE3	2.29	0.68
1:A:163:ASP:HB2	1:B:39:CYS:O	1.92	0.68
1:B:271:GLN:HE22	1:B:302:PHE:H	1.41	0.68
1:B:64:ALA:HB2	1:B:246:VAL:HG23	1.74	0.67
1:B:557:LYS:HD3	1:B:557:LYS:O	1.94	0.67
1:B:271:GLN:NE2	1:B:302:PHE:H	1.93	0.67
1:A:483:GLY:O	1:A:494:LEU:HA	1.95	0.67
1:B:429:VAL:HB	1:B:561:LEU:HD21	1.77	0.66
1:A:23:ARG:HA	1:A:37:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LEU:CB	1:B:644:ARG:HB3	2.22	0.66
1:A:22:PHE:HD2	1:A:37:VAL:HG21	1.60	0.66
1:A:424:ALA:HB3	1:A:581:ARG:CZ	2.26	0.66
1:A:112:LEU:HD12	1:A:135:LEU:HD21	1.78	0.66
1:B:417:ASN:O	1:B:421:THR:HG22	1.95	0.66
1:B:61:THR:CG2	1:B:249:HIS:CD2	2.78	0.66
1:A:429:VAL:HG21	1:A:561:LEU:HD13	1.78	0.66
1:B:133:GLY:HA2	1:B:326:LEU:HD13	1.79	0.65
1:A:304:LYS:HG3	1:A:305:VAL:N	2.11	0.65
1:A:347:LEU:N	1:A:347:LEU:HD23	2.12	0.65
1:B:308:ARG:HB2	1:B:669:SER:HB3	1.79	0.65
1:B:535:HIS:CD2	1:B:536:GLN:HG2	2.32	0.65
1:A:440:THR:HG22	1:A:441:TRP:H	1.62	0.64
1:B:483:GLY:HA2	1:B:497:LEU:HD12	1.78	0.64
1:B:489:LYS:H	1:B:489:LYS:HE2	1.61	0.64
1:A:347:LEU:H	1:A:347:LEU:HD23	1.63	0.64
1:A:333:GLU:O	1:A:335:PRO:HD3	1.96	0.64
1:B:61:THR:HG21	1:B:249:HIS:CD2	2.32	0.64
1:B:470:LYS:O	1:B:471:ILE:HG23	1.98	0.64
1:A:521:PHE:O	1:A:525:VAL:HG23	1.97	0.64
1:B:107:PHE:HA	1:B:111:GLN:NE2	2.12	0.64
1:A:109:MSE:HE2	1:A:226:LEU:HB3	1.80	0.63
1:A:440:THR:HG22	1:A:441:TRP:N	2.13	0.63
1:A:116:LYS:HG2	1:A:173:LEU:HD11	1.80	0.63
1:B:542:THR:OG1	1:B:556:GLU:HG2	1.99	0.63
1:A:514:TYR:CE1	1:A:522:ARG:HG2	2.33	0.63
1:B:26:MSE:O	1:B:30:ILE:HG12	1.98	0.63
1:A:524:LEU:HD12	1:A:528:GLY:O	1.99	0.63
1:A:112:LEU:O	1:A:115:LYS:HB2	1.98	0.63
1:B:641:LEU:HD12	1:B:644:ARG:HB2	1.81	0.63
1:A:37:VAL:HB	1:A:266:LEU:HD11	1.81	0.62
1:B:7:ARG:HH22	1:B:55:ASN:ND2	1.96	0.62
1:A:509:ASN:N	1:A:509:ASN:HD22	1.96	0.62
1:A:538:VAL:HG11	1:A:571:VAL:HG21	1.81	0.62
1:A:216:ASN:HB2	1:A:219:ASP:OD2	2.00	0.62
1:B:240:ASP:OD1	1:B:678:ARG:NH2	2.32	0.62
1:B:467:LEU:O	1:B:471:ILE:HG12	2.00	0.62
1:B:429:VAL:HG12	1:B:578:HIS:HA	1.80	0.62
1:B:309:MSE:SE	1:B:313:MSE:HE3	2.50	0.62
1:B:473:HIS:HB2	1:B:475:ARG:CZ	2.29	0.61
1:A:179:CYS:H	1:B:20:GLN:HE22	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:OD1	1:B:231:THR:HB	2.00	0.61
1:B:408:LEU:HD23	1:B:640:LYS:HA	1.81	0.61
1:B:267:LEU:HB3	1:B:302:PHE:CD2	2.35	0.61
1:A:22:PHE:O	1:A:26:MSE:HG2	2.00	0.61
1:B:133:GLY:HA2	1:B:326:LEU:CD1	2.31	0.61
1:A:445:LYS:C	1:A:445:LYS:HD3	2.21	0.61
1:A:411:ASN:OD1	1:A:639:ALA:HB2	2.01	0.61
1:A:564:LEU:HD11	1:A:579:LEU:O	2.01	0.61
1:B:309:MSE:HA	1:B:313:MSE:HE2	1.81	0.60
1:B:375:GLU:OE1	1:B:668:SER:HB2	2.00	0.60
1:B:453:ALA:HB3	1:B:456:ARG:HG3	1.84	0.60
1:B:454:VAL:HG23	1:B:486:PRO:O	2.00	0.60
1:B:389:MSE:HE2	1:B:391:LEU:HD21	1.82	0.60
1:B:451:HIS:CD2	1:B:485:ALA:HB2	2.35	0.60
1:A:213:ASN:O	1:A:214:LEU:HD13	2.00	0.60
1:A:22:PHE:CD2	1:A:37:VAL:HG21	2.36	0.60
1:B:29:VAL:HB	1:B:273:HIS:CE1	2.36	0.60
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.83	0.60
1:B:489:LYS:N	1:B:489:LYS:HE2	2.17	0.59
1:B:358:TRP:HE1	1:B:604:GLN:CG	2.15	0.59
1:B:462:ILE:HD13	1:B:580:ALA:HB3	1.82	0.59
1:A:624:SER:HB3	1:A:629:LEU:HG	1.84	0.59
1:A:195:LEU:HD12	1:A:200:GLY:O	2.02	0.59
1:A:267:LEU:HD22	1:A:302:PHE:CZ	2.37	0.59
1:A:451:HIS:CD2	1:A:485:ALA:HB2	2.38	0.59
1:A:488:SER:HB2	1:A:495:CYS:SG	2.43	0.59
1:A:409:ALA:HB2	1:A:641:LEU:HD21	1.84	0.59
1:B:210:ILE:HD13	1:B:235:VAL:HG11	1.85	0.59
1:B:124:ARG:HG2	2:B:9206:CIT:H22	1.84	0.59
1:B:224:GLU:OE2	1:B:232:ARG:HD2	2.03	0.58
1:B:430:ALA:HB2	1:B:579:LEU:HD11	1.85	0.58
1:B:148:LYS:HB2	1:B:167:PHE:CE1	2.39	0.58
