



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:04 PM UTC

PDB ID : 2HAV / pdb_00002hav
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

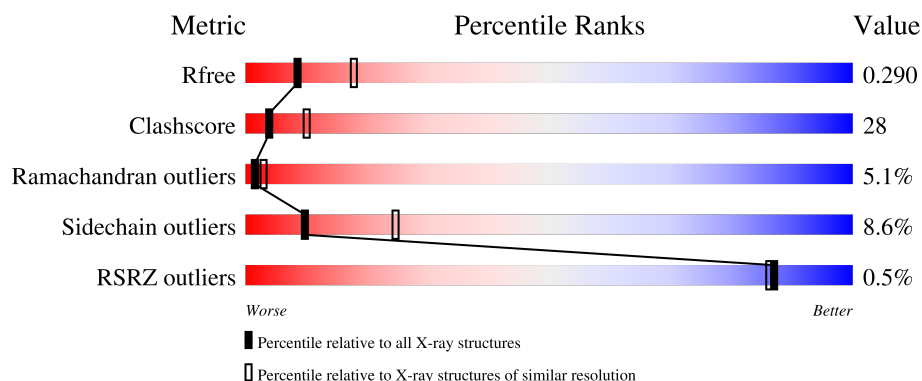
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	9207	-	X	-	-
2	CIT	B	9201	-	X	-	-
2	CIT	B	9206	-	-	X	-
3	GOL	A	9103	-	-	X	-

2 Entry composition [i](#)

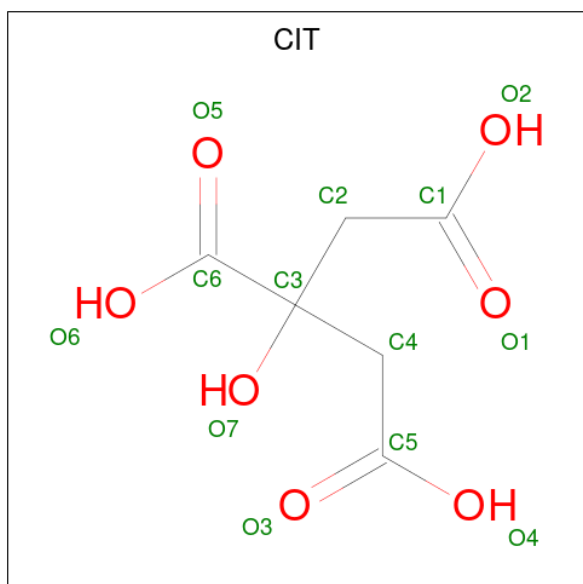
There are 3 unique types of molecules in this entry. The entry contains 10601 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

