



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:40 PM GMT

PDB ID : 1UOR  
Title : X-RAY STUDY OF RECOMBINANT HUMAN SERUM ALBUMIN.  
PHASES DETERMINED BY MOLECULAR REPLACEMENT METHOD,  
USING LOW RESOLUTION STRUCTURE MODEL OF TETRAGONAL  
FORM OF HUMAN SERUM ALBUMIN  
Authors : Carter, D.C.; Ho, J.X.  
Deposited on : 1998-03-10  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

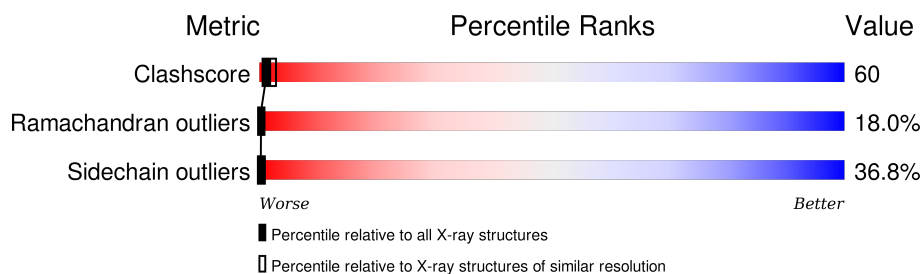
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.


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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4616 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 SERUM ALBUMIN.

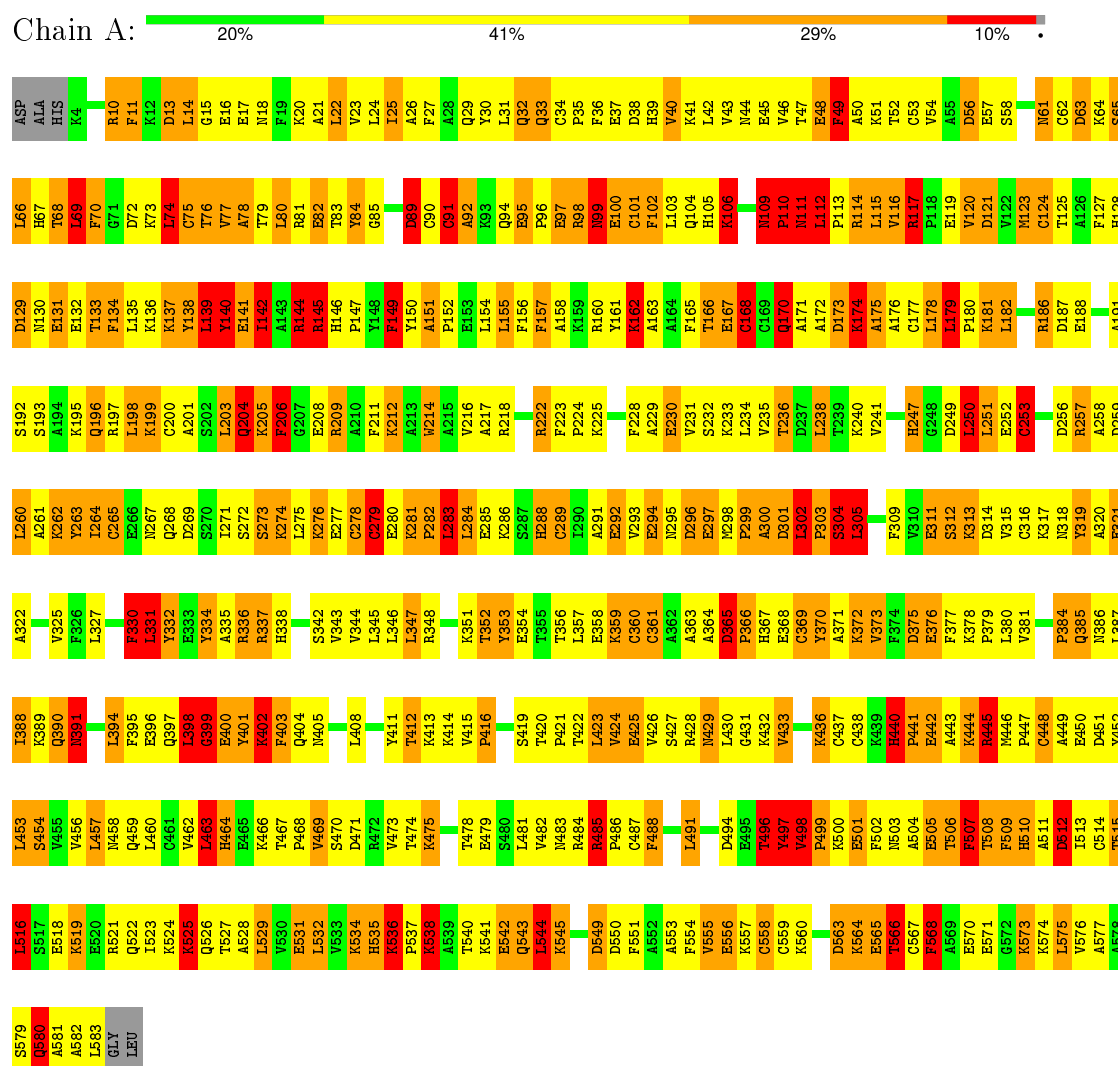
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	580	4616	2915	779	881	41	0	0	0

### 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.

Note EDS was not executed.

#### • Molecule 1: SERUM ALBUMIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.86 Å   88.28 Å   60.68 Å 90.00°   101.85°   90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.0 (6.00-2.80)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.231 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.66	0/4705	0.88	8/6346 (0.1%)

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	A	0	69

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	250	LEU	CA-CB-CG	7.42	132.38	115.30
1	A	516	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	265	CYS	CA-CB-SG	-5.80	103.56	114.00
1	A	491	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	399	GLY	N-CA-C	5.28	126.31	113.10
1	A	145	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	583	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	506	THR	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (69) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Peptide
1	A	105	HIS	Sidechain,Peptide
1	A	106	LYS	Peptide
1	A	109	ASN	Peptide
1	A	110	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	111	ASN	Mainchain
1	A	117	ARG	Sidechain
1	A	119	GLU	Peptide
1	A	138	TYR	Sidechain
1	A	140	TYR	Sidechain
1	A	144	ARG	Sidechain
1	A	145	ARG	Sidechain
1	A	168	CYS	Peptide
1	A	17	GLU	Mainchain
1	A	204	GLN	Peptide
1	A	206	PHE	Sidechain
1	A	229	ALA	Mainchain
1	A	263	TYR	Sidechain
1	A	279	CYS	Peptide
1	A	288	HIS	Peptide
1	A	292	GLU	Peptide
1	A	295	ASN	Mainchain
1	A	297	GLU	Peptide
1	A	301	ASP	Peptide
1	A	302	LEU	Peptide
1	A	305	LEU	Mainchain
1	A	319	TYR	Sidechain
1	A	330	PHE	Mainchain
1	A	352	THR	Peptide
1	A	353	TYR	Sidechain
1	A	360	CYS	Peptide
1	A	363	ALA	Peptide
1	A	365	ASP	Peptide
1	A	370	TYR	Sidechain
1	A	372	LYS	Peptide
1	A	375	ASP	Peptide
1	A	390	GLN	Peptide
1	A	391	ASN	Mainchain
1	A	399	GLY	Mainchain
1	A	401	TYR	Sidechain
1	A	403	PHE	Peptide
1	A	440	HIS	Peptide
1	A	445	ARG	Sidechain
1	A	464	HIS	Peptide
1	A	485	ARG	Peptide
1	A	488	PHE	Sidechain
1	A	497	TYR	Sidechain,Peptide

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Mol	Chain	Res	Type	Group
1	A	498	VAL	Peptide
1	A	505	GLU	Peptide
1	A	506	THR	Mainchain
1	A	507	PHE	Mainchain
1	A	509	PHE	Sidechain
1	A	515	THR	Peptide
1	A	516	LEU	Mainchain
1	A	536	LYS	Peptide
1	A	544	LEU	Peptide
1	A	551	PHE	Sidechain
1	A	573	LYS	Mainchain
1	A	580	GLN	Mainchain
1	A	62	CYS	Mainchain
1	A	70	PHE	Sidechain
1	A	78	ALA	Mainchain
1	A	84	TYR	Sidechain
1	A	89	ASP	Mainchain
1	A	91	CYS	Mainchain
1	A	95	GLU	Peptide
1	A	99	ASN	Mainchain

## 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	4616	0	4542	554	0
All	All	4616	0	4542	554	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 60.

