



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 1KCW / pdb_00001kcw
Title : X-RAY CRYSTAL STRUCTURE OF HUMAN CERULOPLASMIN AT 3.0
ANGSTROMS
Authors : Card, G.L.; Zaitsev, V.N.; Lindley, P.F.
Deposited on : 1996-09-25
Resolution : 3.00 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

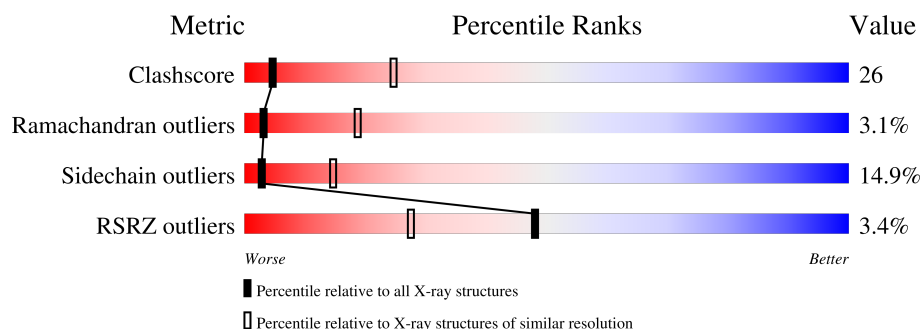
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1046	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8228 atoms, of which 3 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 CERULOPLASMIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1017	Total	C	H	N	O	S	0	0	0
			8190	5225	3	1361	1563	38			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



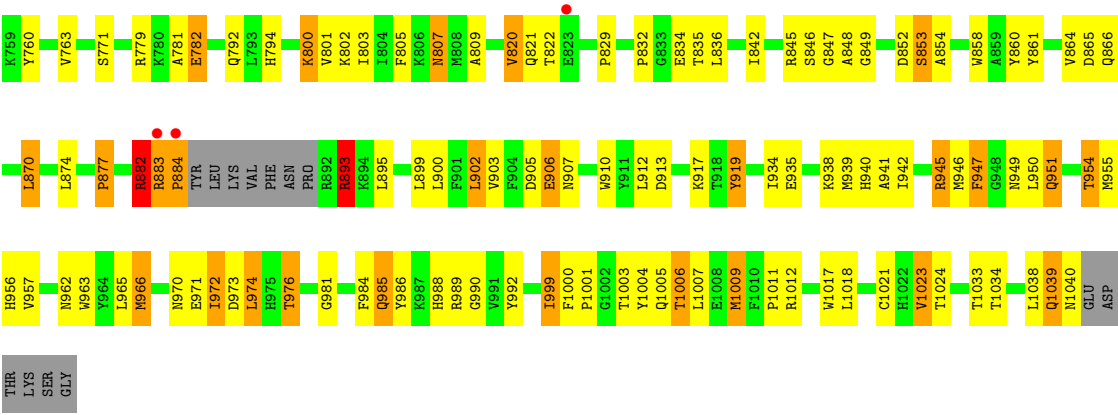
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	Cu	0	0
			8	8		

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.92Å 213.92Å 85.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.00 12.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (12.00-3.00) 96.8 (12.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.286 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8228	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: CU, O, NAG

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	0.86	16/8417 (0.2%)	1.34	118/11429 (1.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	SER	CA-C	-9.56	1.40	1.52
1	A	243	VAL	N-CA	-9.02	1.35	1.46
1	A	586	ASP	N-CA	-8.29	1.35	1.46
1	A	28	VAL	N-CA	-7.71	1.36	1.46
1	A	704	GLU	N-CA	7.48	1.55	1.46
1	A	636	VAL	CA-CB	6.63	1.62	1.53
1	A	287	ASN	CA-C	6.42	1.61	1.52
1	A	287	ASN	C-N	6.08	1.41	1.33
1	A	704	GLU	CA-C	5.91	1.59	1.52
1	A	288	LYS	N-CA	5.80	1.53	1.46
1	A	1009	MET	SD-CE	-5.67	1.65	1.79
1	A	27	SER	C-N	-5.60	1.26	1.33
1	A	976	THR	CA-CB	-5.46	1.46	1.53
1	A	585	PRO	C-N	-5.46	1.26	1.33
1	A	854	ALA	CA-CB	-5.40	1.44	1.53
1	A	242	SER	C-N	-5.16	1.26	1.33