1:B:521:PHE:O	1:B:525:VAL:HG23	2.04	0.58
1:B:427:PHE:HB2	1:B:535:HIS:HB3	1.86	0.58
1:B:334:ALA:O	1:B:338:GLU:HB3	2.04	0.58
1:A:151:ALA:HB2	1:A:170:LEU:HD21	1.86	0.57
1:A:83:GLU:OE2	1:A:249:HIS:HD2	1.87	0.57
1:A:78:LYS:HG2	1:A:255:SER:HA	1.85	0.57
1:A:504:ASN:HA	1:A:507:GLU:HG3	1.85	0.57
1:B:424:ALA:HB3	1:B:581:ARG:CZ	2.35	0.57
1:B:425:GLY:HA3	1:B:582:ALA:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ARG:NH2	1:B:640:LYS:HE2	2.20	0.57
1:A:25:HIS:CD2	1:A:282:PHE:HB2	2.39	0.57
1:A:231:THR:HG22	1:A:232:ARG:N	2.20	0.56
1:A:592:ASP:C	1:A:594:GLU:H	2.08	0.56
1:B:192:PHE:O	1:B:195:LEU:N	2.33	0.56
1:B:641:LEU:HD12	1:B:644:ARG:CB	2.35	0.56
1:B:16:ALA:O	1:B:20:GLN:HG3	2.05	0.56
1:B:157:SER:HA	1:B:173:LEU:HD22	1.87	0.56
1:B:286:SER:O	1:B:288:PRO:HD3	2.06	0.56
1:A:453:ALA:HA	1:A:486:PRO:HG2	1.86	0.56
1:A:452:THR:O	1:A:453:ALA:HB2	2.05	0.56
1:A:440:THR:HG23	1:A:566:GLY:O	2.06	0.56
1:A:445:LYS:HD3	1:A:446:GLY:N	2.21	0.56
1:B:117:SER:O	1:B:157:SER:HB2	2.06	0.56
1:B:405:VAL:HG11	1:B:591:LYS:HD3	1.86	0.56
1:A:26:MSE:O	1:A:30:ILE:HB	2.06	0.56
1:B:391:LEU:HD22	1:B:395:PHE:CB	2.36	0.56
1:B:158:CYS:O	1:B:160:PRO:HD3	2.06	0.56
1:A:122:LEU:C	1:A:122:LEU:HD23	2.25	0.56
1:A:550:TRP:CZ3	1:A:551:ALA:HB2	2.41	0.56
1:B:514:TYR:CG	1:B:523:CYS:HB2	2.41	0.56
1:A:81:VAL:HG11	1:A:267:LEU:HD13	1.87	0.55
1:A:372:GLU:HG2	1:A:373:THR:HG23	1.88	0.55
1:A:471:ILE:HG22	1:A:473:HIS:O	2.06	0.55
1:B:514:TYR:CD2	1:B:523:CYS:HB2	2.42	0.55
1:B:27:LYS:HA	1:B:27:LYS:CE	2.36	0.55
1:A:568:ARG:O	1:A:569:LYS:HG3	2.07	0.55
1:B:640:LYS:HB2	1:B:644:ARG:HH12	1.71	0.55
1:A:605:GLN:OE1	1:A:638:LEU:N	2.36	0.55
1:A:81:VAL:HG21	1:A:267:LEU:HD12	1.88	0.55
1:A:546:ASN:ND2	1:A:548:ASP:HB2	2.21	0.54
1:A:110:ASN:HD22	1:A:110:ASN:N	2.05	0.54
1:B:471:ILE:HB	1:B:473:HIS:NE2	2.22	0.54
1:A:119:HIS:HB3	1:A:127:GLY:O	2.07	0.54
1:B:27:LYS:NZ	1:B:30:ILE:HD11	2.21	0.54
1:A:450:CYS:HB2	1:A:531:ALA:HA	1.89	0.54
1:B:291:LYS:HD2	1:B:297:ASP:OD2	2.06	0.54
1:A:152:ASN:HD22	1:A:152:ASN:N	2.06	0.54
1:B:80:VAL:HG23	1:B:81:VAL:HG23	1.90	0.54
1:B:23:ARG:HG3	1:B:37:VAL:O	2.08	0.54
1:B:141:GLU:HA	1:B:142:PRO:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ALA:O	1:B:581:ARG:HG2	2.08	0.54
1:B:641:LEU:N	1:B:641:LEU:HD23	2.22	0.54
1:A:108:GLN:HB2	1:A:110:ASN:ND2	2.23	0.54
1:B:342:VAL:HB	1:B:366:ILE:HD13	1.90	0.54
1:B:383:ASN:HD22	1:B:384:GLY:N	2.06	0.54
1:B:418:CYS:HA	1:B:421:THR:CG2	2.38	0.54
1:B:68:TYR:CD2	1:B:323:ILE:HD13	2.43	0.54
1:A:105:SER:HB3	1:A:107:PHE:CE1	2.43	0.54
1:A:490:LYS:HE3	1:A:507:GLU:OE2	2.07	0.54
1:B:448:LYS:HB3	1:B:528:GLY:HA2	1.88	0.54
1:B:462:ILE:O	1:B:466:LEU:HD23	2.08	0.53
1:A:437:SER:HA	1:A:568:ARG:NH1	2.23	0.53
1:B:556:GLU:HB3	1:B:572:GLU:OE2	2.07	0.53
1:A:538:VAL:HB	1:A:539:PRO:CD	2.27	0.53
1:A:347:LEU:HD23	1:A:351:GLU:OE2	2.09	0.53
1:B:550:TRP:O	1:B:554:LEU:HD11	2.08	0.53
1:B:440:THR:HG22	1:B:568:ARG:HD2	1.89	0.53
1:A:471:ILE:O	1:A:473:HIS:N	2.42	0.53
1:A:280:LYS:NZ	1:A:280:LYS:HB3	2.24	0.53
1:B:640:LYS:C	1:B:641:LEU:HD23	2.29	0.53
1:B:555:ASN:O	1:B:558:ASP:HB2	2.08	0.53
1:A:154:PHE:O	1:A:156:GLY:N	2.41	0.53
1:B:411:ASN:ND2	1:B:639:ALA:HB2	2.24	0.53
1:B:658:ALA:O	1:B:659:VAL:HB	2.09	0.53
1:A:427:PHE:H	1:A:535:HIS:CD2	2.23	0.53
1:A:509:ASN:HD22	1:A:509:ASN:H	1.57	0.53
1:B:333:GLU:HG2	1:B:334:ALA:N	2.24	0.52
1:B:437:SER:HA	1:B:568:ARG:NH1	2.23	0.52
1:B:468:TYR:C	1:B:470:LYS:H	2.13	0.52
1:B:475:ARG:HG3	1:B:478:GLU:OE2	2.09	0.52
1:B:378:ILE:HG23	1:B:404:LEU:HD22	1.91	0.52
1:B:8:TRP:HH2	1:B:267:LEU:HD11	1.74	0.52