All (554) 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:112:LEU:HB3	1:A:113:PRO:HD3	1.35	1.05
1:A:302:LEU:HD22	1:A:304:SER:HB2	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:HB3	1:A:177:CYS:SG	1.99	1.03
1:A:174:LYS:HB2	1:A:178:LEU:HD12	1.40	1.00
1:A:20:LYS:HE2	1:A:47:THR:HG21	1.45	0.96
1:A:130:ASN:HB2	1:A:134:PHE:HD2	1.32	0.95
1:A:365:ASP:HB2	1:A:366:PRO:HA	1.47	0.93
1:A:470:SER:HB3	1:A:473:VAL:HG23	1.49	0.93
1:A:144:ARG:HH11	1:A:144:ARG:HG2	1.30	0.93
1:A:18:ASN:HA	1:A:21:ALA:HB3	1.50	0.91
1:A:537:PRO:HB2	1:A:580:GLN:HE22	1.33	0.91
1:A:25:ILE:HG22	1:A:142:ILE:HG21	1.54	0.89
1:A:401:TYR:OH	1:A:521:ARG:HA	1.73	0.88
1:A:112:LEU:HB3	1:A:113:PRO:CD	2.05	0.86
1:A:37:GLU:HA	1:A:40:VAL:HG23	1.57	0.86
1:A:519:LYS:HE2	1:A:521:ARG:HG3	1.57	0.85
1:A:481:LEU:HD12	1:A:484:ARG:NH1	1.93	0.84
1:A:302:LEU:HB2	1:A:304:SER:N	1.93	0.83
1:A:408:LEU:HG	1:A:427:SER:HB3	1.61	0.83
1:A:315:VAL:HB	1:A:319:TYR:HB3	1.59	0.83
1:A:537:PRO:HB2	1:A:580:GLN:NE2	1.92	0.82
1:A:440:HIS:NE2	1:A:444:LYS:HB3	1.95	0.82
1:A:36:PHE:CZ	1:A:135:LEU:HD21	2.15	0.81
1:A:317:LYS:HE3	1:A:361:CYS:HB3	1.60	0.81
1:A:531:GLU:O	1:A:534:LYS:HG3	1.81	0.80
1:A:504:ALA:O	1:A:507:PHE:HB2	1.82	0.80
1:A:505:GLU:HA	1:A:507:PHE:HB2	1.63	0.80
1:A:301:ASP:N	1:A:302:LEU:HG	1.95	0.80
1:A:388:ILE:HG21	1:A:445:ARG:HD3	1.64	0.79
1:A:276:LYS:HD3	1:A:277:GLU:H	1.44	0.79
1:A:133:THR:HG21	1:A:165:PHE:CZ	2.17	0.79
1:A:384:PRO:HB2	1:A:446:MET:SD	2.23	0.79
1:A:130:ASN:HB2	1:A:134:PHE:CD2	2.16	0.79
1:A:89:ASP:OD2	1:A:91:CYS:SG	2.41	0.79
1:A:230:GLU:O	1:A:234:LEU:HG	1.83	0.78
1:A:82:GLU:HG3	1:A:82:GLU:O	1.83	0.77
1:A:70:PHE:O	1:A:74:LEU:HB2	1.84	0.77
1:A:172:ALA:CB	1:A:177:CYS:SG	2.73	0.77
1:A:514:CYS:HB3	1:A:556:GLU:HG3	1.65	0.77
1:A:212:LYS:O	1:A:216:VAL:HG23	1.85	0.75
1:A:317:LYS:N	1:A:361:CYS:SG	2.60	0.75
1:A:186:ARG:HG3	1:A:187:ASP:N	2.02	0.74
1:A:98:ARG:HG2	1:A:99:ASN:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD22	1:A:304:SER:CB	2.17	0.73
1:A:541:LYS:HB2	1:A:545:LYS:NZ	2.04	0.73
1:A:305:LEU:H	1:A:305:LEU:HD23	1.52	0.72
1:A:531:GLU:HG3	1:A:534:LYS:NZ	2.03	0.72
1:A:178:LEU:O	1:A:181:LYS:HG3	1.87	0.72
1:A:544:LEU:HD22	1:A:544:LEU:H	1.55	0.72
1:A:441:PRO:HB3	1:A:445:ARG:NH2	2.05	0.72
1:A:313:LYS:HG2	1:A:315:VAL:HG22	1.71	0.72
1:A:222:ARG:HA	1:A:296:ASP:HB3	1.72	0.71
1:A:137:LYS:HD2	1:A:161:TYR:CD2	2.26	0.70
1:A:212:LYS:NZ	1:A:236:THR:HG23	2.06	0.70
1:A:302:LEU:CD2	1:A:304:SER:HB2	2.20	0.70
1:A:542:GLU:HG3	1:A:543:GLN:H	1.55	0.70
1:A:555:VAL:HG13	1:A:556:GLU:OE1	1.90	0.69
1:A:22:LEU:O	1:A:25:ILE:HG12	1.91	0.69
1:A:36:PHE:CE2	1:A:135:LEU:HD21	2.27	0.69
1:A:535:HIS:HA	1:A:537:PRO:O	1.93	0.69
1:A:445:ARG:HH11	1:A:445:ARG:HG3	1.58	0.69
1:A:34:CYS:SG	1:A:82:GLU:HB2	2.33	0.69
1:A:109:ASN:CB	1:A:463:LEU:HD13	2.23	0.68
1:A:402:LYS:HG3	1:A:403:PHE:CD1	2.27	0.68
1:A:558:CYS:C	1:A:567:CYS:SG	2.71	0.68
1:A:448:CYS:SG	1:A:449:ALA:N	2.66	0.68
1:A:474:THR:O	1:A:478:THR:HG22	1.93	0.68
1:A:365:ASP:CB	1:A:366:PRO:HA	2.22	0.68
1:A:192:SER:HA	1:A:195:LYS:HB2	1.76	0.68
1:A:74:LEU:O	1:A:78:ALA:HB3	1.94	0.67
1:A:231:VAL:O	1:A:235:VAL:HG12	1.95	0.67
1:A:49:PHE:HZ	1:A:61:ASN:ND2	1.92	0.67
1:A:538:LYS:HD3	1:A:580:GLN:HG3	1.75	0.67
1:A:304:SER:HB3	1:A:337:ARG:NH2	2.09	0.67
1:A:22:LEU:HD13	1:A:25:ILE:HD11	1.77	0.67
1:A:570:GLU:O	1:A:574:LYS:HG2	1.95	0.67
1:A:420:THR:O	1:A:424:VAL:HG23	1.95	0.67
1:A:519:LYS:CE	1:A:521:ARG:HG3	2.25	0.66
1:A:51:LYS:O	1:A:54:VAL:HB	1.95	0.66
1:A:558:CYS:SG	1:A:558:CYS:O	2.53	0.66
1:A:478:THR:HG23	1:A:479:GLU:N	2.10	0.66
1:A:481:LEU:HA	1:A:484:ARG:HH11	1.59	0.66
1:A:42:LEU:O	1:A:46:VAL:HG23	1.95	0.66
1:A:541:LYS:HB3	1:A:544:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:CYS:HB2	1:A:102:PHE:HB2	1.78	0.66
1:A:68:THR:HG23	1:A:98:ARG:HH12	1.60	0.65
1:A:317:LYS:O	1:A:320:ALA:N	2.29	0.65
1:A:388:ILE:HA	1:A:391:ASN:HB2	1.77	0.65
1:A:505:GLU:HA	1:A:507:PHE:CB	2.25	0.65
1:A:369:CYS:SG	1:A:370:TYR:N	2.69	0.65
1:A:415:VAL:HG13	1:A:415:VAL:O	1.96	0.65