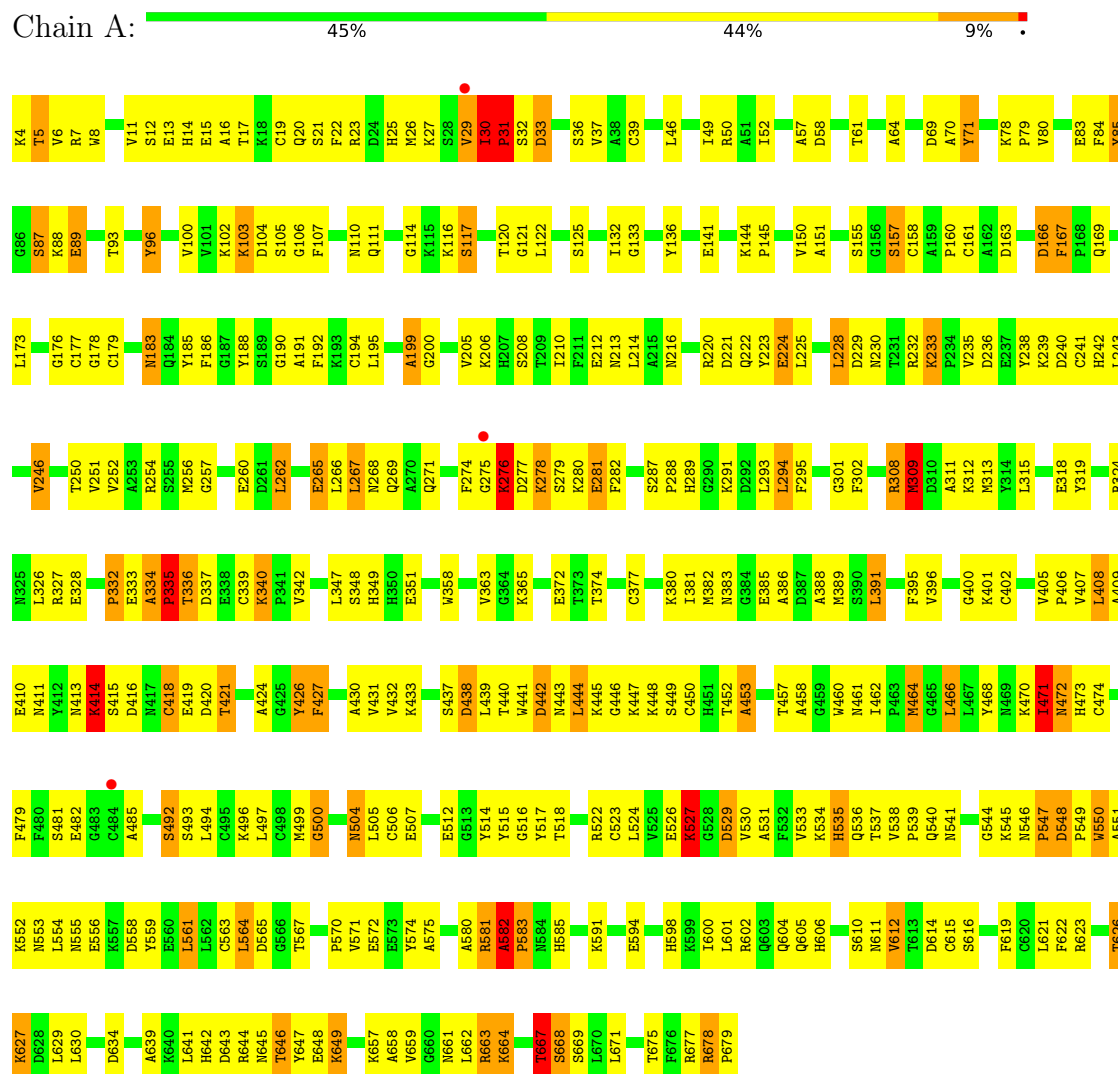


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



S669	T589	E512	M443	R351	G257	T181	F107	K4
L670	G513	G513	L444	R352	G258	L182	Q108	A10
L671	Y514	Y514	K445	R353	K259	M183	M109	N110
T675	Y515	Y515	W358	W358		Q184	N110	N111
	G516	G516	K447	V363	L267	Y188	Q111	S12
	Y517	Y517	K448	V364	M268	S189	R113	E13
			S449	T366	Q269	G190	G114	H14
	F521	F521	V454	E367	A270	A191		E15
	L524	L524	T457	S370	Q271	F193	S117	C19
	E525	E525	A371	E372	F274	C194	T120	F22
	K527	K527	M460	A371	G275	L195	R124	H25
	G528	G528	M461	E372	K276	K196	S125	M26
	D529	D529	P463	T378	K280	D197	A126	K27
	H535	H535	M464	I381		G198	G127	S28
			G465	I381	Q283	D201	W128	V29
	V538	V538	L466	K389	L284		M129	I30
	P539	P539	L467	D392	F285	F204	I130	P31
	Q540	Q540	Y468	D392	S286	V205	P131	S32
	N541	N541	M469	G393	S287	K206	I132	P35
	T542	T542	K470	G394	P288	H207	L135	
	G543	G543	I471	F395	H289	S208	Y136	I49
	G544	G544	N472	V396	G290	T209		
	R545	R545	H473	Y397	K291	I210	L139	I52
	N546	N546	C474	L404	D292	F211	P140	N55
			R475		L293	E212	E141	
	P549	P549	E478	V407	L294	L214	P142	V60
	N550	N550	F479	L408	G301	N213	R143	T61
	A551	A551	F480	L408	P306	N216	K144	
	K552	K552	S481	N411	P307	K217	P145	Y71
	N553	N553	E482	N412	R308		K148	
	L554	L554	E482	N413	D310	R220	A149	L77
	N555	N555	A485	K414	M309	D221	V150	K78
	E556	E556	P486	S415	D311	Q222	A151	P79
	Y559	Y559	G487	D416	A311	Y223	M152	
	E560	E560	S488	N417	K312	E224	F153	F84
	L561	L561	K489	C418	M313	L225	F154	Y85
	L562	L562	K490	E419	Y314		G158	G86
	C563	C563	D420	D421	L315	L228	A159	S87
	L564	L564	S492	T421	Y319	D229	P160	E88
			S493		T320	N230	D163	E89
	R568	R568	K496	A424	T321	T231	D163	D90
	K569	K569	L497	G425	A322	R232	D166	Q92
	P570	P570	C498	Y426	I323	K233	P167	T93
	V571	V571	M499	F427	E328	P234	Q169	F94
	E572	E572	G500	V429		D236	Y95	
	E573	E573	S501		E333	E237		
	Y574	Y574	N504	V432	A334	Y238	L173	A99
	A575	A575	L505	K433	P335	V246	V100	
	N576	N576	K434	K434	T336	P247	V101	
	C577	C577	E506	D438		S248	K102	
	A580	A580	E507	L439	K340	H249	C177	
	R581	R581	N509	T440	P341	T250	C178	
	L662	L662	N510	W441			C179	
	R663	R663		D442	H350		S180	
	N584	N584						
	T667	T667						
	S668	S668						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.32Å 103.26Å 200.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.70) 96.1 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.293 0.237 , 0.290	Depositor DCC
R_{free} test set	2534 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/5362	1.08	48/7247 (0.7%)
1	B	0.51	1/5362 (0.0%)	1.09	33/7247 (0.5%)
All	All	0.51	1/10724 (0.0%)	1.09	81/14494 (0.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	MET	SD-CE	-5.54	1.65	1.79

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	SER	N-CA-C	11.57	127.24	112.89
1	A	405	VAL	N-CA-C	9.35	116.86	109.19
1	B	439	LEU	N-CA-C	-9.34	95.86	109.59
1	B	415	SER	N-CA-C	9.19	125.42	109.80
1	A	85	TYR	N-CA-C	8.96	122.35	110.88
1	B	30	ILE	CA-C-N	8.85	130.90	119.84
1	B	30	ILE	C-N-CA	8.85	130.90	119.84
1	A	87	SER	N-CA-C	-8.14	98.23	109.95
1	A	444	LEU	N-CA-C	8.07	122.08	111.75
1	A	257	GLY	N-CA-C	-7.84	98.58	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	501	SER	N-CA-C	7.80	121.67	109.96
1	B	246	VAL	N-CA-C	7.46	116.12	107.77
1	B	290	GLY	N-CA-C	7.39	119.75	110.96
1	B	280	LYS	N-CA-C	-7.29	104.38	113.28
1	A	167	PHE	CA-C-N	7.27	127.61	119.32
1	A	167	PHE	C-N-CA	7.27	127.61	119.32
1	B	248	SER	N-CA-C	7.25	118.83	111.07
1	A	89	GLU	N-CA-C	-7.22	103.44	112.90
1	A	479	PHE	N-CA-C	-7.15	103.67	113.18
1	B	117	SER	N-CA-C	7.02	121.11	109.95
1	B	292	ASP	N-CA-C	6.99	121.03	111.39
1	A	246	VAL	N-CA-C	6.93	115.45	107.89
1	B	474	CYS	N-CA-C	6.71	121.30	113.18
1	B	546	ASN	CA-C-N	6.66	126.44	119.05
1	B	546	ASN	C-N-CA	6.66	126.44	119.05
1	A	426	TYR	N-CA-C	6.54	119.25	110.88
1	B	396	VAL	N-CA-C	-6.52	103.97	110.62
1	A	117	SER	N-CA-C	6.50	120.63	110.17
1	A	622	PHE	N-CA-C	6.43	120.83	112.92
1	A	535	HIS	N-CA-C	6.43	119.98	111.75
1	B	563	CYS	N-CA-C	6.38	118.89	109.69
1	A	582	ALA	CA-C-N	6.27	126.72	120.52
1	A	582	ALA	C-N-CA	6.27	126.72	120.52
1	B	457	THR	N-CA-C	6.26	117.79	110.97
1	A	526	GLU	N-CA-C	6.25	120.94	112.88
1	B	590	ARG	N-CA-C	-6.24	102.13	110.55
1	B	306	PRO	CA-C-N	6.16	125.84	119.56
1	B	306	PRO	C-N-CA	6.16	125.84	119.56
1	A	437	SER	N-CA-C	6.15	118.47	108.63
1	A	256	MET	N-CA-C	-6.06	99.84	109.59
1	A	667	THR	N-CA-C	6.05	123.70	110.80
1	A	418	CYS	N-CA-C	6.03	123.65	110.80
1	A	17	THR	N-CA-C	-5.95	104.49	110.97
1	B	216	ASN	N-CA-C	5.92	118.38	108.96
1	B	444	LEU	N-CA-C	5.85	117.46	111.14
1	A	349	HIS	N-CA-C	-5.72	105.04	111.28
1	A	664	LYS	N-CA-C	-5.69	105.06	112.23
1	A	166	ASP	N-CA-C	5.68	118.68	111.69
1	B	429	VAL	N-CA-C	5.68	115.75	108.82
1	A	372	GLU	N-CA-C	5.68	117.55	111.36
1	A	449	SER	N-CA-C	5.56	118.76	110.14
1	A	21	SER	N-CA-C	-5.55	105.14	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	CA-C-N	5.51	125.79	119.83
1	A	233	LYS	C-N-CA	5.51	125.79	119.83
1	A	199	ALA	N-CA-C	-5.47	105.33	112.23
1	A	583	PRO	N-CA-C	5.46	119.27	111.13
1	B	85	TYR	N-CA-C	5.46	120.30	113.43
1	B	233	LYS	N-CA-C	5.45	113.04	108.13
1	B	259	LYS	N-CA-C	5.45	119.10	111.74
1	A	581	ARG	N-CA-C	5.44	118.03	111.40
1	A	396	VAL	N-CA-C	-5.41	104.33	111.09
1	A	334	ALA	N-CA-C	-5.38	103.14	110.36
1	B	11	VAL	N-CA-C	5.34	117.24	112.17
1	B	257	GLY	N-CA-C	-5.33	101.05	110.86
1	A	646	THR	N-CA-C	-5.31	100.66	108.99
1	A	96	TYR	N-CA-C	5.29	117.58	109.07
1	A	281	GLU	N-CA-C	-5.25	105.00	111.40
1	A	339	CYS	N-CA-C	5.25	117.64	110.24
1	A	474	CYS	N-CA-C	5.24	119.30	113.02
1	B	307	PRO	N-CA-C	5.21	120.61	113.84
1	A	39	CYS	N-CA-C	5.16	117.05	108.02
1	B	372	GLU	N-CA-C	5.14	116.88	111.28
1	A	33	ASP	N-CA-C	-5.13	105.91	113.61
1	A	216	ASN	N-CA-C	5.12	117.08	108.73
1	A	309	MET	N-CA-C	5.12	118.55	109.96
1	B	461	ASN	N-CA-C	5.10	117.25	111.02
1	B	193	LYS	N-CA-C	-5.05	105.22	111.33
1	B	328	GLU	N-CA-C	5.05	119.31	112.04
1	A	645	ASN	N-CA-C	5.03	120.04	113.20
1	A	458	ALA	N-CA-C	5.03	116.76	111.28
1	A	388	ALA	N-CA-C	5.03	116.71	109.07