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	PHE	CB-CA-C	-16.71	77.17	110.42
1	A	28	VAL	CB-CA-C	15.04	135.96	111.29
1	A	705	ASP	CB-CA-C	-13.03	92.11	111.91
1	A	705	ASP	N-CA-C	11.53	128.56	110.70
1	A	28	VAL	N-CA-C	-11.05	86.35	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ILE	N-CA-C	-10.14	101.52	110.74
1	A	247	THR	CB-CA-C	-9.67	93.31	109.55
1	A	247	THR	N-CA-C	9.47	126.03	113.72
1	A	684	ASP	O-C-N	9.21	134.84	122.59
1	A	524	VAL	N-CA-C	-9.20	101.43	110.72
1	A	986	TYR	N-CA-C	9.10	125.00	114.62
1	A	273	VAL	N-CA-C	-9.05	102.36	111.77
1	A	985	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	A	283	GLN	OE1-CD-NE2	-8.88	113.72	122.60
1	A	320	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	A	552	GLN	OE1-CD-NE2	-8.72	113.88	122.60
1	A	951	GLN	OE1-CD-NE2	-8.58	114.02	122.60
1	A	327	ALA	N-CA-C	-8.45	103.09	112.72
1	A	974	LEU	N-CA-C	-8.11	95.51	108.73
1	A	243	VAL	O-C-N	-8.11	112.43	122.57
1	A	187	ASP	CB-CA-C	-7.93	101.60	111.43
1	A	553	LYS	N-CA-C	7.60	119.65	111.36
1	A	702	GLN	N-CA-C	7.54	120.78	108.26
1	A	910	TRP	N-CA-C	-7.54	103.34	112.54
1	A	96	ARG	CA-C-N	7.53	127.96	119.83
1	A	96	ARG	C-N-CA	7.53	127.96	119.83
1	A	701	ARG	N-CA-C	-7.44	96.19	108.76
1	A	883	ARG	N-CA-C	7.44	118.68	110.13
1	A	703	SER	N-CA-C	7.30	126.34	110.80
1	A	23	LYS	N-CA-C	-7.10	105.08	113.38
1	A	708	PHE	N-CA-C	7.09	125.91	110.80
1	A	410	THR	N-CA-C	6.98	118.97	111.36
1	A	405	VAL	N-CA-C	6.98	119.26	108.44
1	A	334	GLN	N-CA-C	6.76	120.32	108.75
1	A	704	GLU	N-CA-CB	-6.74	99.35	110.68
1	A	234	PHE	N-CA-C	-6.74	103.86	111.14
1	A	163	HIS	N-CA-C	6.69	118.97	110.61
1	A	33	SER	N-CA-C	-6.67	103.17	112.45
1	A	29	ASP	N-CA-CB	-6.65	99.01	109.51
1	A	744	VAL	N-CA-C	6.64	118.63	109.80
1	A	270	GLY	N-CA-C	6.63	118.87	110.38
1	A	941	ALA	N-CA-C	6.61	119.92	109.81
1	A	66	GLU	N-CA-C	6.43	119.19	108.96
1	A	684	ASP	CA-C-N	-6.43	111.67	120.28
1	A	684	ASP	C-N-CA	-6.43	111.67	120.28
1	A	283	GLN	N-CA-C	6.43	120.54	108.65
1	A	919	TYR	N-CA-C	6.38	121.09	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	283	GLN	CG-CD-NE2	6.36	125.93	116.40
1	A	985	GLN	CG-CD-NE2	6.35	125.92	116.40
1	A	877	PRO	CA-N-CD	-6.35	103.12	112.00
1	A	882	ARG	N-CA-C	6.34	121.26	111.56
1	A	52	LEU	N-CA-C	6.29	118.73	108.55
1	A	552	GLN	CG-CD-NE2	6.26	125.80	116.40
1	A	580	MET	N-CA-C	6.25	117.90	111.14
1	A	612	GLN	CA-C-N	6.21	127.60	119.84
1	A	612	GLN	C-N-CA	6.21	127.60	119.84
1	A	970	ASN	N-CA-C	6.18	119.06	109.60