1:A:437:CYS:O	1:A:440:HIS:HB3	1.97	0.64
1:A:272:SER:O	1:A:274:LYS:N	2.29	0.64
1:A:413:LYS:HD3	1:A:540:THR:HB	1.79	0.64
1:A:408:LEU:HG	1:A:427:SER:CB	2.27	0.64
1:A:413:LYS:HD3	1:A:540:THR:CB	2.28	0.64
1:A:440:HIS:CE1	1:A:444:LYS:HB3	2.33	0.63
1:A:327:LEU:HD11	1:A:354:GLU:HB2	1.80	0.63
1:A:144:ARG:HH11	1:A:144:ARG:CG	2.08	0.63
1:A:481:LEU:HA	1:A:484:ARG:NH1	2.14	0.63
1:A:315:VAL:O	1:A:315:VAL:HG23	1.99	0.63
1:A:558:CYS:SG	1:A:570:GLU:OE1	2.56	0.63
1:A:49:PHE:CZ	1:A:61:ASN:ND2	2.67	0.63
1:A:265:CYS:SG	1:A:265:CYS:O	2.56	0.63
1:A:179:LEU:HD23	1:A:180:PRO:HD3	1.80	0.63
1:A:441:PRO:O	1:A:442:GLU:HB2	2.00	0.62
1:A:559:CYS:O	1:A:559:CYS:SG	2.56	0.62
1:A:97:GLU:HA	1:A:100:GLU:OE1	1.98	0.62
1:A:288:HIS:HA	1:A:291:ALA:HB3	1.80	0.62
1:A:26:ALA:O	1:A:30:TYR:HD2	1.82	0.62
1:A:75:CYS:HA	1:A:79:THR:OG1	2.00	0.62
1:A:168:CYS:SG	1:A:177:CYS:C	2.78	0.62
1:A:90:CYS:SG	1:A:102:PHE:N	2.72	0.62
1:A:145:ARG:NE	1:A:146:HIS:NE2	2.46	0.62
1:A:322:ALA:HB1	1:A:325:VAL:HG22	1.81	0.61
1:A:304:SER:HB3	1:A:337:ARG:HH22	1.63	0.61
1:A:571:GLU:O	1:A:575:LEU:N	2.34	0.61
1:A:167:GLU:O	1:A:170:GLN:HB2	2.01	0.61
1:A:137:LYS:HE2	1:A:157:PHE:O	2.01	0.60
1:A:368:GLU:HA	1:A:371:ALA:HB2	1.83	0.60
1:A:576:VAL:O	1:A:579:SER:HB2	2.01	0.60
1:A:113:PRO:O	1:A:114:ARG:HG3	2.01	0.60
1:A:75:CYS:O	1:A:79:THR:HB	2.01	0.60
1:A:33:GLN:HE22	1:A:112:LEU:HD13	1.66	0.60
1:A:448:CYS:SG	1:A:449:ALA:HB2	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:PHE:O	1:A:491:LEU:HB2	2.02	0.60
1:A:311:GLU:O	1:A:370:TYR:HE1	1.85	0.60
1:A:471:ASP:O	1:A:475:LYS:HD3	2.01	0.60
1:A:137:LYS:O	1:A:141:GLU:HB2	2.01	0.60
1:A:228:PHE:HB2	1:A:332:TYR:CE2	2.36	0.60
1:A:395:PHE:HE1	1:A:404:GLN:HA	1.66	0.60
1:A:537:PRO:CB	1:A:580:GLN:HE22	2.13	0.60
1:A:502:PHE:CE1	1:A:580:GLN:OE1	2.55	0.60
1:A:313:LYS:HG3	1:A:314:ASP:N	2.17	0.59
1:A:316:CYS:C	1:A:361:CYS:SG	2.81	0.59
1:A:563:ASP:O	1:A:565:GLU:N	2.36	0.59
1:A:173:ASP:O	1:A:174:LYS:HG3	2.02	0.59
1:A:134:PHE:O	1:A:137:LYS:HG2	2.02	0.59
1:A:394:LEU:O	1:A:398:LEU:HB3	2.03	0.59
1:A:498:VAL:HA	1:A:500:LYS:HE3	1.84	0.59
1:A:300:ALA:HB3	1:A:302:LEU:HD11	1.83	0.59
1:A:543:GLN:HG2	1:A:544:LEU:H	1.68	0.59
1:A:156:PHE:HZ	1:A:160:ARG:NH2	2.01	0.59
1:A:531:GLU:HG3	1:A:534:LYS:HZ1	1.68	0.59
1:A:395:PHE:CE1	1:A:404:GLN:HA	2.38	0.58
1:A:440:HIS:CG	1:A:440:HIS:O	2.56	0.58
1:A:260:LEU:O	1:A:263:TYR:N	2.37	0.58
1:A:401:TYR:HH	1:A:521:ARG:HA	1.66	0.58
1:A:426:VAL:HG13	1:A:456:VAL:CG1	2.34	0.58
1:A:457:LEU:O	1:A:460:LEU:HB3	2.03	0.58
1:A:176:ALA:O	1:A:180:PRO:HD2	2.03	0.58
1:A:278:CYS:O	1:A:279:CYS:SG	2.61	0.58
1:A:22:LEU:HD11	1:A:151:ALA:HB1	1.86	0.58
1:A:138:TYR:C	1:A:140:TYR:H	2.08	0.57
1:A:168:CYS:SG	1:A:178:LEU:N	2.76	0.57
1:A:18:ASN:HA	1:A:21:ALA:CB	2.27	0.57
1:A:166:THR:HG22	1:A:166:THR:O	2.03	0.57
1:A:137:LYS:HD3	1:A:158:ALA:HA	1.86	0.57
1:A:384:PRO:O	1:A:386:ASN:N	2.37	0.57
1:A:512:ASP:OD1	1:A:514:CYS:SG	2.62	0.57
1:A:30:TYR:HD1	1:A:103:LEU:O	1.87	0.57
1:A:260:LEU:O	1:A:262:LYS:N	2.38	0.57
1:A:440:HIS:HE2	1:A:444:LYS:HB3	1.69	0.57
1:A:138:TYR:O	1:A:142:ILE:HG22	2.05	0.57
1:A:537:PRO:HB2	1:A:580:GLN:CD	2.24	0.57
1:A:27:PHE:HE2	1:A:46:VAL:HG21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HA	1:A:321:GLU:OE1	2.04	0.57
1:A:365:ASP:HB2	1:A:366:PRO:CA	2.28	0.57
1:A:412:THR:O	1:A:416:PRO:HB3	2.04	0.57
1:A:251:LEU:H	1:A:251:LEU:HD12	1.69	0.57
1:A:537:PRO:HB2	1:A:580:GLN:OE1	2.04	0.57
1:A:445:ARG:HH11	1:A:445:ARG:CG	2.16	0.56
1:A:101:CYS:SG	1:A:102:PHE:N	2.78	0.56
1:A:283:LEU:O	1:A:286:LYS:HB2	2.05	0.56
1:A:133:THR:HG21	1:A:165:PHE:HZ	1.69	0.56
1:A:401:TYR:CE2	1:A:521:ARG:HD2	2.40	0.56
1:A:302:LEU:HD12	1:A:302:LEU:O	2.05	0.56
1:A:196:GLN:O	1:A:199:LYS:N	2.38	0.56
1:A:144:ARG:O	1:A:146:HIS:N	2.38	0.56
1:A:149:PHE:CE2	1:A:193:SER:HB3	2.41	0.56
1:A:524:LYS:O	1:A:527:THR:N	2.39	0.56
1:A:334:TYR:CE1	1:A:338:HIS:CD2	2.93	0.56
1:A:90:CYS:CB	1:A:102:PHE:HB2	2.35	0.56
1:A:317:LYS:HG3	1:A:361:CYS:SG	2.45	0.56