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	318	0
1	B	5243	0	5068	262	0
2	A	39	0	15	17	0
2	B	52	0	20	15	0
3	A	18	0	24	9	0
3	B	6	0	8	2	0
All	All	10601	0	10203	589	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 (589) 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:HE2	1:B:88:LYS:H	1.38	0.88
1:A:461:ASN:HA	1:A:662:LEU:HD11	1.53	0.87
1:B:108:GLN:HE21	1:B:108:GLN:CA	1.91	0.84
1:A:25:HIS:ND1	1:A:282:PHE:HB2	1.92	0.84
2:B:9201:CIT:O6	2:B:9201:CIT:O1	1.98	0.81
1:A:471:ILE:HB	1:A:473:HIS:CD2	2.15	0.81
1:B:188:TYR:OH	2:B:9206:CIT:H21	1.81	0.81
1:B:108:GLN:HA	1:B:108:GLN:NE2	1.93	0.80
1:B:517:TYR:HB2	2:B:9205:CIT:O2	1.82	0.79
1:B:26:MET:HE1	1:B:270:ALA:HA	1.66	0.78
1:B:144:LYS:HA	1:B:145:PRO:C	2.09	0.78
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:HA	1:A:271:GLN:HE21	1.51	0.76
1:B:109:MET:HE3	1:B:135:LEU:HD21	1.66	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:HA	1:A:365:LYS:HE2	1.68	0.75
1:A:462:ILE:HD13	1:A:580:ALA:HB3	1.69	0.75
1:B:504:ASN:C	1:B:504:ASN:HD22	1.94	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
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:B:309:MET:HE3	1:B:313:MET:SD	2.29	0.73
1:A:564:LEU:CD1	3:A:9103:GOL:O3	2.37	0.73
1:B:181:THR:C	1:B:183:ASN:H	1.97	0.72
1:A:563:CYS:HB3	3:A:9103:GOL:O2	1.90	0.72
1:A:31:PRO:C	1:A:33:ASP:H	1.98	0.72
1:A:332:PRO:C	1:A:334:ALA:H	1.95	0.71
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: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:293:LEU:O	1:B:294:LEU:HB2	1.93	0.69
1:B:460:TRP:O	1:B:464:MET:HB2	1.92	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: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:B:468:TYR:HB3	1:B:661:ASN:HD22	1.60	0.67
1:B:591:LYS:C	1:B:593:LYS:H	2.01	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:A:334:ALA:HB1	1:A:335:PRO:HD2	1.78	0.65
1:B:678:ARG:O	1:B:679:PRO:O	2.14	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:308:ARG:HG3	1:A:669:SER:OG	1.97	0.65
1:A:407:VAL:HG13	1:A:598:HIS:NE2	2.12	0.65
1:A:442:ASP:HB3	1:A:470:LYS:HZ2	1.59	0.65
1:B:352:ARG:HD3	1:B:370: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:196:LYS:C	1:B:198:GLY:H	2.04	0.64
1:A:514:TYR:HE1	1:A:522:ARG:HG2	1.63	0.64
1:B:644:ARG:HA	1:B:649:LYS:HD3	1.79	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:A:413:ASN:CG	1:A:414:LYS:H	2.06	0.63
1:B:434:LYS:HG3	1:B:560:GLU:OE2	1.99	0.63
1:B:551:ALA:HA	1:B:554:LEU:CD1	2.28	0.63
1:B:663:ARG:HG2	1:B:671:LEU:CD2	2.28	0.63
1:B:446:GLY:O	1:B:481:SER:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ILE:O	1:B:473:HIS:CD2	2.52	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:334:ALA:O	1:A:335:PRO:C	2.42	0.62
1:A:552:LYS:HE3	1:A:553:ASN:HD21	1.64	0.62
1:A:46:LEU:HB3	1:A:50:ARG:HH21	1.65	0.62
1:A:413:ASN:ND2	1:A:414:LYS:HG2	2.15	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: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:103:LYS:HB2	1:A:222:GLN:O	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: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:13:GLU:HG2	1:B:179:CYS:SG	2.41	0.61
1:A:107:PHE:HA	1:A:111:GLN:OE1	1.99	0.61
1:A:391:LEU:HG	1:A:395:PHE:HB3	1.82	0.61
1:A:433:LYS:HG2	1:A:559:TYR:CE2	2.34	0.61
1:B:89:GLU:CD	1:B:89:GLU:H	2.07	0.61
1:B:475:ARG:HE	1:B:478:GLU:CD	2.08	0.61
1:B:192:PHE:CZ	1:B:210:ILE:HG13	2.36	0.60
1:A:383:ASN:OD1	1:A:385:GLU:HG3	2.02	0.60
1:A:407:VAL:HG22	1:A:594:GLU:HG3	1.82	0.60
1:B:678:ARG:HB3	1:B:679:PRO:HD3	1.84	0.60
1:A:602:ARG:HA	1:A:605:GLN:HE21	1.67	0.60
1:B:105:SER:HB2	1:B:107:PHE:HE2	1.67	0.60
1:B:315:LEU:HB3	1:B:319:TYR:HD2	1.68	0.59
1:A:381:ILE:HA	1:A:386:ALA:O	2.02	0.59
1:A:551:ALA:HA	1:A:554:LEU:HG	1.83	0.59
2:A:9202:CIT:O1	2:A:9202:CIT:C6	2.50	0.59
1:A:471:ILE:HG13	1:A:472:ASN:H	1.67	0.59
1:B:413:ASN:O	1:B:414:LYS:C	2.46	0.59
1:B:468:TYR:O	1:B:470:LYS:N	2.36	0.59
2:B:9201:CIT:O6	2:B:9201:CIT:C1	2.50	0.59
1:A:262:LEU:O	1:A:262:LEU:HD12	2.03	0.59
1:A:574:TYR:CD1	1:A:575:ALA:N	2.71	0.59
1:B:49:ILE:HG23	1:B:77:LEU:CD1	2.33	0.59
1:B:675:THR:HG23	1:B:679:PRO:HG2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:315:LEU:HD22	1:A:319:TYR:CE2	2.38	0.58
1:B:517:TYR:N	2:B:9205:CIT:O1	2.36	0.58
1:A:413:ASN:O	1:A:414:LYS:C	2.46	0.58
1:A:457:THR:OG1	2:A:9202:CIT:H22	2.03	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:424:ALA:HB3	1:B:581:ARG:CZ	2.34	0.58
1:B:71:TYR:CZ	1:B:312:LYS:HD3	2.38	0.57
1:B:678:ARG:CB	1:B:679:PRO:CD	2.82	0.57
1:A:214:LEU:HD11	1:A:223:TYR:CE1	2.37	0.57
2:A:9207:CIT:O6	2:A:9207:CIT:C5	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:267:LEU:HB3	1:A:302:PHE:CD2	2.39	0.57
1:A:444:LEU:O	1:A:447:LYS:HB2	2.04	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:158:CYS:HB2	1:A:173:LEU:HB2	1.86	0.56
1:A:363:VAL:HG12	1:A:363:VAL:O	2.05	0.56
1:B:105:SER:HB2	1:B:107:PHE:CE2	2.39	0.56
1:A:117:SER:OG	1:A:157:SER:HB3	2.05	0.56
1:A:439:LEU:HD23	1:A:443:ASN:HD22	1.71	0.56