1:B:283:GLN:HB2	1:B:286:SER:HB3	1.91	0.52
1:B:551:ALA:HA	1:B:554:LEU:CD1	2.39	0.52
1:B:91:PRO:O	1:B:92:GLN:HB2	2.10	0.52
1:A:534:LYS:CE	1:A:536:GLN:HE21	2.23	0.52
1:A:542:THR:O	1:A:545:LYS:HE3	2.10	0.52
1:B:191:ALA:O	1:B:194:CYS:HB3	2.10	0.52
1:A:181:THR:C	1:A:183:ASN:N	2.63	0.52
1:B:108:GLN:N	1:B:111:GLN:HE21	2.02	0.52
1:A:151:ALA:HB2	1:A:170:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:VAL:O	1:B:601:LEU:HB2	2.10	0.52
1:B:466:LEU:CD2	1:B:658:ALA:HB2	2.39	0.52
1:B:249:HIS:ND1	1:B:296:LYS:HE2	2.25	0.52
1:B:524:LEU:HB2	1:B:531:ALA:HB2	1.92	0.52
1:B:188:TYR:OH	1:B:206:LYS:HG3	2.10	0.52
1:B:473:HIS:HB2	1:B:475:ARG:HE	1.72	0.52
1:A:380:LYS:HG2	1:A:385:GLU:HB2	1.92	0.52
1:B:22:PHE:O	1:B:26:MSE:HG2	2.09	0.51
1:B:407:VAL:HG21	1:B:597:VAL:HG11	1.93	0.51
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.76	0.51
1:A:41:LYS:HG2	1:A:42:LYS:N	2.24	0.51
1:B:102:LYS:O	1:B:105:SER:OG	2.28	0.51
1:B:535:HIS:CD2	1:B:536:GLN:H	2.28	0.51
1:B:309:MSE:HA	1:B:313:MSE:HE3	1.87	0.51
1:B:117:SER:OG	1:B:157:SER:CB	2.59	0.51
1:A:592:ASP:O	1:A:594:GLU:N	2.44	0.51
1:A:192:PHE:CZ	1:A:210:ILE:HG13	2.46	0.51
1:A:148:LYS:O	1:A:151:ALA:HB3	2.10	0.51
1:A:225:LEU:HD13	1:A:235:VAL:HG12	1.93	0.51
1:A:108:GLN:HA	1:A:226:LEU:HD21	1.93	0.50
1:B:61:THR:HG22	1:B:249:HIS:CD2	2.45	0.50
1:B:323:ILE:HG12	1:B:327:ARG:HD3	1.94	0.50
1:A:267:LEU:HB3	1:A:302:PHE:CD2	2.46	0.50
1:B:188:TYR:HB3	1:B:209:THR:HG23	1.94	0.50
1:A:225:LEU:HD22	1:A:235:VAL:HA	1.93	0.50
1:A:352:ARG:HD3	1:A:370:SER:OG	2.11	0.50
1:B:565:ASP:OD2	1:B:567:THR:HG23	2.11	0.50
1:B:283:GLN:N	1:B:283:GLN:OE1	2.45	0.50
1:B:70:ALA:HB1	1:B:77:LEU:HD12	1.94	0.50
1:A:441:TRP:CE2	1:A:467:LEU:HD13	2.47	0.49
1:B:509:ASN:HD22	1:B:509:ASN:N	2.11	0.49
1:B:129:ASN:O	1:B:133:GLY:N	2.45	0.49
1:B:534:LYS:HE3	1:B:536:GLN:HG3	1.94	0.49
1:B:551:ALA:HA	1:B:554:LEU:HD12	1.94	0.49
1:B:482:GLU:HA	1:B:493:SER:HB2	1.94	0.49
1:A:109:MSE:H	1:A:226:LEU:HD22	1.77	0.49
1:A:534:LYS:HE3	1:A:536:GLN:HE21	1.78	0.49
1:B:439:LEU:HD21	1:B:529:ASP:HB3	1.95	0.49
1:A:550:TRP:CE3	1:A:551:ALA:HB2	2.48	0.49
1:B:668:SER:HG	1:B:671:LEU:CB	2.24	0.49
1:B:117:SER:OG	1:B:157:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:O	1:A:263:ILE:HG13	2.11	0.49
1:B:641:LEU:H	1:B:644:ARG:NH1	2.11	0.49
1:A:109:MSE:CE	1:A:226:LEU:HB3	2.41	0.49
1:B:468:TYR:O	1:B:470:LYS:N	2.46	0.49
1:B:8:TRP:CZ3	1:B:267:LEU:HD21	2.47	0.49
1:A:387:ASP:OD1	1:A:593:LYS:HE2	2.13	0.49
1:B:535:HIS:CD2	1:B:536:GLN:N	2.80	0.49
1:A:37:VAL:HB	1:A:266:LEU:CD1	2.42	0.49
1:B:121:GLY:HA2	1:B:160:PRO:HB2	1.95	0.49
1:A:590:ARG:O	1:A:592:ASP:O	2.30	0.48
1:A:451:HIS:O	1:A:486:PRO:HD2	2.13	0.48
1:B:499:MSE:HG3	1:B:500:GLY:N	2.28	0.48
1:B:383:ASN:HD21	1:B:385:GLU:HB2	1.77	0.48
1:A:15:GLU:HG2	1:A:294:LEU:HD12	1.92	0.48
1:B:451:HIS:HD2	1:B:485:ALA:HB2	1.77	0.48
1:B:352:ARG:HD3	1:B:370:SER:OG	2.13	0.48
1:A:365:LYS:HE2	1:A:603:GLN:NE2	2.28	0.48
1:A:108:GLN:H	1:A:111:GLN:HG3	1.78	0.48
1:B:431:VAL:HG13	1:B:524:LEU:HD22	1.95	0.48
1:A:562:LEU:HD23	1:A:563:CYS:N	2.28	0.48
1:A:589:THR:CG2	1:A:597:VAL:HG21	2.21	0.48
1:B:70:ALA:HB1	1:B:77:LEU:HB2	1.95	0.48
1:A:552:LYS:HG2	1:A:553:ASN:CG	2.34	0.48
1:B:214:LEU:HD11	1:B:223:TYR:HE2	1.79	0.48
1:A:483:GLY:N	1:A:497:LEU:HD13	2.28	0.48
1:A:120:THR:OG1	1:A:127:GLY:HA3	2.13	0.48
1:A:157:SER:N	1:A:173:LEU:HD13	2.29	0.48
1:A:268:ASN:C	1:A:270:ALA:H	2.16	0.48
1:B:341:PRO:HB3	1:B:364:GLY:O	2.14	0.48
1:A:347:LEU:CD2	1:A:351:GLU:OE2	2.62	0.48
1:A:157:SER:CA	1:A:173:LEU:HD13	2.44	0.48
1:B:358:TRP:HE1	1:B:604:GLN:HG2	1.78	0.48