1:A:498:VAL:O	1:A:500:LYS:N	2.38	0.56
1:A:494:ASP:HB3	1:A:496:THR:OG1	2.06	0.56
1:A:485:ARG:NH2	1:A:486:PRO:HD3	2.20	0.56
1:A:543:GLN:HG2	1:A:544:LEU:N	2.21	0.56
1:A:534:LYS:HE2	1:A:535:HIS:HB3	1.88	0.56
1:A:212:LYS:HZ1	1:A:236:THR:HG23	1.69	0.56
1:A:497:TYR:O	1:A:499:PRO:HD2	2.05	0.56
1:A:420:THR:HG23	1:A:532:LEU:HD13	1.87	0.55
1:A:388:ILE:CG2	1:A:445:ARG:HD3	2.35	0.55
1:A:42:LEU:CD1	1:A:78:ALA:HB2	2.36	0.55
1:A:144:ARG:HB3	1:A:145:ARG:HD3	1.88	0.55
1:A:256:ASP:O	1:A:260:LEU:N	2.39	0.55
1:A:131:GLU:HA	1:A:135:LEU:HD22	1.89	0.55
1:A:223:PHE:CG	1:A:272:SER:HB2	2.42	0.55
1:A:234:LEU:O	1:A:238:LEU:HB2	2.07	0.55
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.88	0.55
1:A:510:HIS:CE1	1:A:567:CYS:HB2	2.41	0.55
1:A:33:GLN:OE1	1:A:112:LEU:HB2	2.07	0.55
1:A:525:LYS:HE2	1:A:526:GLN:HE21	1.71	0.55
1:A:570:GLU:C	1:A:574:LYS:HG2	2.26	0.55
1:A:137:LYS:NZ	1:A:137:LYS:HB2	2.22	0.54
1:A:412:THR:HG21	1:A:532:LEU:HA	1.89	0.54
1:A:422:THR:HG22	1:A:422:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ASN:HB2	1:A:463:LEU:HD13	1.90	0.54
1:A:558:CYS:O	1:A:567:CYS:SG	2.64	0.54
1:A:384:PRO:CB	1:A:446:MET:SD	2.95	0.54
1:A:343:VAL:HG13	1:A:344:VAL:H	1.72	0.54
1:A:267:ASN:O	1:A:269:ASP:N	2.41	0.54
1:A:302:LEU:HD13	1:A:303:PRO:O	2.07	0.54
1:A:563:ASP:HA	1:A:566:THR:OG1	2.06	0.54
1:A:348:ARG:NH2	1:A:486:PRO:HG2	2.23	0.54
1:A:373:VAL:HA	1:A:376:GLU:OE2	2.06	0.54
1:A:137:LYS:HD2	1:A:161:TYR:HD2	1.70	0.54
1:A:179:LEU:HA	1:A:182:LEU:HB2	1.90	0.54
1:A:412:THR:HB	1:A:535:HIS:NE2	2.22	0.54
1:A:92:ALA:HB3	1:A:95:GLU:OE2	2.08	0.54
1:A:356:THR:HA	1:A:359:LYS:HB2	1.90	0.54
1:A:114:ARG:O	1:A:144:ARG:NH1	2.36	0.54
1:A:168:CYS:SG	1:A:178:LEU:HB2	2.48	0.54
1:A:535:HIS:O	1:A:536:LYS:HG3	2.07	0.54
1:A:511:ALA:HA	1:A:564:LYS:HD3	1.88	0.53
1:A:433:VAL:HG23	1:A:452:TYR:CD1	2.43	0.53
1:A:77:VAL:HA	1:A:80:LEU:HD23	1.90	0.53
1:A:250:LEU:O	1:A:253:CYS:N	2.41	0.53
1:A:304:SER:O	1:A:305:LEU:C	2.47	0.53
1:A:443:ALA:O	1:A:445:ARG:N	2.41	0.53
1:A:155:LEU:HD23	1:A:155:LEU:H	1.73	0.53
1:A:401:TYR:CD1	1:A:524:LYS:HD3	2.43	0.53
1:A:155:LEU:HD23	1:A:155:LEU:N	2.24	0.53
1:A:449:ALA:O	1:A:453:LEU:HD12	2.09	0.53
1:A:149:PHE:CD2	1:A:193:SER:HB3	2.43	0.53
1:A:69:LEU:O	1:A:72:ASP:N	2.41	0.53
1:A:354:GLU:O	1:A:354:GLU:HG2	2.09	0.53
1:A:425:GLU:O	1:A:429:ASN:HB2	2.07	0.53
1:A:168:CYS:O	1:A:168:CYS:SG	2.67	0.53
1:A:135:LEU:HD23	1:A:136:LYS:HG3	1.90	0.53
1:A:519:LYS:O	1:A:522:GLN:N	2.37	0.53
1:A:510:HIS:CD2	1:A:567:CYS:HB2	2.44	0.53
1:A:70:PHE:HB3	1:A:74:LEU:HD12	1.89	0.53
1:A:175:ALA:O	1:A:179:LEU:HD22	2.09	0.53
1:A:377:PHE:O	1:A:379:PRO:N	2.42	0.53
1:A:276:LYS:O	1:A:279:CYS:HB2	2.09	0.53
1:A:485:ARG:HH21	1:A:486:PRO:HD3	1.73	0.53
1:A:299:PRO:O	1:A:300:ALA:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:HE2	1:A:188:GLU:O	1.91	0.53
1:A:524:LYS:O	1:A:526:GLN:N	2.42	0.53
1:A:99:ASN:O	1:A:104:GLN:N	2.40	0.53
1:A:303:PRO:HB2	1:A:305:LEU:HD23	1.91	0.53
1:A:288:HIS:O	1:A:288:HIS:CD2	2.62	0.53
1:A:109:ASN:O	1:A:145:ARG:HA	2.09	0.52
1:A:462:VAL:HG23	1:A:463:LEU:N	2.23	0.52
1:A:37:GLU:CA	1:A:40:VAL:HG23	2.36	0.52
1:A:421:PRO:O	1:A:424:VAL:N	2.42	0.52
1:A:34:CYS:SG	1:A:82:GLU:CB	2.97	0.52
1:A:505:GLU:HG3	1:A:505:GLU:O	2.10	0.52
1:A:571:GLU:O	1:A:574:LYS:N	2.42	0.52
1:A:114:ARG:HG2	1:A:144:ARG:HG3	1.90	0.52
1:A:441:PRO:HA	1:A:445:ARG:NH1	2.24	0.52
1:A:128:HIS:O	1:A:128:HIS:ND1	2.43	0.52
1:A:206:PHE:HZ	1:A:481:LEU:H	1.56	0.52
1:A:368:GLU:O	1:A:371:ALA:HB3	2.08	0.52
1:A:146:HIS:HB3	1:A:149:PHE:HB2	1.92	0.52
1:A:22:LEU:CD1	1:A:25:ILE:HD11	2.38	0.52
1:A:27:PHE:CE1	1:A:74:LEU:HG	2.45	0.52
1:A:334:TYR:HE1	1:A:338:HIS:NE2	2.08	0.52
1:A:156:PHE:HE1	1:A:285:GLU:CG	2.23	0.52
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.75	0.52
1:A:130:ASN:O	1:A:132:GLU:O	2.28	0.52
1:A:109:ASN:HB3	1:A:110:PRO:CD	2.38	0.51
1:A:556:GLU:O	1:A:559:CYS:N	2.44	0.51
1:A:172:ALA:O	1:A:175:ALA:N	2.41	0.51
1:A:550:ASP:HA	1:A:553:ALA:HB3	1.91	0.51
1:A:276:LYS:CD	1:A:277:GLU:H	2.18	0.51