2:A:9202:CIT:O1	2:A:9202:CIT:O5	2.23	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: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
1:B:19:CYS:O	1:B:22:PHE:HB3	2.05	0.55
1:B:188:TYR:CZ	1:B:206:LYS:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:OD1	1:B:231:THR:HG23	2.06	0.55
1:B:283:GLN:CD	1:B:283:GLN:N	2.64	0.55
1:A:220:ARG:C	1:A:222:GLN:H	2.15	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:333:GLU:H	1:A:333:GLU:CD	2.15	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:O3	2:B:9204:CIT:O7	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: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:B:591:LYS:C	1:B:593:LYS:N	2.66	0.54
1:A:100:VAL:HG22	1:A:225:LEU:CD2	2.37	0.54
1:A:275:GLY:H	1:A:278:LYS:CB	2.16	0.54
1:B:132:ILE:HD12	1:B:150:VAL:HG22	1.90	0.54
1:B:526:GLU:C	1:B:527:LYS:HG3	2.32	0.54
1:A:358:TRP:HE1	1:A:604:GLN:NE2	2.06	0.54
1:A:332:PRO:C	1:A:334:ALA:N	2.65	0.53
1:A:426:TYR:OH	2:A:9202:CIT:O5	2.23	0.53
1:B:181:THR:C	1:B:183:ASN:N	2.64	0.53
1:B:408:LEU:HD23	1:B:640:LYS:HA	1.90	0.53
1:B:521:PHE:O	1:B:524:LEU:HB3	2.08	0.53
1:A:324:ARG:HD2	1:A:328:GLU:OE2	2.07	0.53
1:B:192:PHE:HD2	1:B:213:ASN:HD22	1.56	0.53
1:A:471:ILE:O	1:A:472:ASN:HB2	2.07	0.53
1:A:31:PRO:C	1:A:33:ASP:N	2.66	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:A:381:ILE:HD12	1:A:389:MET:HE2	1.91	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:544:GLY:C	1:A:546:ASN:H	2.16	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:B:196:LYS:C	1:B:198:GLY:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:544:GLY:C	1:A:546:ASN:N	2.66	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: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:516:GLY:HA3	2:A:9203:CIT:C5	2.40	0.52
1:A:564:LEU:HD12	3:A:9103:GOL:O3	2.09	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:A:87:SER:OG	1:A:89:GLU:HB2	2.09	0.52
1:B:26:MET:CE	1:B:270:ALA:HA	2.39	0.52
1:B:341:PRO:HB2	1:B:367:GLU:HG3	1.91	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:A:517:TYR:N	2:A:9203:CIT:O4	2.43	0.52
1:B:561:LEU:HD12	1:B:577:CYS:SG	2.50	0.52
1:A:185:TYR:HA	1:A:190:GLY:O	2.09	0.51
1:A:240:ASP:CG	1:A:678:ARG:HH22	2.18	0.51
1:A:555:ASN:HB2	1:A:558:ASP:OD2	2.09	0.51
1:B:89:GLU:CD	1:B:89:GLU:N	2.67	0.51
1:A:535:HIS:HB2	1:A:574:TYR:CG	2.44	0.51
1:B:504:ASN:HA	1:B:507:GLU:HG2	1.92	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:B:434:LYS:HG3	1:B:560:GLU:CD	2.35	0.51
1:A:374:THR:HG21	1:A:395:PHE:CD1	2.46	0.51
1:B:350:HIS:HD2	2:B:9201:CIT:O3	1.93	0.51
1:A:144:LYS:HA	1:A:145:PRO:C	2.36	0.51
1:A:410:GLU:CD	1:A:585:HIS:HB2	2.36	0.51
1:A:629:LEU:O	1:A:630:LEU:HB2	2.10	0.51
1:B:308:ARG:HB2	1:B:669:SER:HB3	1.92	0.51
1:B:574:TYR:CD1	1:B:575:ALA:N	2.79	0.51
1:A:5:THR:HB	1:A:36:SER:OG	2.11	0.51
1:B:169:GLN:CD	1:B:169:GLN:H	2.19	0.51
1:B:418:CYS:O	1:B:420:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:GLU:O	1:B:527:LYS:HG3	2.11	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:A:426:TYR:OH	2:A:9202:CIT:O1	2.28	0.50
1:A:426:TYR:HD1	1:A:426:TYR:O	1.94	0.50
1:B:538:VAL:HB	1:B:571:VAL:HG11	1.93	0.50
1:A:485:ALA:HB3	1:A:494:LEU:HB3	1.92	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:598:HIS:O	1:B:602:ARG:CG	2.59	0.50
1:A:11:VAL:O	1:A:12:SER:HB3	2.10	0.50
1:B:651:LEU:HD22	1:B:655:TYR:CD2	2.47	0.50
1:B:30:ILE:O	1:B:32:SER:N	2.39	0.50
1:B:214:LEU:HD11	1:B:223:TYR:CE1	2.46	0.50
1:B:420:ASP:O	1:B:421:THR:HG23	2.12	0.50
1:A:151:ALA:HB1	1:A:169:GLN:CG	2.42	0.50
1:A:380:LYS:HG2	1:A:385:GLU:HB2	1.94	0.50
1:B:626:THR:HG22	1:B:627:LYS:N	2.27	0.49
1:A:176:GLY:O	1:A:177:CYS:HB2	2.12	0.49
1:A:228:LEU:HD22	3:A:9104:GOL:H2	1.95	0.49
1:A:675:THR:HA	1:A:679:PRO:HD2	1.93	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:A:662:LEU:C	1:A:664:LYS:H	2.19	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:107:PHE:O	1:A:232:ARG:NH2	2.44	0.49
1:A:441:TRP:O	1:A:444:LEU:HD13	2.11	0.49
1:B:538:VAL:O	1:B:540:GLN:N	2.41	0.49
1:A:335:PRO:O	1:A:336:THR:HB	2.13	0.49
1:B:142:PRO:O	1:B:144:LYS:N	2.44	0.49
1:B:188:TYR:OH	2:B:9206:CIT:C2	2.58	0.49
1:B:319:TYR:O	1:B:323:ILE:HG12	2.12	0.49
1:B:413:ASN:HD22	1:B:414:LYS:HD2	1.78	0.49
1:B:471:ILE:HG21	1:B:479:PHE:HD1	1.77	0.49
1:A:468:TYR:C	1:A:470:LYS:H	2.20	0.49
1:B:125:SER:C	1:B:130:ILE:HD12	2.37	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:B:30:ILE:CD1	1:B:35:PRO:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:O	1:A:178:GLY:C	2.56	0.49
1:A:677:ARG:HB3	1:A:677:ARG:NH1	2.27	0.49
1:A:678:ARG:CB	1:A:679:PRO:CD	2.87	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:B:285:PHE:O	1:B:286:SER:HB3	2.13	0.49
1:A:64:ALA:CB	1:A:246:VAL:HG13	2.43	0.48
1:A:482:GLU:OE2	1:A:496:LYS:HB3	2.13	0.48
1:B:358:TRP:CE2	1:B:366:ILE:HG13	2.48	0.48
1:B:598:HIS:CD2	1:B:640:LYS:HG2	2.48	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
2:B:9204:CIT:O1	2:B:9204:CIT:O5	2.31	0.48
1:A:220:ARG:O	1:A:222:GLN:N	2.46	0.48
1:B:629:LEU:O	1:B:630:LEU:HB2	2.13	0.48
1:A:22:PHE:CE2	1:A:37:VAL:HG21	2.48	0.48
1:A:547:PRO:O	1:A:548:ASP:O	2.31	0.48