1:A:291:LYS:HG3	1:A:297:ASP:OD1	2.14	0.48
1:A:283:GLN:CB	1:A:286:SER:HB3	2.39	0.47
1:B:421:THR:O	1:B:421:THR:HG23	2.15	0.47
1:A:201:ASP:N	1:A:201:ASP:OD2	2.47	0.47
1:A:417:ASN:O	1:A:421:THR:HG22	2.13	0.47
1:A:429:VAL:HG22	1:A:430:ALA:N	2.29	0.47
1:A:605:GLN:O	1:A:609:GLY:HA3	2.14	0.47
1:A:59:ALA:HB2	1:A:263:ILE:HD13	1.96	0.47
1:B:272:GLU:O	1:B:278:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:HA	1:A:145:PRO:C	2.34	0.47
1:A:259:LYS:HE2	1:A:262:LEU:HD23	1.95	0.47
1:B:174:CYS:HB2	1:B:183:ASN:HD21	1.79	0.47
1:A:90:ASP:OD2	1:A:92:GLN:HG3	2.14	0.47
1:A:120:THR:HG21	1:A:188:TYR:CD1	2.50	0.47
1:A:112:LEU:HD12	1:A:135:LEU:CD2	2.44	0.47
1:A:471:ILE:O	1:A:473:HIS:ND1	2.47	0.47
1:A:388:ALA:O	1:A:389:MSE:HB3	2.14	0.47
1:B:228:LEU:C	1:B:230:ASN:H	2.17	0.47
1:A:433:LYS:C	1:A:435:SER:H	2.17	0.47
1:B:117:SER:O	1:B:157:SER:CB	2.62	0.47
1:B:533:VAL:HB	1:B:537:THR:OG1	2.15	0.47
1:B:383:ASN:HD21	1:B:385:GLU:H	1.60	0.47
1:A:84:PHE:HB2	1:A:91:PRO:O	2.15	0.47
1:B:569:LYS:HD3	1:B:577:CYS:SG	2.55	0.47
1:A:23:ARG:HB2	1:A:37:VAL:O	2.15	0.47
1:A:460:TRP:O	1:A:463:PRO:HG2	2.14	0.47
1:A:462:ILE:HD13	1:A:580:ALA:HB3	1.97	0.47
1:A:414:LYS:C	1:A:414:LYS:HD2	2.35	0.47
1:B:548:ASP:HB3	1:B:549:PRO:HD2	1.96	0.47
1:A:133:GLY:HA2	1:A:326:LEU:HD13	1.97	0.47
1:B:468:TYR:C	1:B:470:LYS:N	2.68	0.47
1:B:267:LEU:O	1:B:302:PHE:HD2	1.98	0.47
1:B:342:VAL:HG23	1:B:600:ILE:HD12	1.96	0.47
1:A:414:LYS:HD2	1:A:414:LYS:O	2.15	0.47
1:A:632:ARG:NH2	2:A:9202:CIT:H42	2.30	0.47
1:B:130:ILE:HD11	1:B:319:TYR:HE1	1.80	0.47
1:B:407:VAL:HG12	1:B:594:GLU:HG3	1.97	0.47
1:A:460:TRP:HD1	1:A:461:ASN:HD22	1.63	0.47
1:B:398:ILE:HG12	1:B:671:LEU:HG	1.96	0.46
1:B:144:LYS:HA	1:B:145:PRO:C	2.36	0.46
1:A:518:THR:HG22	1:A:541:ASN:OD1	2.15	0.46
1:A:382:MSE:SE	1:A:402:CYS:HB3	2.65	0.46
1:A:108:GLN:HB2	1:A:110:ASN:HD21	1.79	0.46
1:A:361:ASN:O	1:A:608:PHE:CZ	2.69	0.46
1:A:643:ASP:O	1:A:645:ASN:N	2.43	0.46
1:B:545:LYS:O	1:B:547:PRO:HD3	2.15	0.46
1:A:602:ARG:HH11	1:A:602:ARG:CB	2.09	0.46
1:A:497:LEU:HD21	1:A:527:LYS:HB2	1.97	0.46
1:A:287:SER:HB2	1:A:290:GLY:O	2.16	0.46
1:A:439:LEU:HA	1:A:443:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ASP:C	1:A:594:GLU:N	2.69	0.46
1:A:605:GLN:CD	1:A:638:LEU:H	2.19	0.46
1:B:378:ILE:O	1:B:382:MSE:HG2	2.16	0.46
1:A:121:GLY:HA2	1:A:160:PRO:HD2	1.97	0.46
1:A:499:MSE:O	1:A:505:LEU:HD12	2.16	0.46
1:B:22:PHE:HA	1:B:282:PHE:CE2	2.51	0.46
1:A:574:TYR:CD1	1:A:575:ALA:N	2.83	0.46
1:B:489:LYS:H	1:B:489:LYS:HD3	1.81	0.46
1:A:538:VAL:HB	1:A:571:VAL:HG11	1.97	0.45
1:B:184:GLN:O	1:B:190:GLY:HA2	2.16	0.45
1:B:342:VAL:HB	1:B:366:ILE:CD1	2.45	0.45
1:A:562:LEU:HD23	1:A:563:CYS:O	2.16	0.45
1:A:290:GLY:C	1:A:291:LYS:HD2	2.36	0.45
1:A:171:CYS:O	1:A:174:CYS:C	2.55	0.45
1:A:109:MSE:N	1:A:226:LEU:HD22	2.31	0.45
1:B:192:PHE:CZ	1:B:210:ILE:HG13	2.50	0.45
1:A:363:VAL:O	1:A:363:VAL:HG12	2.17	0.45
1:A:217:LYS:HA	1:A:220:ARG:HD2	1.98	0.45
1:B:641:LEU:O	1:B:642:HIS:C	2.54	0.45
1:A:283:GLN:OE1	1:A:283:GLN:N	2.49	0.45
1:B:418:CYS:HA	1:B:421:THR:HG22	1.97	0.45
1:B:98:VAL:HB	1:B:225:LEU:HG	1.98	0.45
1:B:394:GLY:O	1:B:397:TYR:HB3	2.17	0.45
1:B:344:TRP:CE2	1:B:389:MSE:HA	2.52	0.45
1:A:120:THR:HG22	1:A:188:TYR:HA	1.98	0.45
1:B:173:LEU:HG	1:B:199:ALA:HB1	1.98	0.45
1:A:448:LYS:O	1:A:529:ASP:HB2	2.16	0.45
1:A:374:THR:HG21	1:A:395:PHE:CD2	2.51	0.45
1:B:4:LYS:HB3	1:B:4:LYS:NZ	2.32	0.45
1:B:452:THR:HG22	1:B:517:TYR:HA	1.98	0.45
1:B:64:ALA:HB2	1:B:246:VAL:CG2	2.46	0.45
1:A:192:PHE:CD1	1:A:213:ASN:HB2	2.52	0.45
1:A:60:VAL:HG22	1:A:61:THR:H	1.82	0.45