1:A:397:GLN:O	1:A:398:LEU:HB2	2.10	0.51
1:A:206:PHE:CZ	1:A:481:LEU:HB2	2.45	0.51
1:A:283:LEU:HD23	1:A:284:LEU:H	1.74	0.51
1:A:34:CYS:SG	1:A:82:GLU:OE1	2.67	0.51
1:A:41:LYS:O	1:A:44:ASN:HB2	2.10	0.51
1:A:317:LYS:O	1:A:319:TYR:N	2.44	0.51
1:A:228:PHE:HD1	1:A:332:TYR:CD2	2.29	0.51
1:A:315:VAL:CB	1:A:319:TYR:HB3	2.37	0.51
1:A:294:GLU:OE1	1:A:294:GLU:HA	2.09	0.51
1:A:156:PHE:HE1	1:A:285:GLU:HG2	1.74	0.51
1:A:69:LEU:O	1:A:70:PHE:C	2.49	0.51
1:A:459:GLN:O	1:A:463:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:HZ	1:A:61:ASN:HD22	1.59	0.50
1:A:130:ASN:CB	1:A:134:PHE:HD2	2.15	0.50
1:A:48:GLU:O	1:A:50:ALA:N	2.44	0.50
1:A:222:ARG:C	1:A:224:PRO:HD3	2.32	0.50
1:A:372:LYS:HB3	1:A:375:ASP:HB2	1.94	0.50
1:A:253:CYS:O	1:A:256:ASP:HB2	2.11	0.50
1:A:526:GLN:O	1:A:529:LEU:N	2.44	0.50
1:A:531:GLU:HG3	1:A:534:LYS:HZ3	1.76	0.50
1:A:123:MET:O	1:A:165:PHE:CE2	2.65	0.50
1:A:98:ARG:CG	1:A:99:ASN:N	2.74	0.50
1:A:541:LYS:HE2	1:A:544:LEU:CD2	2.42	0.50
1:A:431:GLY:O	1:A:433:VAL:N	2.45	0.50
1:A:33:GLN:NE2	1:A:112:LEU:HD13	2.27	0.50
1:A:302:LEU:HB2	1:A:303:PRO:C	2.31	0.50
1:A:142:ILE:HG23	1:A:142:ILE:O	2.12	0.50
1:A:157:PHE:HZ	1:A:188:GLU:HG2	1.76	0.50
1:A:420:THR:HG23	1:A:532:LEU:HD22	1.94	0.50
1:A:571:GLU:HA	1:A:574:LYS:HG3	1.93	0.50
1:A:258:ALA:HB2	1:A:283:LEU:HD11	1.94	0.49
1:A:509:PHE:O	1:A:568:PHE:HE1	1.94	0.49
1:A:345:LEU:O	1:A:348:ARG:HB2	2.12	0.49
1:A:81:ARG:CZ	1:A:81:ARG:HB2	2.42	0.49
1:A:263:TYR:CD2	1:A:264:ILE:N	2.80	0.49
1:A:510:HIS:O	1:A:511:ALA:HB3	2.11	0.49
1:A:233:LYS:O	1:A:234:LEU:HD23	2.11	0.49
1:A:331:LEU:O	1:A:335:ALA:N	2.40	0.49
1:A:283:LEU:O	1:A:286:LYS:N	2.45	0.49
1:A:502:PHE:HB3	1:A:503:ASN:ND2	2.28	0.49
1:A:470:SER:HB3	1:A:473:VAL:CG2	2.31	0.49
1:A:357:LEU:O	1:A:361:CYS:HB2	2.13	0.49
1:A:413:LYS:HD3	1:A:540:THR:OG1	2.13	0.49
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.43	0.49
1:A:176:ALA:O	1:A:180:PRO:CD	2.60	0.49
1:A:401:TYR:OH	1:A:521:ARG:HD2	2.13	0.49
1:A:440:HIS:H	1:A:441:PRO:HD3	1.76	0.49
1:A:342:SER:H	1:A:446:MET:HE2	1.78	0.49
1:A:212:LYS:HZ3	1:A:236:THR:HG23	1.77	0.49
1:A:22:LEU:HD22	1:A:155:LEU:HD11	1.95	0.48
1:A:11:PHE:CE1	1:A:16:GLU:HB2	2.48	0.48
1:A:204:GLN:OE1	1:A:247:HIS:CD2	2.66	0.48
1:A:283:LEU:O	1:A:284:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:CB	1:A:325:VAL:HG22	2.43	0.48
1:A:142:ILE:HG12	1:A:154:LEU:HD12	1.95	0.48
1:A:42:LEU:HD11	1:A:78:ALA:HB2	1.95	0.48
1:A:545:LYS:HZ2	1:A:545:LYS:HB3	1.78	0.48
1:A:364:ALA:O	1:A:365:ASP:O	2.30	0.48
1:A:317:LYS:CE	1:A:361:CYS:HB3	2.37	0.48
1:A:510:HIS:O	1:A:513:ILE:HG12	2.14	0.48
1:A:23:VAL:HG22	1:A:251:LEU:HD21	1.94	0.48
1:A:402:LYS:HE2	1:A:403:PHE:CE1	2.48	0.48
1:A:36:PHE:O	1:A:39:HIS:HB2	2.13	0.48
1:A:512:ASP:O	1:A:516:LEU:HG	2.13	0.48
1:A:343:VAL:HG13	1:A:344:VAL:N	2.28	0.48
1:A:250:LEU:O	1:A:252:GLU:N	2.47	0.48
1:A:553:ALA:CA	1:A:555:VAL:HG12	2.43	0.48
1:A:575:LEU:HG	1:A:575:LEU:O	2.12	0.48
1:A:22:LEU:HD12	1:A:250:LEU:HD23	1.95	0.48
1:A:538:LYS:HD3	1:A:580:GLN:CG	2.43	0.48
1:A:313:LYS:HG3	1:A:314:ASP:H	1.79	0.48
1:A:450:GLU:O	1:A:454:SER:OG	2.30	0.48
1:A:149:PHE:HD1	1:A:150:TYR:N	2.11	0.48
1:A:446:MET:O	1:A:447:PRO:C	2.52	0.47
1:A:99:ASN:O	1:A:104:GLN:HB2	2.14	0.47
1:A:191:ALA:O	1:A:195:LYS:N	2.46	0.47
1:A:115:LEU:O	1:A:116:VAL:O	2.32	0.47
1:A:478:THR:HG23	1:A:479:GLU:H	1.78	0.47
1:A:45:GLU:O	1:A:48:GLU:HB2	2.15	0.47
1:A:401:TYR:HE2	1:A:521:ARG:HD2	1.79	0.47
1:A:401:TYR:HD1	1:A:524:LYS:HD3	1.79	0.47
1:A:170:GLN:HB3	1:A:171:ALA:H	1.58	0.47
1:A:111:ASN:N	1:A:111:ASN:ND2	2.61	0.47
1:A:424:VAL:HG22	1:A:532:LEU:HD21	1.96	0.47
1:A:508:THR:C	1:A:510:HIS:H	2.18	0.47
1:A:305:LEU:HD23	1:A:305:LEU:N	2.27	0.47
1:A:426:VAL:HG13	1:A:456:VAL:HG12	1.97	0.47
1:A:528:ALA:O	1:A:531:GLU:N	2.40	0.47
1:A:510:HIS:HB3	1:A:568:PHE:HD1	1.79	0.47
1:A:124:CYS:SG	1:A:127:PHE:HZ	2.37	0.47
1:A:124:CYS:SG	1:A:127:PHE:CZ	3.07	0.47
1:A:514:CYS:SG	1:A:514:CYS:O	2.72	0.47
1:A:168:CYS:O	1:A:178:LEU:HG	2.15	0.47