1:A:564:LEU:HD12	1:A:565:ASP:N	2.28	0.48
1:B:658:ALA:O	1:B:662:LEU:HB2	2.13	0.48
1:A:220:ARG:C	1:A:222:GLN:N	2.71	0.48
1:B:471:ILE:HG21	1:B:479:PHE:CD1	2.48	0.48
1:B:471:ILE:CG2	1:B:479:PHE:HD1	2.27	0.48
1:A:536:GLN:HB2	1:A:540:GLN:HE21	1.79	0.48
1:B:413:ASN:O	1:B:414:LYS:O	2.31	0.48
1:B:552:LYS:HG3	1:B:553:ASN:H	1.78	0.48
1:A:450:CYS:SG	1:A:523:CYS:C	2.97	0.48
1:A:564:LEU:HD12	1:A:564:LEU:N	2.29	0.48
1:A:646:THR:CG2	1:A:649:LYS:HE2	2.42	0.48
1:B:613:THR:C	1:B:615:CYS:N	2.72	0.48
1:B:426:TYR:O	1:B:535:HIS:ND1	2.44	0.48
1:A:309:MET:HE3	1:A:313:MET:SD	2.54	0.47
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:N	1:B:85:TYR:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASN:ND2	1:B:230:ASN:CG	2.72	0.47
1:A:347:LEU:HD21	1:A:374:THR:HA	1.96	0.47
1:A:547:PRO:O	1:A:552:LYS:HB3	2.13	0.47
1:B:234:PRO:HB2	1:B:237:GLU:HG3	1.96	0.47
1:B:468:TYR:HD2	1:B:661:ASN:ND2	2.13	0.47
1:A:426:TYR:O	1:A:427:PHE:O	2.32	0.47
1:A:530:VAL:O	1:A:530:VAL:HG13	2.13	0.47
1:B:482:GLU:HB3	1:B:497:LEU:HG	1.95	0.47
1:B:509:ASN:HA	1:B:515:TYR:CE2	2.50	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:107:PHE:H	1:A:232:ARG:NH2	2.11	0.47
1:B:378:ILE:CG1	1:B:389:MET:HE1	2.45	0.47
1:A:52:ILE:O	1:A:254:ARG:NE	2.48	0.47
1:A:206:LYS:NZ	2:A:9207:CIT:O6	2.48	0.47
1:B:25:HIS:HB3	1:B:274:PHE:CZ	2.50	0.47
1:A:169:GLN:H	1:A:169:GLN:CD	2.17	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:432:VAL:HG21	1:B:562:LEU:HD21	1.96	0.46
1:B:570:PRO:HD2	1:B:573:GLU:CD	2.39	0.46
1:A:407:VAL:HG13	1:A:598:HIS:CD2	2.50	0.46
1:A:441:TRP:C	1:A:443:ASN:H	2.23	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:418:CYS:O	1:B:419:GLU:C	2.57	0.46
1:B:514:TYR:CE1	1:B:527:LYS:HD3	2.50	0.46
1:A:25:HIS:ND1	1:A:282:PHE:CB	2.73	0.46
1:A:457:THR:N	2:A:9202:CIT:O2	2.46	0.46
1:B:600:ILE:HD12	1:B:600:ILE:H	1.81	0.46
1:A:570:PRO:C	1:A:572:GLU:N	2.74	0.46
1:B:163:ASP:OD2	1:B:166:ASP:OD2	2.33	0.46
1:B:210:ILE:HD11	1:B:223:TYR:CD1	2.50	0.46
1:B:471:ILE:CG2	1:B:479:PHE:CD1	2.99	0.46
1:A:333:GLU:OE2	1:A:333:GLU:N	2.46	0.46
1:B:499:MET:O	1:B:505:LEU:HG	2.15	0.46
1:A:229:ASP:OD1	1:A:229:ASP:C	2.59	0.46
1:A:400:GLY:HA3	1:A:647:TYR:CD2	2.51	0.46
1:A:493:SER:HA	1:A:496:LYS:HE3	1.97	0.46
1:A:614:ASP:C	1:A:616:SER:N	2.72	0.46
1:A:659:VAL:O	1:A:663:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD12	1:A:262:LEU:C	2.42	0.45
1:B:28:SER:O	1:B:29:VAL:HG23	2.16	0.45
1:B:468:TYR:C	1:B:470:LYS:N	2.75	0.45
1:B:613:THR:O	1:B:615:CYS:N	2.45	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:A:662:LEU:C	1:A:664:LYS:N	2.75	0.45
1:B:142:PRO:C	1:B:144:LYS:H	2.23	0.45
1:A:30:ILE:O	1:A:31:PRO:C	2.59	0.45
1:B:84:PHE:CZ	1:B:301:GLY:HA3	2.51	0.45
1:B:102:LYS:HG3	1:B:223:TYR:HE2	1.81	0.45
1:B:444:LEU:O	1:B:445:LYS:C	2.59	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
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:A:377:CYS:HB3	1:A:389:MET:SD	2.57	0.45
1:A:614:ASP:C	1:A:616:SER:H	2.24	0.45
1:B:542:THR:OG1	1:B:556:GLU:HB2	2.16	0.45
1:B:591:LYS:NZ	1:B:594:GLU:OE1	2.33	0.45
1:A:539:PRO:HG3	1:A:556:GLU:OE1	2.16	0.45
1:B:538:VAL:HG11	1:B:571:VAL:HG21	1.99	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: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:599:LYS:C	1:B:599:LYS:HD3	2.40	0.45
1:A:444:LEU:O	1:A:445:LYS:C	2.59	0.44
1:B:512:GLU:OE2	1:B:514:TYR:HB2	2.18	0.44
1:B:598:HIS:O	1:B:602:ARG:HG2	2.17	0.44
1:A:186:PHE:O	1:A:190:GLY:HA3	2.17	0.44
1:B:196:LYS:O	1:B:198:GLY:N	2.51	0.44
1:B:485:ALA:O	1:B:486:PRO:C	2.59	0.44
1:B:109:MET:HE3	1:B:135:LEU:CD2	2.41	0.44
1:B:321:THR:O	1:B:322:ALA:C	2.61	0.44
1:A:132:ILE:HD12	1:A:150:VAL:CG2	2.47	0.44
1:A:522:ARG:HB2	1:A:550:TRP:CH2	2.53	0.44
1:A:634:ASP:OD1	1:A:634:ASP:N	2.44	0.44
1:B:438:ASP:O	1:B:438:ASP:CG	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LYS:HE2	1:A:527:LYS:O	2.17	0.44
1:A:83:GLU:OE2	1:A:295:PHE:HB3	2.17	0.44
1:B:188:TYR:CE2	1:B:206:LYS:HG3	2.52	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:A:8:TRP:CH2	1:A:267:LEU:HD21	2.53	0.44
1:A:110:ASN:CG	1:A:230:ASN:OD1	2.61	0.44
1:A:229:ASP:C	1:A:230:ASN:HD22	2.26	0.44
1:A:540:GLN:C	1:A:541:ASN:HD22	2.25	0.44
1:B:469:ASN:ND2	1:B:661:ASN:HD21	2.16	0.44
1:A:426:TYR:O	1:A:427:PHE:C	2.61	0.43
1:B:87:SER:O	1:B:88:LYS:C	2.60	0.43
1:A:163:ASP:OD2	1:A:166:ASP:OD2	2.36	0.43
1:A:183:ASN:HD22	1:A:186:PHE:HB2	1.83	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:133:GLY:O	1:A:136:TYR:HB2	2.18	0.43
1:A:208:SER:O	1:A:212:GLU:HG3	2.18	0.43
1:B:136:TYR:O	1:B:139:LEU:HB2	2.18	0.43
1:B:473:HIS:HE1	1:B:478:GLU:OE1	2.01	0.43
1:A:8:TRP:HH2	1:A:267:LEU:HD21	1.83	0.43
1:A:440:THR:O	1:A:443:ASN:HB3	2.17	0.43
1:B:55:ASN:CG	1:B:55:ASN:O	2.62	0.43
1:B:177:CYS:O	1:B:178:GLY:C	2.59	0.43
1:B:589:THR:OG1	1:B:590:ARG:N	2.51	0.43
1:B:602:ARG:NH1	1:B:602:ARG:HB3	2.32	0.43
1:A:85:TYR:CD1	1:A:85:TYR:N	2.87	0.43
1:A:183:ASN:ND2	1:A:186:PHE:HB2	2.33	0.43
1:A:238:TYR:CD1	1:A:239:LYS:N	2.87	0.43
1:B:120:THR:OG1	1:B:127:GLY:HA3	2.18	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:277:ASP:C	1:A:279:SER:N	2.76	0.43