1:A:407:VAL:HG23	1:A:408:LEU:N	2.31	0.45
1:B:645:ASN:HD22	1:B:645:ASN:HA	1.66	0.45
1:B:27:LYS:HZ2	1:B:30:ILE:HD11	1.82	0.45
1:A:632:ARG:HB3	1:A:634:ASP:OD2	2.16	0.44
1:B:600:ILE:O	1:B:603:GLN:HG2	2.17	0.44
1:B:52:ILE:HA	1:B:57:ALA:O	2.17	0.44
1:B:589:THR:HG21	1:B:597:VAL:HG21	1.99	0.44
1:B:475:ARG:N	1:B:475:ARG:CD	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:HIS:HB2	1:A:574:TYR:CD2	2.51	0.44
1:B:451:HIS:HB3	1:B:459:GLY:O	2.17	0.44
1:A:417:ASN:OD1	1:A:417:ASN:N	2.50	0.44
1:B:487:GLY:HA2	1:B:508:PRO:HD3	1.99	0.44
1:A:338:GLU:O	1:A:339:CYS:HB2	2.16	0.44
1:B:336:THR:HB	1:B:337:ASP:H	1.44	0.44
1:A:191:ALA:O	1:A:194:CYS:HB3	2.17	0.44
1:B:534:LYS:HE3	1:B:536:GLN:CG	2.48	0.44
1:A:60:VAL:HG22	1:A:61:THR:N	2.31	0.44
1:B:432:VAL:HG22	1:B:433:LYS:N	2.32	0.44
1:A:81:VAL:HB	1:A:251:VAL:HB	1.98	0.44
1:A:192:PHE:HD1	1:A:213:ASN:HB2	1.83	0.44
1:B:591:LYS:HB2	1:B:591:LYS:HE2	1.79	0.44
1:A:181:THR:C	1:A:183:ASN:H	2.19	0.44
1:B:42:LYS:HE3	1:B:51:ALA:HB2	1.98	0.44
1:A:615:CYS:O	1:A:616:SER:HB2	2.18	0.44
1:A:112:LEU:O	1:A:113:ARG:C	2.55	0.44
1:B:405:VAL:CG1	1:B:591:LYS:HD3	2.47	0.44
1:A:552:LYS:HD3	1:A:553:ASN:H	1.82	0.44
1:A:671:LEU:O	1:A:671:LEU:HD22	2.17	0.44
1:B:26:MSE:HE2	1:B:266:LEU:HD12	1.98	0.44
1:A:429:VAL:HG23	1:A:577:CYS:O	2.17	0.44
1:A:406:PRO:O	1:A:641:LEU:HD12	2.18	0.44
1:B:327:ARG:HH11	1:B:327:ARG:HG2	1.81	0.44
1:B:71:TYR:HB2	1:B:311:ALA:CB	2.48	0.44
1:A:634:ASP:N	1:A:634:ASP:OD2	2.49	0.44
1:A:509:ASN:N	1:A:509:ASN:ND2	2.64	0.44
1:B:499:MSE:HG3	1:B:500:GLY:H	1.83	0.44
1:A:602:ARG:NH1	1:A:602:ARG:CB	2.77	0.44
1:A:482:GLU:HA	1:A:493:SER:OG	2.17	0.44
1:A:140:PRO:HG3	1:A:152:ASN:HB2	2.00	0.44
1:A:101:VAL:HG22	1:A:224:GLU:O	2.17	0.44
1:A:539:PRO:HD3	1:A:571:VAL:HG11	2.00	0.43
1:B:85:TYR:CD1	1:B:85:TYR:N	2.85	0.43
1:B:389:MSE:HE2	1:B:391:LEU:CD2	2.47	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD12	1.79	0.43
1:B:91:PRO:HG2	1:B:92:GLN:H	1.82	0.43
1:B:177:CYS:O	1:B:178:GLY:C	2.56	0.43
1:A:268:ASN:O	1:A:271:GLN:HG2	2.19	0.43
1:A:194:CYS:O	1:A:199:ALA:HB3	2.18	0.43
1:A:309:MSE:HE1	1:A:677:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HG	1:B:322:ALA:HB2	1.99	0.43
1:A:351:GLU:HG2	1:A:630:LEU:HD21	1.93	0.43
1:A:110:ASN:HD22	1:A:110:ASN:H	1.64	0.43
1:A:110:ASN:HB3	1:A:230:ASN:OD1	2.18	0.43
1:B:29:VAL:CB	1:B:273:HIS:ND1	2.76	0.43
1:A:365:LYS:HE2	1:A:603:GLN:HE22	1.84	0.43
1:B:371:ALA:HB3	1:B:377:CYS:SG	2.58	0.43
1:A:316:GLY:O	1:A:320:VAL:HG23	2.17	0.43
1:A:308:ARG:HB2	1:A:669:SER:CB	2.43	0.43
1:B:258:GLY:O	1:B:259:LYS:HB2	2.18	0.43
1:A:23:ARG:CA	1:A:37:VAL:HG13	2.39	0.43
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.88	0.43
1:B:462:ILE:N	1:B:463:PRO:HD2	2.34	0.43
1:B:79:PRO:HB3	1:B:250:THR:HG21	1.99	0.43
1:B:127:GLY:HA2	1:B:204:PHE:O	2.19	0.43
1:A:510:ASN:C	1:A:512:GLU:H	2.21	0.43
1:A:592:ASP:O	1:A:593:LYS:HB2	2.19	0.43
1:A:440:THR:CG2	1:A:441:TRP:N	2.81	0.43
1:A:381:ILE:O	1:A:381:ILE:HG22	2.19	0.43
1:B:163:ASP:OD2	1:B:163:ASP:C	2.56	0.43
1:B:400:GLY:HA3	1:B:647:TYR:CD2	2.54	0.43
1:B:407:VAL:O	1:B:408:LEU:HG	2.18	0.43
1:B:355:CYS:HA	1:B:630:LEU:HD11	2.00	0.43
1:A:85:TYR:HD1	1:A:298:SER:O	2.01	0.43
1:B:471:ILE:C	1:B:473:HIS:H	2.21	0.43
1:A:113:ARG:HG2	1:A:113:ARG:NH1	2.33	0.43
1:A:274:PHE:HB3	1:A:282:PHE:O	2.18	0.43
1:A:544:GLY:HA2	1:A:553:ASN:HA	2.01	0.43
1:A:591:LYS:HD2	1:A:591:LYS:O	2.18	0.43
1:B:640:LYS:CB	1:B:644:ARG:HH12	2.32	0.43
1:A:15:GLU:HA	1:A:293:LEU:HD23	2.00	0.43
1:A:647:TYR:O	1:A:651:LEU:HG	2.18	0.43
1:B:535:HIS:HB2	1:B:574:TYR:CD2	2.54	0.43