1	A	350	LYS	N-CA-C	6.16	118.80	111.71
1	A	951	GLN	CG-CD-NE2	6.13	125.60	116.40
1	A	422	PRO	N-CA-C	-6.10	106.23	113.86
1	A	632	ASN	N-CA-C	6.09	117.96	109.31
1	A	756	ILE	CB-CA-C	6.09	118.46	110.91
1	A	534	LEU	N-CA-C	6.08	119.13	108.56
1	A	853	SER	N-CA-C	-6.00	103.03	110.41
1	A	250	SER	N-CA-C	5.96	119.81	112.54
1	A	289	ASN	O-C-N	5.90	130.44	122.59
1	A	947	PHE	N-CA-C	5.84	117.74	110.91
1	A	282	GLY	N-CA-C	5.77	119.47	112.49
1	A	171	ALA	N-CA-C	-5.76	105.00	111.28
1	A	491	ALA	CA-C-N	5.76	127.04	119.84
1	A	491	ALA	C-N-CA	5.76	127.04	119.84
1	A	29	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	59	GLU	N-CA-C	-5.63	106.26	113.01
1	A	367	ALA	CA-C-N	5.61	126.85	119.84
1	A	367	ALA	C-N-CA	5.61	126.85	119.84
1	A	242	SER	CA-C-N	-5.56	111.96	121.97
1	A	242	SER	C-N-CA	-5.56	111.96	121.97
1	A	695	THR	N-CA-C	5.55	118.01	109.07
1	A	251	LEU	CA-C-N	5.49	126.70	119.84
1	A	251	LEU	C-N-CA	5.49	126.70	119.84
1	A	578	ILE	N-CA-C	-5.45	105.41	110.53
1	A	240	MET	N-CA-C	5.44	118.21	107.98
1	A	460	GLY	N-CA-C	5.44	122.25	114.64
1	A	985	GLN	CA-C-N	-5.44	111.25	121.63
1	A	985	GLN	C-N-CA	-5.44	111.25	121.63
1	A	945	ARG	N-CA-C	5.40	118.25	109.06
1	A	40	GLY	CA-C-N	5.40	126.59	119.84
1	A	40	GLY	C-N-CA	5.40	126.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	O-C-N	-5.39	114.96	122.19
1	A	705	ASP	O-C-N	-5.38	115.51	122.61
1	A	954	THR	N-CA-C	5.33	117.77	108.76
1	A	26	ILE	N-CA-C	-5.32	104.44	111.09
1	A	161	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
1	A	37	LEU	N-CA-C	5.24	119.36	112.92
1	A	115	ILE	N-CA-C	5.22	115.42	108.11
1	A	781	ALA	N-CA-C	5.22	116.65	111.07
1	A	893	ARG	N-CA-C	5.21	117.94	109.86
1	A	858	TRP	N-CA-C	-5.21	101.16	109.23
1	A	981	GLY	N-CA-C	5.20	122.27	115.40
1	A	286	THR	CA-C-N	-5.17	113.10	122.50
1	A	286	THR	C-N-CA	-5.17	113.10	122.50
1	A	187	ASP	N-CA-C	5.16	115.97	107.20
1	A	985	GLN	O-C-N	-5.13	116.48	123.10
1	A	95	SER	N-CA-C	5.13	119.29	113.19
1	A	860	TYR	N-CA-C	-5.12	101.34	109.59
1	A	67	LYS	CA-C-N	5.12	126.24	119.84
1	A	67	LYS	C-N-CA	5.12	126.24	119.84
1	A	57	THR	CB-CA-C	-5.10	102.84	110.90
1	A	285	LEU	N-CA-C	-5.10	99.94	110.80
1	A	846	SER	N-CA-C	-5.09	106.48	113.30
1	A	268	GLY	N-CA-C	-5.07	104.80	112.41
1	A	245	GLY	N-CA-C	-5.06	107.67	114.25
1	A	281	HIS	N-CA-C	5.06	121.57	110.80
1	A	704	GLU	CA-C-N	5.05	129.69	122.21
1	A	704	GLU	C-N-CA	5.05	129.69	122.21
1	A	243	VAL	CA-C-N	-5.05	113.17	122.31
1	A	243	VAL	C-N-CA	-5.05	113.17	122.31