1:A:533:VAL:HG23	1:A:534:LYS:N	2.33	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:315:LEU:HB3	1:B:319:TYR:CD2	2.52	0.43
1:B:381:ILE:HD12	1:B:389:MET:HE2	2.01	0.43
1:B:416:ASP:O	1:B:417:ASN:HB2	2.17	0.43
1:B:493:SER:HA	1:B:496:LYS:HG3	1.99	0.43
1:B:552:LYS:HE3	1:B:553:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:HA	2:B:9206:CIT:O5	2.19	0.43
1:A:61:THR:HA	1:A:250:THR:O	2.18	0.43
1:B:407:VAL:HG13	1:B:408:LEU:HG	2.01	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:120:THR:O	1:A:160:PRO:HG2	2.18	0.43
1:A:504:ASN:HA	1:A:507:GLU:CG	2.46	0.43
1:B:193:LYS:HD3	1:B:197:ASP:OD2	2.19	0.43
1:A:407:VAL:CG2	1:A:594:GLU:HG3	2.47	0.42
1:A:497:LEU:HD22	1:A:527:LYS:HD3	2.00	0.42
1:A:615:CYS:SG	1:A:623:ARG:NH1	2.92	0.42
1:B:152:ASN:O	1:B:153:PHE:C	2.62	0.42
1:A:340:LYS:HA	1:A:340:LYS:HD2	1.91	0.42
1:B:232:ARG:O	1:B:233:LYS:CG	2.66	0.42
1:B:584:ASN:O	1:B:650:TYR:OH	2.32	0.42
1:A:49:ILE:HD13	1:A:70:ALA:HB2	2.00	0.42
1:A:79:PRO:HB3	1:A:250:THR:HG21	2.01	0.42
1:A:275:GLY:N	1:A:278:LYS:HB2	2.19	0.42
1:A:446:GLY:O	1:A:481:SER:HB3	2.19	0.42
1:A:461:ASN:HA	1:A:662:LEU:CD1	2.36	0.42
1:A:19:CYS:O	1:A:22:PHE:HB3	2.19	0.42
1:A:96:TYR:CD1	1:A:96:TYR:N	2.87	0.42
1:A:441:TRP:CD1	1:A:564:LEU:HA	2.55	0.42
1:A:544:GLY:O	1:A:546:ASN:N	2.52	0.42
1:B:207:HIS:HB2	1:B:238:TYR:CD2	2.54	0.42
1:B:283:GLN:N	1:B:283:GLN:OE1	2.53	0.42
1:A:107:PHE:N	1:A:232:ARG:NH2	2.66	0.42
1:A:406:PRO:HB2	1:A:641:LEU:CD1	2.49	0.42
1:B:490:LYS:NZ	1:B:507:GLU:OE2	2.43	0.42
1:A:7:ARG:HB2	1:A:58:ASP:OD2	2.20	0.42
1:A:71:TYR:O	1:A:71:TYR:CD1	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:A:612:VAL:O	1:A:612:VAL:CG1	2.67	0.42
1:B:504:ASN:C	1:B:504:ASN:ND2	2.67	0.42
1:A:358:TRP:HB2	1:A:619:PHE:CZ	2.54	0.42
1:B:468:TYR:CD2	1:B:661:ASN:ND2	2.88	0.42
1:A:6:VAL:HG22	1:A:262:LEU:HG	2.02	0.42
1:A:103:LYS:HD2	1:A:104:ASP:CG	2.45	0.42
1:A:547:PRO:O	1:A:548:ASP:C	2.61	0.42
1:B:461:ASN:HA	1:B:662:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:THR:HB	1:B:556:GLU:N	2.35	0.42
1:A:4:LYS:O	1:A:4:LYS:HG3	2.19	0.42
1:A:206:LYS:HZ1	2:A:9207:CIT:C6	2.33	0.42
1:A:71:TYR:CD1	1:A:71:TYR:C	2.97	0.42
1:A:420:ASP:C	1:A:421:THR:HG1	2.28	0.42
1:A:448:LYS:O	1:A:530:VAL:HG12	2.20	0.42
1:A:527:LYS:HA	1:A:527:LYS:CE	2.49	0.42
1:B:457:THR:N	2:B:9204:CIT:O4	2.32	0.42
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: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: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:84:PHE:CE2	1:A:301:GLY:C	2.98	0.41
1:A:224:GLU:OE1	1:A:232:ARG:HD2	2.20	0.41
1:B:60:VAL:HG22	1:B:61:THR:N	2.35	0.41
1:B:538:VAL:C	1:B:540:GLN:H	2.24	0.41
1:A:293:LEU:O	1:A:294:LEU:HB2	2.18	0.41
1:A:612:VAL:O	1:A:612:VAL:HG13	2.20	0.41
1:B:176:GLY:O	1:B:177:CYS:HB2	2.19	0.41
1:B:394:GLY:O	1:B:397:TYR:HB3	2.20	0.41
1:B:467:LEU:HD13	1:B:479:PHE:CE2	2.56	0.41
1:B:623:ARG:HD3	1:B:623:ARG:HA	1.81	0.41
1:A:210:ILE:HD11	1:A:223:TYR:CD1	2.56	0.41
1:A:277:ASP:O	1:A:278:LYS:C	2.64	0.41
1:B:10:ALA:HB1	1:B:15:GLU:HB2	2.02	0.41
1:B:27:LYS:C	1:B:29:VAL:H	2.29	0.41
1:B:71:TYR:HB2	1:B:311:ALA:CB	2.51	0.41
1:B:504:ASN:HA	1:B:507:GLU:CG	2.50	0.41
1:B:509:ASN:O	1:B:510:ASN:C	2.63	0.41
1:A:195:LEU:HD12	1:A:200:GLY:O	2.20	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:276:LYS:O	1:A:276:LYS:HD3	2.20	0.41
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.84	0.41
1:B:95:TYR:CD1	1:B:95:TYR:C	2.98	0.41
1:B:457:THR:HA	1:B:461:ASN:HB2	2.03	0.41
1:A:13:GLU:O	1:A:14:HIS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:H	1:A:351:GLU:HB2	1.86	0.41
1:A:591:LYS:HA	1:A:591:LYS:HD2	1.90	0.41
1:B:124:ARG:HB3	2:B:9206:CIT:O5	2.21	0.41
1:B:128:TRP:CH2	1:B:150:VAL:HG21	2.56	0.41
1:B:442:ASP:OD1	1:B:442:ASP:N	2.53	0.41
1:A:78:LYS:O	1:A:252:VAL:HA	2.20	0.40
1:A:318:GLU:CD	1:A:318:GLU:H	2.29	0.40
1:A:382:MET:SD	1:A:402:CYS:HB3	2.60	0.40
1:B:228:LEU:HD12	1:B:228:LEU:HA	1.85	0.40
1:B:378:ILE:HG13	1:B:389:MET:HE1	2.03	0.40
1:B:439:LEU:HD23	1:B:443:ASN:HD22	1.85	0.40
1:B:481:SER:OG	1:B:482:GLU:N	2.52	0.40
1:A:102:LYS:HG2	1:A:223:TYR:CD2	2.56	0.40
1:B:378:ILE:HG12	1:B:389:MET:HE3	2.02	0.40
1:B:419:GLU:CD	1:B:419:GLU:H	2.29	0.40
1:B:498:CYS:HA	1:B:514:TYR:CD1	2.56	0.40
1:A:80:VAL:HG22	1:A:251:VAL:O	2.22	0.40
1:A:121:GLY:HA2	1:A:160:PRO:HB2	2.02	0.40
1:A:430:ALA:O	1:A:561:LEU:HA	2.21	0.40
1:A:522:ARG:HE	1:A:550:TRP:CD1	2.39	0.40
1:B:99:ALA:O	1:B:225:LEU:HA	2.22	0.40
1:B:141:GLU:H	1:B:141:GLU:HG2	1.53	0.40
1:B:378:ILE:HG23	1:B:404:LEU:HD12	2.02	0.40
1:B:623:ARG:HG2	1:B:623:ARG:NH1	2.36	0.40
1:A:69:ASP:OD1	1:A:327:ARG:NH2	2.46	0.40
1:A:533:VAL:HG11	1:A:537:THR:HG21	2.03	0.40
1:B:85:TYR:OH	1:B:249:HIS:HB2	2.21	0.40
1:B:139:LEU:HD23	1:B:153:PHE:HB2	2.03	0.40
1:B:144:LYS:CB	1:B:144:LYS:NZ	2.85	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	674/676 (100%)	552 (82%)	85 (13%)	37 (6%)	1	2
1	B	674/676 (100%)	554 (82%)	88 (13%)	32 (5%)	2	3
All	All	1348/1352 (100%)	1106 (82%)	173 (13%)	69 (5%)	1	3