1:A:43:VAL:O	1:A:45:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:N	1:A:251:LEU:HD12	2.29	0.47
1:A:498:VAL:C	1:A:500:LYS:N	2.68	0.47
1:A:34:CYS:O	1:A:39:HIS:CE1	2.68	0.47
1:A:70:PHE:C	1:A:74:LEU:HD12	2.35	0.47
1:A:29:GLN:O	1:A:32:GLN:HB3	2.15	0.46
1:A:205:LYS:O	1:A:205:LYS:HG3	2.14	0.46
1:A:478:THR:CG2	1:A:479:GLU:N	2.79	0.46
1:A:98:ARG:O	1:A:99:ASN:C	2.53	0.46
1:A:10:ARG:O	1:A:14:LEU:HD23	2.15	0.46
1:A:535:HIS:O	1:A:535:HIS:CG	2.68	0.46
1:A:264:ILE:HG22	1:A:265:CYS:N	2.29	0.46
1:A:332:TYR:CE1	1:A:336:ARG:NH1	2.83	0.46
1:A:106:LYS:HD3	1:A:147:PRO:CB	2.46	0.46
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.76	0.46
1:A:348:ARG:HH21	1:A:483:ASN:HD22	1.63	0.46
1:A:563:ASP:C	1:A:565:GLU:H	2.18	0.46
1:A:125:THR:O	1:A:129:ASP:O	2.33	0.46
1:A:345:LEU:HD23	1:A:384:PRO:HG3	1.97	0.46
1:A:332:TYR:HE1	1:A:336:ARG:NH1	2.14	0.46
1:A:204:GLN:OE1	1:A:247:HIS:NE2	2.49	0.46
1:A:53:CYS:HA	1:A:56:ASP:O	2.16	0.46
1:A:138:TYR:O	1:A:140:TYR:N	2.49	0.45
1:A:470:SER:O	1:A:473:VAL:N	2.49	0.45
1:A:436:LYS:O	1:A:437:CYS:SG	2.74	0.45
1:A:541:LYS:HB2	1:A:545:LYS:HZ3	1.81	0.45
1:A:200:CYS:O	1:A:203:LEU:N	2.50	0.45
1:A:140:TYR:O	1:A:142:ILE:N	2.50	0.45
1:A:422:THR:HG23	1:A:463:LEU:HG	1.98	0.45
1:A:332:TYR:O	1:A:335:ALA:HB3	2.17	0.45
1:A:111:ASN:HD22	1:A:111:ASN:N	2.13	0.45
1:A:30:TYR:CD1	1:A:103:LEU:O	2.67	0.45
1:A:140:TYR:C	1:A:142:ILE:H	2.19	0.45
1:A:31:LEU:O	1:A:33:GLN:N	2.49	0.45
1:A:372:LYS:NZ	1:A:375:ASP:CG	2.70	0.45
1:A:424:VAL:HG21	1:A:529:LEU:HG	1.98	0.45
1:A:518:GLU:O	1:A:522:GLN:HB2	2.17	0.45
1:A:538:LYS:NZ	1:A:581:ALA:HB2	2.31	0.45
1:A:556:GLU:O	1:A:558:CYS:N	2.50	0.45
1:A:384:PRO:C	1:A:386:ASN:N	2.70	0.45
1:A:111:ASN:ND2	1:A:114:ARG:HD2	2.31	0.45
1:A:121:ASP:C	1:A:174:LYS:HZ3	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ALA:O	1:A:293:VAL:N	2.47	0.45
1:A:196:GLN:O	1:A:198:LEU:N	2.50	0.45
1:A:525:LYS:O	1:A:529:LEU:HB2	2.17	0.45
1:A:511:ALA:O	1:A:516:LEU:HG	2.16	0.45
1:A:146:HIS:N	1:A:147:PRO:HD3	2.31	0.45
1:A:212:LYS:C	1:A:216:VAL:HG23	2.37	0.45
1:A:573:LYS:O	1:A:577:ALA:HB3	2.17	0.45
1:A:558:CYS:O	1:A:566:THR:HB	2.17	0.44
1:A:199:LYS:HG2	1:A:211:PHE:CE1	2.52	0.44
1:A:209:ARG:NE	1:A:209:ARG:O	2.50	0.44
1:A:281:LYS:HA	1:A:282:PRO:HD2	1.65	0.44
1:A:301:ASP:CA	1:A:302:LEU:HG	2.47	0.44
1:A:99:ASN:C	1:A:104:GLN:HB2	2.38	0.44
1:A:67:HIS:NE2	1:A:249:ASP:HB3	2.32	0.44
1:A:311:GLU:HB3	1:A:312:SER:H	1.52	0.44
1:A:162:LYS:HD3	1:A:166:THR:OG1	2.17	0.44
1:A:462:VAL:CG2	1:A:463:LEU:N	2.80	0.44
1:A:201:ALA:O	1:A:206:PHE:HB2	2.17	0.44
1:A:478:THR:HG23	1:A:479:GLU:HG2	1.99	0.44
1:A:157:PHE:CZ	1:A:188:GLU:HG2	2.51	0.44
1:A:223:PHE:CD1	1:A:223:PHE:N	2.85	0.44
1:A:228:PHE:CD1	1:A:332:TYR:CD2	3.06	0.44
1:A:111:ASN:HD21	1:A:114:ARG:HD2	1.83	0.44
1:A:111:ASN:H	1:A:111:ASN:ND2	2.16	0.44
1:A:334:TYR:HE1	1:A:338:HIS:CD2	2.36	0.44
1:A:258:ALA:C	1:A:260:LEU:N	2.70	0.44
1:A:133:THR:O	1:A:136:LYS:N	2.50	0.44
1:A:209:ARG:HA	1:A:209:ARG:HD2	1.70	0.44
1:A:174:LYS:O	1:A:178:LEU:HB3	2.18	0.44
1:A:504:ALA:O	1:A:507:PHE:CB	2.61	0.44
1:A:441:PRO:O	1:A:442:GLU:OE1	2.36	0.43
1:A:288:HIS:O	1:A:288:HIS:HD2	2.01	0.43
1:A:199:LYS:HG2	1:A:211:PHE:CZ	2.52	0.43
1:A:356:THR:O	1:A:359:LYS:N	2.50	0.43
1:A:441:PRO:HB3	1:A:445:ARG:HH22	1.81	0.43
1:A:214:TRP:O	1:A:217:ALA:HB3	2.18	0.43
1:A:214:TRP:CZ3	1:A:218:ARG:NH1	2.86	0.43
1:A:142:ILE:HD11	1:A:146:HIS:O	2.19	0.43
1:A:150:TYR:O	1:A:151:ALA:C	2.56	0.43
1:A:179:LEU:N	1:A:180:PRO:HD2	2.34	0.43
1:A:553:ALA:HA	1:A:555:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LYS:HD3	1:A:277:GLU:HG2	2.00	0.43
1:A:149:PHE:CD1	1:A:150:TYR:N	2.87	0.43
1:A:11:PHE:CD2	1:A:50:ALA:HB1	2.53	0.43
1:A:559:CYS:O	1:A:560:LYS:HG3	2.18	0.43
1:A:483:ASN:O	1:A:487:CYS:HB2	2.19	0.43
1:A:139:LEU:O	1:A:140:TYR:CD1	2.72	0.43
1:A:436:LYS:HE2	1:A:436:LYS:O	2.18	0.43
1:A:301:ASP:HB3	1:A:302:LEU:HD23	1.99	0.43
1:A:142:ILE:HD11	1:A:149:PHE:HB3	2.00	0.43
1:A:131:GLU:CA	1:A:135:LEU:HD22	2.48	0.43
1:A:79:THR:O	1:A:82:GLU:O	2.36	0.43