1:A:152:ASN:ND2	1:A:152:ASN:N	2.66	0.43
1:B:11:VAL:HG11	1:B:45:TYR:CD1	2.53	0.43
1:B:84:PHE:C	1:B:85:TYR:CD1	2.92	0.42
1:B:225:LEU:HD13	1:B:235:VAL:HG12	2.00	0.42
1:A:618:ASN:HA	1:A:618:ASN:HD22	1.58	0.42
1:A:107:PHE:CE2	1:A:226:LEU:HD11	2.53	0.42
1:B:111:GLN:C	1:B:113:ARG:H	2.22	0.42
1:B:535:HIS:HB2	1:B:574:TYR:CG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:HA	1:A:235:VAL:HG13	2.00	0.42
1:B:172:GLN:HG2	1:B:172:GLN:O	2.20	0.42
1:A:266:LEU:HD23	1:A:267:LEU:CA	2.48	0.42
1:A:490:LYS:HA	1:A:495:CYS:SG	2.60	0.42
1:B:663:ARG:HD3	1:B:663:ARG:HA	1.79	0.42
1:B:27:LYS:CA	1:B:27:LYS:HE3	2.43	0.42
1:B:489:LYS:HG2	1:B:492:SER:HB2	2.00	0.42
1:A:91:PRO:O	1:A:92:GLN:HB2	2.20	0.42
1:A:243:LEU:HD12	1:A:243:LEU:N	2.35	0.42
1:B:108:GLN:HA	1:B:108:GLN:HE21	1.84	0.42
1:B:483:GLY:HA2	1:B:497:LEU:CD1	2.48	0.42
1:A:653:GLU:O	1:A:656:VAL:HG22	2.20	0.42
1:B:546:ASN:ND2	1:B:548:ASP:HB2	2.34	0.42
1:A:35:PRO:HB2	1:A:266:LEU:HB2	2.02	0.42
1:B:341:PRO:HB3	1:B:367:GLU:HG3	2.02	0.42
1:A:462:ILE:CG2	1:A:580:ALA:HB3	2.50	0.42
1:A:610:SER:HB2	1:A:636:VAL:O	2.20	0.42
1:A:254:ARG:HB2	1:A:258:GLY:HA2	2.01	0.42
1:B:641:LEU:HG	1:B:644:ARG:HD3	2.02	0.42
1:A:110:ASN:ND2	1:A:111:GLN:HG2	2.35	0.42
1:B:383:ASN:ND2	1:B:385:GLU:N	2.62	0.42
1:A:651:LEU:HD12	1:A:656:VAL:HG12	2.02	0.42
1:A:391:LEU:HD13	1:A:395:PHE:HB3	2.02	0.42
1:B:412:TYR:HA	1:B:636:VAL:HG23	2.01	0.42
1:B:344:TRP:O	1:B:369:VAL:HG12	2.20	0.42
1:B:485:ALA:HB3	1:B:494:LEU:HB3	2.01	0.42
1:A:371:ALA:HB3	1:A:377:CYS:SG	2.60	0.42
1:A:499:MSE:HB2	1:A:500:GLY:H	1.56	0.42
1:A:412:TYR:CE1	1:A:632:ARG:NH1	2.88	0.41
1:B:148:LYS:HB2	1:B:167:PHE:HE1	1.85	0.41
1:B:214:LEU:HD11	1:B:223:TYR:CE2	2.54	0.41
1:A:391:LEU:HB3	1:A:395:PHE:HB2	2.02	0.41
1:A:646:THR:O	1:A:647:TYR:C	2.59	0.41
1:A:483:GLY:CA	1:A:497:LEU:HD13	2.50	0.41
1:B:499:MSE:CG	1:B:500:GLY:H	2.33	0.41
1:A:309:MSE:SE	1:A:314:TYR:HD1	2.53	0.41
1:A:71:TYR:HB2	1:A:311:ALA:CB	2.50	0.41
1:B:14:HIS:HB3	1:B:293:LEU:HD21	2.02	0.41
1:A:381:ILE:HA	1:A:386:ALA:O	2.20	0.41
1:B:644:ARG:O	1:B:645:ASN:C	2.59	0.41
1:A:627:LYS:O	1:A:628:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:C	1:A:233:LYS:HG3	2.41	0.41
1:A:22:PHE:CE1	1:A:284:LEU:HD13	2.56	0.41
1:B:111:GLN:C	1:B:113:ARG:N	2.74	0.41
1:A:25:HIS:NE2	1:A:282:PHE:HB2	2.35	0.41
1:B:569:LYS:HB3	1:B:573:GLU:OE1	2.20	0.41
1:A:342:VAL:HG23	1:A:600:ILE:CD1	2.42	0.41
1:B:308:ARG:HD2	1:B:308:ARG:HA	1.75	0.41
1:B:192:PHE:O	1:B:195:LEU:HB3	2.21	0.41
1:A:171:CYS:O	1:A:175:PRO:N	2.53	0.41
1:A:254:ARG:HB2	1:A:258:GLY:CA	2.50	0.41
1:B:542:THR:HB	1:B:555:ASN:C	2.41	0.41
1:A:534:LYS:NZ	1:A:536:GLN:HE21	2.19	0.41
1:B:83:GLU:OE1	1:B:299:ALA:HB2	2.20	0.41
1:A:428:ALA:O	1:A:579:LEU:HB2	2.20	0.41
1:A:552:LYS:HG2	1:A:553:ASN:N	2.36	0.41
1:B:574:TYR:CD1	1:B:575:ALA:N	2.89	0.41
1:B:188:TYR:HD1	1:B:205:VAL:HB	1.86	0.41
1:A:374:THR:HG21	1:A:395:PHE:CG	2.55	0.41
1:A:524:LEU:C	1:A:526:GLU:H	2.22	0.41
1:A:524:LEU:HB2	1:A:531:ALA:HB2	2.02	0.41
1:A:342:VAL:HB	1:A:366:ILE:HD13	2.02	0.41
1:A:216:ASN:HB2	1:A:219:ASP:CG	2.40	0.41
1:B:456:ARG:O	1:B:460:TRP:HB3	2.21	0.41
1:A:248:SER:O	1:A:249:HIS:HB2	2.21	0.41
1:B:603:GLN:O	1:B:606:HIS:HB2	2.20	0.41
1:B:381:ILE:HB	1:B:404:LEU:HD21	2.02	0.41
1:A:399:ALA:HB1	1:A:404:LEU:HD12	2.02	0.41
1:A:621:LEU:HD21	1:A:631:PHE:HE2	1.86	0.41
1:B:217:LYS:HD3	1:B:221:ASP:OD2	2.20	0.41
1:A:514:TYR:OH	1:A:526:GLU:OE1	2.33	0.41
1:B:210:ILE:HG23	1:B:211:PHE:N	2.36	0.41
1:A:83:GLU:CD	1:A:249:HIS:HD2	2.24	0.41
1:A:377:CYS:HB3	1:A:389:MSE:SE	2.71	0.41
1:A:454:VAL:O	1:A:454:VAL:HG23	2.21	0.41