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
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

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Mol	Chain	Res	Type
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
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%)	512 (90%)	57 (10%)	7	19
1	B	569/569 (100%)	528 (93%)	41 (7%)	13	32
All	All	1138/1138 (100%)	1040 (91%)	98 (9%)	10	25

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	27	LYS
1	A	30	ILE
1	A	31	PRO
1	A	71	TYR
1	A	88	LYS
1	A	93	THR
1	A	103	LYS
1	A	105	SER
1	A	122	LEU
1	A	141	GLU
1	A	157	SER
1	A	161	CYS
1	A	167	PHE
1	A	183	ASN
1	A	224	GLU
1	A	228	LEU
1	A	236	ASP
1	A	243	LEU
1	A	260	GLU
1	A	262	LEU
1	A	265	GLU
1	A	267	LEU
1	A	276	LYS
1	A	280	LYS
1	A	291	LYS
1	A	294	LEU
1	A	308	ARG
1	A	309	MET
1	A	326	LEU
1	A	335	PRO
1	A	337	ASP
1	A	340	LYS

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Mol	Chain	Res	Type
1	A	391	LEU
1	A	408	LEU
1	A	414	LYS
1	A	416	ASP
1	A	421	THR
1	A	464	MET
1	A	466	LEU
1	A	471	ILE
1	A	492	SER
1	A	504	ASN
1	A	527	LYS
1	A	529	ASP
1	A	561	LEU
1	A	564	LEU
1	A	583	PRO
1	A	601	LEU
1	A	610	SER
1	A	612	VAL
1	A	621	LEU
1	A	626	THR
1	A	643	ASP
1	A	649	LYS
1	A	663	ARG
1	A	667	THR
1	B	29	VAL
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

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Mol	Chain	Res	Type
1	B	310	ASP
1	B	312	LYS
1	B	336	THR
1	B	340	LYS
1	B	407	VAL
1	B	442	ASP
1	B	464	MET
1	B	466	LEU
1	B	488	SER
1	B	496	LYS
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	598	HIS
1	B	599	LYS
1	B	618	ASN
1	B	621	LEU
1	B	640	LYS
1	B	663	ARG
1	B	667	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	152	ASN
1	A	216	ASN
1	A	230	ASN
1	A	268	ASN
1	A	271	GLN
1	A	411	ASN
1	A	413	ASN
1	A	443	ASN
1	A	540	GLN
1	A	604	GLN
1	A	611	ASN
1	A	661	ASN
1	B	110	ASN
1	B	152	ASN

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Mol	Chain	Res	Type
1	B	213	ASN
1	B	222	GLN
1	B	230	ASN
1	B	273	HIS
1	B	300	HIS
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	540	GLN
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 oligosaccharides 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
2	CIT	B	9206	-	12,12,12	2.02	6 (50%)	17,17,17	1.53	4 (23%)
3	GOL	A	9104	-	5,5,5	0.50	0	5,5,5	1.16	1 (20%)
3	GOL	A	9103	-	5,5,5	0.59	0	5,5,5	0.75	0
2	CIT	A	9203	-	12,12,12	1.92	2 (16%)	17,17,17	1.70	5 (29%)
2	CIT	A	9207	-	12,12,12	2.45	5 (41%)	17,17,17	1.59	4 (23%)
2	CIT	B	9205	-	12,12,12	2.10	2 (16%)	17,17,17	1.28	3 (17%)
3	GOL	A	9101	-	5,5,5	0.69	0	5,5,5	0.47	0
3	GOL	B	9102	-	5,5,5	0.55	0	5,5,5	0.28	0
2	CIT	A	9202	-	12,12,12	2.02	2 (16%)	17,17,17	1.79	5 (29%)
2	CIT	B	9204	-	12,12,12	1.78	3 (25%)	17,17,17	1.68	4 (23%)
2	CIT	B	9201	-	12,12,12	2.78	5 (41%)	17,17,17	1.84	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	B	9206	-	-	7/16/16/16	-
3	GOL	A	9104	-	-	2/4/4/4	-
3	GOL	A	9103	-	-	0/4/4/4	-
2	CIT	A	9203	-	-	5/16/16/16	-
2	CIT	A	9207	-	-	11/16/16/16	-
2	CIT	B	9205	-	-	3/16/16/16	-
3	GOL	A	9101	-	-	2/4/4/4	-
3	GOL	B	9102	-	-	2/4/4/4	-
2	CIT	A	9202	-	-	5/16/16/16	-
2	CIT	B	9204	-	-	6/16/16/16	-
2	CIT	B	9201	-	-	12/16/16/16	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9201	CIT	C3-C6	6.16	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9202	CIT	C3-C6	5.30	1.59	1.53
2	A	9207	CIT	C3-C6	5.19	1.58	1.53
2	B	9205	CIT	C3-C6	4.37	1.58	1.53
2	B	9201	CIT	C2-C3	4.04	1.59	1.54
2	B	9206	CIT	O7-C3	3.81	1.50	1.43
2	B	9201	CIT	O7-C3	3.81	1.50	1.43
2	B	9205	CIT	O7-C3	3.78	1.50	1.43
2	B	9204	CIT	O7-C3	3.46	1.49	1.43
2	A	9203	CIT	C4-C3	3.33	1.58	1.54
2	A	9203	CIT	C4-C5	3.23	1.60	1.50
2	A	9207	CIT	C2-C1	3.04	1.59	1.50
2	B	9201	CIT	C2-C1	2.75	1.59	1.50
2	B	9204	CIT	C3-C6	2.73	1.56	1.53
2	A	9207	CIT	C2-C3	2.69	1.57	1.54
2	A	9207	CIT	C4-C3	2.62	1.57	1.54
2	B	9206	CIT	C4-C5	2.47	1.58	1.50
2	B	9201	CIT	C4-C5	2.44	1.58	1.50
2	B	9206	CIT	C2-C3	2.39	1.56	1.54
2	B	9206	CIT	O1-C1	2.36	1.29	1.22
2	A	9207	CIT	O7-C3	2.25	1.47	1.43
2	B	9206	CIT	O3-C5	2.20	1.29	1.22
2	B	9204	CIT	C2-C3	2.17	1.56	1.54
2	A	9202	CIT	O7-C3	2.15	1.47	1.43
2	B	9206	CIT	C2-C1	2.09	1.57	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9201	CIT	O6-C6-C3	4.39	121.55	113.14
2	B	9204	CIT	O6-C6-C3	3.82	120.48	113.14
2	A	9202	CIT	O6-C6-C3	3.57	119.99	113.14
2	B	9206	CIT	O6-C6-C3	3.55	119.95	113.14
2	A	9207	CIT	O6-C6-C3	3.39	119.64	113.14
2	B	9206	CIT	C4-C3-C6	-3.25	102.84	110.03
2	A	9203	CIT	C3-C2-C1	-3.18	105.23	113.92
2	B	9204	CIT	O7-C3-C6	3.14	113.41	108.96
2	A	9202	CIT	C2-C3-C6	2.87	116.39	110.03
2	A	9203	CIT	C2-C3-C6	-2.77	103.91	110.03
2	A	9202	CIT	C4-C3-C2	-2.67	102.47	109.31
2	A	9202	CIT	O7-C3-C2	-2.65	103.33	109.38
2	A	9207	CIT	O2-C1-C2	2.62	122.64	114.35
2	A	9203	CIT	O6-C6-C3	2.60	118.12	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9201	CIT	O4-C5-C4	2.58	122.51	114.35
2	B	9205	CIT	C2-C3-C6	2.56	115.70	110.03
2	B	9201	CIT	O7-C3-C6	2.50	112.50	108.96
2	A	9207	CIT	O7-C3-C4	-2.48	103.72	109.38
2	A	9202	CIT	O7-C3-C4	2.48	115.03	109.38
2	B	9201	CIT	O3-C5-C4	-2.47	115.94	122.95
2	A	9207	CIT	O1-C1-C2	-2.39	116.17	122.95
2	B	9204	CIT	C4-C3-C6	-2.36	104.81	110.03
2	B	9206	CIT	O7-C3-C6	2.35	112.29	108.96
2	A	9203	CIT	C4-C3-C6	2.32	115.17	110.03
2	B	9205	CIT	O6-C6-C3	2.31	117.56	113.14
3	A	9104	GOL	C3-C2-C1	-2.29	103.40	111.80
2	B	9204	CIT	O5-C6-C3	-2.27	117.70	122.09
2	A	9203	CIT	O4-C5-C4	2.20	121.32	114.35
2	B	9205	CIT	C3-C4-C5	-2.14	108.06	113.92
2	B	9206	CIT	O5-C6-C3	-2.14	117.95	122.09