1:A:293:VAL:O	1:A:293:VAL:HG12	2.19	0.43
1:A:109:ASN:HB3	1:A:110:PRO:HD2	2.00	0.43
1:A:391:ASN:HD22	1:A:391:ASN:HA	1.60	0.43
1:A:438:CYS:O	1:A:440:HIS:N	2.50	0.43
1:A:330:PHE:CZ	1:A:334:TYR:HD2	2.37	0.43
1:A:138:TYR:C	1:A:140:TYR:N	2.72	0.43
1:A:250:LEU:O	1:A:253:CYS:HB2	2.18	0.43
1:A:282:PRO:O	1:A:283:LEU:C	2.57	0.43
1:A:445:ARG:NH1	1:A:445:ARG:HG3	2.29	0.43
1:A:146:HIS:CE1	1:A:193:SER:OG	2.72	0.42
1:A:271:ILE:HG22	1:A:272:SER:N	2.34	0.42
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.01	0.42
1:A:502:PHE:CD1	1:A:580:GLN:OE1	2.72	0.42
1:A:505:GLU:O	1:A:505:GLU:CG	2.67	0.42
1:A:504:ALA:C	1:A:507:PHE:HB2	2.37	0.42
1:A:541:LYS:HE2	1:A:544:LEU:HG	2.01	0.42
1:A:458:ASN:O	1:A:462:VAL:HG13	2.19	0.42
1:A:314:ASP:O	1:A:315:VAL:HG13	2.19	0.42
1:A:330:PHE:CZ	1:A:334:TYR:CD2	3.07	0.42
1:A:36:PHE:CE2	1:A:40:VAL:HG21	2.53	0.42
1:A:519:LYS:HE2	1:A:521:ARG:CG	2.38	0.42
1:A:507:PHE:HB3	1:A:508:THR:H	1.60	0.42
1:A:222:ARG:C	1:A:223:PHE:HD1	2.21	0.42
1:A:197:ARG:HG3	1:A:462:VAL:HG11	2.01	0.42
1:A:253:CYS:O	1:A:256:ASP:N	2.53	0.42
1:A:524:LYS:O	1:A:525:LYS:C	2.58	0.42
1:A:481:LEU:HD12	1:A:484:ARG:HH12	1.77	0.42
1:A:152:PRO:HA	1:A:155:LEU:HG	2.01	0.42
1:A:250:LEU:HD13	1:A:250:LEU:H	1.84	0.42
1:A:423:LEU:O	1:A:426:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:HIS:CD2	1:A:535:HIS:O	2.72	0.42
1:A:348:ARG:CZ	1:A:486:PRO:HG3	2.49	0.42
1:A:348:ARG:NH2	1:A:483:ASN:HD22	2.18	0.42
1:A:573:LYS:O	1:A:577:ALA:CB	2.67	0.42
1:A:510:HIS:CG	1:A:567:CYS:HB2	2.54	0.42
1:A:196:GLN:C	1:A:198:LEU:N	2.73	0.42
1:A:411:TYR:CE1	1:A:414:LYS:HE2	2.55	0.42
1:A:111:ASN:HB2	1:A:112:LEU:H	1.71	0.42
1:A:26:ALA:HB2	1:A:250:LEU:HD22	2.01	0.42
1:A:419:SER:O	1:A:422:THR:N	2.52	0.42
1:A:178:LEU:C	1:A:180:PRO:HD2	2.40	0.42
1:A:537:PRO:CB	1:A:580:GLN:OE1	2.68	0.42
1:A:263:TYR:O	1:A:264:ILE:C	2.58	0.41
1:A:123:MET:O	1:A:165:PHE:HE2	2.01	0.41
1:A:216:VAL:HG22	1:A:235:VAL:HG11	2.02	0.41
1:A:460:LEU:O	1:A:460:LEU:HD12	2.20	0.41
1:A:13:ASP:OD1	1:A:13:ASP:N	2.53	0.41
1:A:26:ALA:O	1:A:30:TYR:CD2	2.67	0.41
1:A:276:LYS:HE3	1:A:276:LYS:HB2	1.71	0.41
1:A:542:GLU:O	1:A:544:LEU:N	2.53	0.41
1:A:124:CYS:O	1:A:124:CYS:SG	2.79	0.41
1:A:149:PHE:CD2	1:A:193:SER:CB	3.04	0.41
1:A:216:VAL:HG13	1:A:231:VAL:HG11	2.02	0.41
1:A:426:VAL:O	1:A:427:SER:C	2.58	0.41
1:A:447:PRO:O	1:A:451:ASP:HB2	2.21	0.41
1:A:334:TYR:CD1	1:A:338:HIS:HD2	2.39	0.41
1:A:65:SER:O	1:A:67:HIS:N	2.53	0.41
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.05	0.41
1:A:511:ALA:HA	1:A:564:LYS:CD	2.51	0.41
1:A:519:LYS:HG2	1:A:521:ARG:HB2	2.02	0.41
1:A:563:ASP:OD1	1:A:563:ASP:N	2.52	0.41
1:A:212:LYS:HA	1:A:235:VAL:CG2	2.50	0.41
1:A:13:ASP:C	1:A:15:GLY:H	2.23	0.41
1:A:134:PHE:CG	1:A:135:LEU:N	2.88	0.41
1:A:408:LEU:C	1:A:412:THR:HG1	2.24	0.41
1:A:23:VAL:HG11	1:A:46:VAL:HG11	2.02	0.41
1:A:117:ARG:HA	1:A:140:TYR:OH	2.20	0.41
1:A:39:HIS:O	1:A:43:VAL:HG23	2.20	0.41
1:A:424:VAL:O	1:A:424:VAL:HG12	2.20	0.41
1:A:70:PHE:HD1	1:A:70:PHE:H	1.68	0.41
1:A:545:LYS:NZ	1:A:545:LYS:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLU:HA	1:A:371:ALA:CB	2.50	0.41
1:A:125:THR:HG22	1:A:125:THR:O	2.21	0.41
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.68	0.41
1:A:510:HIS:HB3	1:A:568:PHE:CD1	2.56	0.41
1:A:334:TYR:CD1	1:A:338:HIS:CD2	3.08	0.41
1:A:113:PRO:C	1:A:114:ARG:HG3	2.41	0.40
1:A:174:LYS:O	1:A:175:ALA:C	2.58	0.40
1:A:510:HIS:NE2	1:A:567:CYS:HB2	2.35	0.40
1:A:225:LYS:HB3	1:A:301:ASP:HA	2.02	0.40
1:A:276:LYS:O	1:A:277:GLU:C	2.59	0.40
1:A:500:LYS:O	1:A:501:GLU:C	2.59	0.40
1:A:400:GLU:OE1	1:A:400:GLU:N	2.54	0.40
1:A:373:VAL:O	1:A:375:ASP:N	2.53	0.40
1:A:43:VAL:O	1:A:44:ASN:C	2.59	0.40
1:A:395:PHE:O	1:A:399:GLY:N	2.55	0.40
1:A:347:LEU:HB3	1:A:482:VAL:CG1	2.51	0.40
1:A:397:GLN:O	1:A:398:LEU:CB	2.70	0.40
1:A:128:HIS:CG	1:A:128:HIS:O	2.74	0.40
1:A:81:ARG:HG3	1:A:81:ARG:NH1	2.36	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	578/585 (99%)	309 (54%)	165 (28%)	104 (18%)	<b>0</b> <b>0</b>