1:B:90:ASP:OD2	1:B:92:GLN:HG3	2.21	0.40
1:B:431:VAL:HG13	1:B:524:LEU:CD2	2.51	0.40
1:B:128:TRP:O	1:B:132:ILE:HB	2.21	0.40
1:B:8:TRP:CH2	1:B:267:LEU:HD11	2.55	0.40
1:B:437:SER:HA	1:B:568:ARG:HH12	1.86	0.40
1:A:597:VAL:O	1:A:601:LEU:HB2	2.22	0.40
1:B:589:THR:OG1	1:B:590:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG13	1:A:37:VAL:O	2.20	0.40
1:B:291:LYS:HA	1:B:291:LYS:HD2	1.83	0.40
1:A:376:ASP:O	1:A:377:CYS:C	2.59	0.40
1:B:292:ASP:HA	1:B:295:PHE:O	2.21	0.40
1:B:657:LYS:HB2	1:B:657:LYS:HE3	1.90	0.40
1:A:440:THR:CG2	1:A:441:TRP:H	2.31	0.40
1:B:533:VAL:HG11	1:B:537:THR:HG21	2.03	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%)	566 (84%)	89 (13%)	19 (3%)	6	15
1	B	674/676 (100%)	572 (85%)	80 (12%)	22 (3%)	5	11
All	All	1348/1352 (100%)	1138 (84%)	169 (12%)	41 (3%)	5	13

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	PRO
1	A	501	SER
1	A	628	ASP
1	B	162	ALA
1	B	338	GLU
1	B	435	SER
1	A	278	LYS
1	A	453	ALA
1	A	499	MSE
1	A	553	ASN
1	A	629	LEU

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Mol	Chain	Res	Type
1	B	125	SER
1	B	178	GLY
1	B	332	PRO
1	B	436	ALA
1	B	471	ILE
1	B	629	LEU
1	A	417	ASN
1	A	472	ASN
1	A	567	THR
1	A	644	ARG
1	B	469	ASN
1	B	549	PRO
1	B	552	LYS
1	B	567	THR
1	B	628	ASP
1	A	329	GLY
1	A	438	ASP
1	A	593	LYS
1	B	163	ASP
1	B	445	LYS
1	B	472	ASN
1	A	527	LYS
1	B	416	ASP
1	B	460	TRP
1	A	420	ASP
1	A	577	CYS
1	B	277	ASP
1	B	486	PRO
1	B	533	VAL
1	A	549	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	569/560 (102%)	531 (93%)	38 (7%)	20 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	569/560 (102%)	513 (90%)	56 (10%)	10	23
All	All	1138/1120 (102%)	1044 (92%)	94 (8%)	14	31

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	32	SER
1	A	33	ASP
1	A	110	ASN
1	A	167	PHE
1	A	184	GLN
1	A	214	LEU
1	A	225	LEU
1	A	246	VAL
1	A	266	LEU
1	A	278	LYS
1	A	283	GLN
1	A	304	LYS
1	A	312	LYS
1	A	326	LEU
1	A	338	GLU
1	A	347	LEU
1	A	348	SER
1	A	351	GLU
1	A	414	LYS
1	A	445	LYS
1	A	473	HIS
1	A	495	CYS
1	A	499	MSE
1	A	509	ASN
1	A	511	LYS
1	A	545	LYS
1	A	552	LYS
1	A	557	LYS
1	A	573	GLU
1	A	602	ARG
1	A	618	ASN
1	A	623	ARG
1	A	628	ASP
1	A	644	ARG
1	A	646	THR

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Mol	Chain	Res	Type
1	A	654	GLU
1	A	670	LEU
1	B	13	GLU
1	B	21	SER
1	B	27	LYS
1	B	41	LYS
1	B	46	LEU
1	B	55	ASN
1	B	74	PRO
1	B	93	THR
1	B	125	SER
1	B	181	THR
1	B	183	ASN
1	B	193	LYS
1	B	225	LEU
1	B	233	LYS
1	B	239	LYS
1	B	240	ASP
1	B	246	VAL
1	B	280	LYS
1	B	281	GLU
1	B	308	ARG
1	B	310	ASP
1	B	317	TYR
1	B	327	ARG
1	B	336	THR
1	B	339	CYS
1	B	347	LEU
1	B	374	THR
1	B	383	ASN
1	B	389	MSE
1	B	414	LYS
1	B	420	ASP
1	B	423	GLU
1	B	442	ASP
1	B	470	LYS
1	B	473	HIS
1	B	475	ARG
1	B	489	LYS
1	B	506	CYS
1	B	509	ASN
1	B	527	LYS

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Mol	Chain	Res	Type
1	B	535	HIS
1	B	538	VAL
1	B	545	LYS
1	B	558	ASP
1	B	565	ASP
1	B	591	LYS
1	B	613	THR
1	B	623	ARG
1	B	624	SER
1	B	641	LEU
1	B	644	ARG
1	B	645	ASN
1	B	646	THR
1	B	654	GLU
1	B	662	LEU
1	B	671	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	75	ASN
1	A	76	ASN
1	A	110	ASN
1	A	152	ASN
1	A	245	GLN
1	A	249	HIS
1	A	411	ASN
1	A	451	HIS
1	A	461	ASN
1	A	509	ASN
1	A	535	HIS
1	A	536	GLN
1	A	546	ASN
1	A	578	HIS
1	A	603	GLN
1	A	606	HIS
1	A	618	ASN
1	A	642	HIS
1	B	20	GLN
1	B	55	ASN
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	111	GLN
1	B	169	GLN
1	B	183	ASN
1	B	245	GLN
1	B	249	HIS
1	B	271	GLN
1	B	325	ASN
1	B	361	ASN
1	B	383	ASN
1	B	417	ASN
1	B	451	HIS
1	B	509	ASN
1	B	535	HIS