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9202	CIT	C1-C2-C3-O7
2	A	9202	CIT	C1-C2-C3-C4
2	A	9207	CIT	O7-C3-C6-O5
2	A	9207	CIT	O7-C3-C6-O6
2	A	9207	CIT	C4-C3-C6-O5
2	A	9207	CIT	C4-C3-C6-O6
2	B	9201	CIT	C1-C2-C3-O7
2	B	9201	CIT	C1-C2-C3-C4
2	B	9201	CIT	C2-C3-C6-O5
2	B	9201	CIT	C2-C3-C6-O6
2	B	9201	CIT	O7-C3-C6-O5
2	B	9201	CIT	O7-C3-C6-O6
2	B	9205	CIT	C1-C2-C3-O7
2	B	9205	CIT	C1-C2-C3-C4
2	B	9206	CIT	C2-C3-C4-C5
2	B	9206	CIT	C6-C3-C4-C5
3	A	9101	GOL	O1-C1-C2-C3
3	A	9104	GOL	O1-C1-C2-C3
3	B	9102	GOL	O1-C1-C2-C3
2	A	9202	CIT	C1-C2-C3-C6
2	B	9201	CIT	C1-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
2	B	9204	CIT	C1-C2-C3-O7
2	B	9204	CIT	C1-C2-C3-C4
2	B	9204	CIT	C1-C2-C3-C6
2	B	9205	CIT	C1-C2-C3-C6
2	A	9203	CIT	O7-C3-C4-C5
2	A	9207	CIT	C1-C2-C3-O7
2	A	9207	CIT	C1-C2-C3-C6
2	B	9206	CIT	C1-C2-C3-O7
2	B	9206	CIT	O7-C3-C4-C5
3	A	9101	GOL	O1-C1-C2-O2
3	B	9102	GOL	O1-C1-C2-O2
2	B	9201	CIT	O7-C3-C4-C5
2	B	9201	CIT	C6-C3-C4-C5
2	B	9204	CIT	O7-C3-C4-C5
2	B	9204	CIT	C6-C3-C4-C5
2	A	9207	CIT	O2-C1-C2-C3
2	B	9201	CIT	C2-C3-C4-C5
3	A	9104	GOL	O1-C1-C2-O2
2	A	9207	CIT	O1-C1-C2-C3
2	A	9203	CIT	C6-C3-C4-C5
2	A	9207	CIT	C2-C3-C4-C5
2	B	9204	CIT	C2-C3-C4-C5
2	B	9201	CIT	C3-C4-C5-O3
2	A	9207	CIT	C1-C2-C3-C4
2	B	9206	CIT	C1-C2-C3-C4
2	B	9201	CIT	C3-C4-C5-O4
2	A	9203	CIT	C2-C3-C4-C5
2	A	9207	CIT	O7-C3-C4-C5
2	A	9203	CIT	C3-C4-C5-O4
2	B	9206	CIT	C1-C2-C3-C6
2	A	9203	CIT	C3-C4-C5-O3
2	A	9202	CIT	C4-C3-C6-O5
2	A	9202	CIT	C4-C3-C6-O6
2	B	9206	CIT	O1-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9206	CIT	6	0
3	A	9104	GOL	2	0
3	A	9103	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9203	CIT	5	0
2	A	9207	CIT	5	0
2	B	9205	CIT	2	0
3	B	9102	GOL	2	0
2	A	9202	CIT	7	0
2	B	9204	CIT	4	0
2	B	9201	CIT	3	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 [i](#)

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

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, 95th 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 ²)	Q<0.9
1	A	676/676 (100%)	-0.23	3 (0%) 88 87	38, 74, 105, 123	0
1	B	676/676 (100%)	-0.27	4 (0%) 85 85	38, 75, 107, 124	0
All	All	1352/1352 (100%)	-0.25	7 (0%) 87 86	38, 75, 106, 124	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	CYS	2.9
1	A	275	GLY	2.3
1	B	612	VAL	2.2
1	B	615	CYS	2.1
1	B	335	PRO	2.1
1	B	414	LYS	2.1
1	A	29	VAL	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	A	9202	13/13	0.38	0.13	76,81,87,90	0
2	CIT	B	9205	13/13	0.49	0.11	81,87,91,94	0
2	CIT	B	9206	13/13	0.51	0.14	76,78,81,81	0
2	CIT	A	9207	13/13	0.54	0.13	80,85,89,90	0
2	CIT	B	9201	13/13	0.61	0.13	68,71,82,84	0
3	GOL	A	9103	6/6	0.61	0.17	79,83,85,86	0
3	GOL	B	9102	6/6	0.61	0.13	78,82,86,88	0
2	CIT	B	9204	13/13	0.64	0.11	73,77,84,86	0
3	GOL	A	9101	6/6	0.65	0.13	82,86,87,88	0
2	CIT	A	9203	13/13	0.67	0.10	77,81,88,89	0
3	GOL	A	9104	6/6	0.82	0.11	73,75,78,80	0

6.5 Other polymers

There are no such residues in this entry.