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	48	GLU

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Mol	Chain	Res	Type
1	A	49	PHE
1	A	66	LEU
1	A	76	THR
1	A	89	ASP
1	A	92	ALA
1	A	96	PRO
1	A	109	ASN
1	A	110	PRO
1	A	112	LEU
1	A	116	VAL
1	A	133	THR
1	A	142	ILE
1	A	151	ALA
1	A	170	GLN
1	A	250	LEU
1	A	251	LEU
1	A	268	GLN
1	A	273	SER
1	A	283	LEU
1	A	284	LEU
1	A	305	LEU
1	A	312	SER
1	A	366	PRO
1	A	385	GLN
1	A	396	GLU
1	A	398	LEU
1	A	402	LYS
1	A	440	HIS
1	A	441	PRO
1	A	466	LYS
1	A	497	TYR
1	A	498	VAL
1	A	499	PRO
1	A	510	HIS
1	A	536	LYS
1	A	538	LYS
1	A	564	LYS
1	A	94	GLN
1	A	97	GLU
1	A	106	LYS
1	A	117	ARG
1	A	139	LEU

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Mol	Chain	Res	Type
1	A	141	GLU
1	A	261	ALA
1	A	274	LYS
1	A	279	CYS
1	A	292	GLU
1	A	381	VAL
1	A	432	LYS
1	A	442	GLU
1	A	496	THR
1	A	501	GLU
1	A	519	LYS
1	A	544	LEU
1	A	555	VAL
1	A	557	LYS
1	A	566	THR
1	A	568	PHE
1	A	580	GLN
1	A	582	ALA
1	A	63	ASP
1	A	74	LEU
1	A	114	ARG
1	A	129	ASP
1	A	149	PHE
1	A	162	LYS
1	A	163	ALA
1	A	174	LYS
1	A	175	ALA
1	A	282	PRO
1	A	300	ALA
1	A	378	LYS
1	A	525	LYS
1	A	543	GLN
1	A	69	LEU
1	A	166	THR
1	A	253	CYS
1	A	257	ARG
1	A	318	ASN
1	A	384	PRO
1	A	445	ARG
1	A	35	PRO
1	A	120	VAL
1	A	179	LEU

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Mol	Chain	Res	Type
1	A	330	PHE
1	A	388	ILE
1	A	400	GLU
1	A	463	LEU
1	A	512	ASP
1	A	542	GLU
1	A	549	ASP
1	A	85	GLY
1	A	167	GLU
1	A	304	SER
1	A	331	LEU
1	A	416	PRO
1	A	241	VAL
1	A	469	VAL
1	A	485	ARG
1	A	303	PRO
1	A	468	PRO
1	A	299	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	508/511 (99%)	321 (63%)	187 (37%)	<b>0</b> <b>0</b>

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	11	PHE
1	A	13	ASP
1	A	14	LEU
1	A	22	LEU
1	A	24	LEU
1	A	25	ILE
1	A	33	GLN

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Mol	Chain	Res	Type
1	A	38	ASP
1	A	40	VAL
1	A	49	PHE
1	A	52	THR
1	A	56	ASP
1	A	57	GLU
1	A	58	SER
1	A	61	ASN
1	A	63	ASP
1	A	64	LYS
1	A	65	SER
1	A	66	LEU
1	A	68	THR
1	A	69	LEU
1	A	73	LYS
1	A	74	LEU
1	A	75	CYS
1	A	76	THR
1	A	77	VAL
1	A	80	LEU
1	A	82	GLU
1	A	83	THR
1	A	84	TYR
1	A	89	ASP
1	A	91	CYS
1	A	98	ARG
1	A	99	ASN
1	A	101	CYS
1	A	102	PHE
1	A	109	ASN
1	A	111	ASN
1	A	112	LEU
1	A	115	LEU
1	A	117	ARG
1	A	120	VAL
1	A	121	ASP
1	A	123	MET
1	A	124	CYS
1	A	131	GLU
1	A	134	PHE
1	A	137	LYS
1	A	139	LEU

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Mol	Chain	Res	Type
1	A	140	TYR
1	A	142	ILE
1	A	144	ARG
1	A	145	ARG
1	A	149	PHE
1	A	155	LEU
1	A	157	PHE
1	A	162	LYS
1	A	168	CYS
1	A	170	GLN
1	A	173	ASP
1	A	174	LYS
1	A	178	LEU
1	A	179	LEU
1	A	181	LYS
1	A	182	LEU
1	A	186	ARG
1	A	196	GLN
1	A	198	LEU
1	A	199	LYS
1	A	203	LEU
1	A	204	GLN
1	A	205	LYS
1	A	206	PHE
1	A	208	GLU
1	A	209	ARG
1	A	212	LYS
1	A	214	TRP
1	A	222	ARG
1	A	230	GLU
1	A	232	SER
1	A	236	THR
1	A	238	LEU
1	A	240	LYS
1	A	247	HIS
1	A	250	LEU
1	A	253	CYS
1	A	257	ARG
1	A	259	ASP
1	A	260	LEU
1	A	262	LYS
1	A	264	ILE

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Mol	Chain	Res	Type
1	A	273	SER
1	A	275	LEU
1	A	276	LYS
1	A	278	CYS
1	A	280	GLU
1	A	281	LYS
1	A	283	LEU
1	A	289	CYS
1	A	294	GLU
1	A	296	ASP
1	A	297	GLU
1	A	298	MET
1	A	302	LEU
1	A	304	SER
1	A	305	LEU
1	A	309	PHE
1	A	311	GLU
1	A	313	LYS
1	A	321	GLU
1	A	331	LEU
1	A	332	TYR
1	A	334	TYR
1	A	336	ARG
1	A	337	ARG
1	A	346	LEU
1	A	347	LEU
1	A	351	LYS
1	A	352	THR
1	A	353	TYR
1	A	358	GLU
1	A	359	LYS
1	A	360	CYS
1	A	361	CYS
1	A	365	ASP
1	A	367	HIS
1	A	369	CYS
1	A	373	VAL
1	A	376	GLU
1	A	380	LEU
1	A	385	GLN
1	A	387	LEU
1	A	389	LYS

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Mol	Chain	Res	Type
1	A	390	GLN
1	A	391	ASN
1	A	394	LEU
1	A	398	LEU
1	A	402	LYS
1	A	405	ASN
1	A	412	THR
1	A	423	LEU
1	A	424	VAL
1	A	425	GLU
1	A	428	ARG
1	A	429	ASN
1	A	430	LEU
1	A	433	VAL
1	A	436	LYS
1	A	444	LYS
1	A	445	ARG
1	A	448	CYS
1	A	453	LEU
1	A	454	SER
1	A	457	LEU
1	A	463	LEU
1	A	464	HIS
1	A	467	THR
1	A	469	VAL
1	A	475	LYS
1	A	485	ARG
1	A	496	THR
1	A	497	TYR
1	A	507	PHE
1	A	508	THR
1	A	512	ASP
1	A	515	THR
1	A	516	LEU
1	A	523	ILE
1	A	525	LYS
1	A	529	LEU
1	A	531	GLU
1	A	532	LEU
1	A	534	LYS
1	A	535	HIS
1	A	538	LYS

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Mol	Chain	Res	Type
1	A	545	LYS
1	A	549	ASP
1	A	554	PHE
1	A	556	GLU
1	A	558	CYS
1	A	563	ASP
1	A	565	GLU
1	A	566	THR
1	A	568	PHE
1	A	575	LEU
1	A	580	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	61	ASN
1	A	99	ASN
1	A	196	GLN
1	A	288	HIS
1	A	295	ASN
1	A	318	ASN
1	A	338	HIS
1	A	385	GLN
1	A	391	ASN
1	A	397	GLN
1	A	404	GLN
1	A	429	ASN
1	A	503	ASN
1	A	526	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.