1	B	536	GLN
1	B	546	ASN
1	B	645	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	0.22	0	5,5,5	0.21	0
2	CIT	A	9202	-	3,12,12	2.15	2 (66%)	3,17,17	2.22	2 (66%)
3	GOL	B	9102	-	5,5,5	0.41	0	5,5,5	0.28	0
2	CIT	B	9201	-	3,12,12	2.29	2 (66%)	3,17,17	2.61	2 (66%)
2	CIT	B	9204	-	3,12,12	2.37	1 (33%)	3,17,17	2.24	2 (66%)
2	CIT	B	9206	-	3,12,12	2.39	2 (66%)	3,17,17	2.30	2 (66%)

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
2	CIT	A	9202	-	-	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	9206	-	-	0/6/16/16	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9201	CIT	C4-C3	2.08	1.57	1.54
2	A	9202	CIT	C4-C3	2.37	1.58	1.54
2	B	9206	CIT	C4-C3	2.46	1.58	1.54
2	A	9202	CIT	C2-C3	2.88	1.59	1.54
2	B	9206	CIT	C2-C3	3.28	1.59	1.54
2	B	9201	CIT	C2-C3	3.33	1.59	1.54
2	B	9204	CIT	C2-C3	3.61	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9201	CIT	C3-C4-C5	-3.81	108.87	114.96
2	A	9202	CIT	C3-C4-C5	-3.15	109.92	114.96
2	B	9204	CIT	C3-C4-C5	-2.94	110.25	114.96
2	B	9206	CIT	C3-C4-C5	-2.94	110.26	114.96
2	A	9202	CIT	C3-C2-C1	2.09	118.30	114.96
2	B	9201	CIT	C3-C2-C1	2.42	118.82	114.96
2	B	9204	CIT	C3-C2-C1	2.51	118.98	114.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9206	CIT	C3-C2-C1	2.65	119.20	114.96

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
2	A	9202	CIT	1	0
2	B	9206	CIT	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	667/676 (98%)	0.54	59 (8%)	12 10	27, 66, 113, 122	0
1	B	667/676 (98%)	0.35	27 (4%)	42 41	26, 62, 102, 113	0
All	All	1334/1352 (98%)	0.44	86 (6%)	23 21	26, 64, 108, 122	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	PRO	9.3
1	A	559	TYR	8.6
1	B	336	THR	7.6
1	B	538	VAL	4.6
1	B	334	ALA	4.4
1	A	547	PRO	4.4
1	A	22	PHE	4.3
1	A	439	LEU	4.1
1	B	337	ASP	3.9
1	A	503	LEU	3.9
1	A	202	VAL	3.9
1	A	336	THR	3.8
1	A	554	LEU	3.8
1	B	443	ASN	3.4
1	A	561	LEU	3.3
1	A	557	LYS	3.3
1	A	100	VAL	3.3
1	B	645	ASN	3.3
1	A	490	LYS	3.2
1	B	547	PRO	3.2
1	A	294	LEU	3.2
1	A	438	ASP	3.0
1	A	284	LEU	3.0
1	A	29	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	521	PHE	2.9
1	B	431	VAL	2.9
1	A	612	VAL	2.9
1	B	644	ARG	2.9
1	A	567	THR	2.9
1	A	560	GLU	2.9
1	A	564	LEU	2.8
1	A	431	VAL	2.8
1	A	420	ASP	2.8
1	B	338	GLU	2.8
1	A	477	ASP	2.7
1	B	571	VAL	2.7
1	A	644	ARG	2.7
1	A	502	GLY	2.7
1	A	27	LYS	2.7
1	A	482	GLU	2.7
1	A	577	CYS	2.6
1	A	550	TRP	2.6
1	A	571	VAL	2.6
1	A	642	HIS	2.6
1	A	437	SER	2.6
1	A	496	LYS	2.6
1	B	613	THR	2.5
1	A	529	ASP	2.5
1	A	572	GLU	2.5
1	A	337	ASP	2.5
1	A	541	ASN	2.5
1	B	679	PRO	2.5
1	A	495	CYS	2.4
1	A	476	PHE	2.4
1	A	570	PRO	2.4
1	A	203	ALA	2.4
1	A	112	LEU	2.4
1	B	266	LEU	2.4
1	B	561	LEU	2.4
1	B	88	LYS	2.3
1	A	558	ASP	2.3
1	B	641	LEU	2.3
1	A	539	PRO	2.3
1	B	472	ASN	2.3
1	B	496	LYS	2.3
1	A	483	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	PHE	2.2
1	B	471	ILE	2.2
1	A	274	PHE	2.2
1	A	524	LEU	2.2
1	A	180	SER	2.2
1	A	113	ARG	2.2
1	B	501	SER	2.2
1	B	432	VAL	2.2
1	B	541	ASN	2.1
1	A	528	GLY	2.1
1	A	333	GLU	2.1
1	A	481	SER	2.1
1	A	153	PHE	2.1
1	A	335	PRO	2.1
1	A	543	GLY	2.1
1	B	438	ASP	2.0
1	B	662	LEU	2.0
1	B	22	PHE	2.0
1	A	226	LEU	2.0
1	A	494	LEU	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	0.64	0.40	15.50	98,101,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	B	9204	13/13	0.68	0.26	5.01	111,112,115,115	0
2	CIT	B	9206	13/13	0.78	0.27	1.83	115,116,116,117	0
2	CIT	A	9202	13/13	0.75	0.20	1.25	104,106,107,107	0
3	GOL	A	9101	6/6	0.74	0.46	-	101,101,101,102	0
3	GOL	B	9102	6/6	0.74	0.26	-	93,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.