There are no chirality outliers.

There are no planarity outliers.

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	8187	3	7732	413	1
2	A	28	0	26	1	0
3	A	8	0	0	0	0
4	A	2	0	0	0	0
All	All	8225	3	7758	414	1

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 26.

All (414) 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:24:LYS:HA	1:A:474:PRO:CG	1.79	1.12
1:A:24:LYS:HA	1:A:474:PRO:HG3	1.29	1.12
1:A:23:LYS:O	1:A:474:PRO:HG3	1.55	1.05
1:A:294:THR:HG21	1:A:661:GLN:HG2	1.39	1.04
1:A:288:LYS:HG3	1:A:303:PHE:CZ	1.99	0.98
1:A:756:ILE:HG12	1:A:919:TYR:HB2	1.46	0.97
1:A:470:THR:HG23	1:A:523:ALA:HB1	1.44	0.96
1:A:201:MET:HE3	1:A:203:SER:HB3	1.56	0.88
1:A:27:SER:C	1:A:28:VAL:O	2.04	0.85
1:A:585:PRO:O	1:A:586:ASP:C	2.14	0.84
1:A:26:ILE:O	1:A:28:VAL:HG23	1.80	0.81
1:A:26:ILE:O	1:A:28:VAL:N	2.13	0.80
1:A:760:TYR:HE1	1:A:939:MET:HE2	1.47	0.80
1:A:551:ARG:HH11	1:A:551:ARG:HB3	1.48	0.79
1:A:485:PRO:HG3	1:A:494:GLU:HB3	1.65	0.78
1:A:749:LEU:HD12	1:A:758:SER:HB3	1.63	0.77
1:A:24:LYS:HA	1:A:474:PRO:HG2	1.67	0.75
1:A:285:LEU:O	1:A:285:LEU:HG	1.87	0.75
1:A:652:ARG:HD3	1:A:845:ARG:O	1.86	0.74
1:A:564:THR:HG22	1:A:565:VAL:N	2.03	0.74
1:A:280:PHE:HB2	1:A:285:LEU:HD22	1.68	0.74
1:A:612:GLN:HE21	1:A:692:GLN:HG3	1.54	0.73
1:A:110:GLU:HG3	1:A:124:GLN:HG2	1.71	0.73
1:A:459:ILE:HD11	1:A:521:TYR:CE1	2.24	0.73
1:A:257:CYS:O	1:A:260:ASP:HB2	1.89	0.72
1:A:229:LYS:HA	1:A:234:PHE:CD2	2.23	0.72
1:A:96:ARG:HB2	1:A:97:PRO:HD2	1.72	0.72
1:A:503:PRO:O	1:A:506:VAL:HG12	1.89	0.72
1:A:24:LYS:CA	1:A:474:PRO:HG3	2.17	0.72
1:A:247:THR:O	1:A:328:GLY:O	2.09	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HG	1:A:27:SER:HB2	1.71	0.71
1:A:564:THR:HG22	1:A:565:VAL:H	1.56	0.70
1:A:42:ASP:HB2	1:A:43:ARG:NH1	2.06	0.69
1:A:503:PRO:HD2	1:A:506:VAL:HG11	1.75	0.68
1:A:807:ASN:C	1:A:807:ASN:HD22	2.02	0.68
1:A:27:SER:HA	1:A:28:VAL:O	1.93	0.68
1:A:23:LYS:O	1:A:23:LYS:HD3	1.94	0.68
1:A:56:TYR:CE2	1:A:64:THR:HG22	2.29	0.67
1:A:208:ASN:ND2	1:A:238:ASN:HB2	2.10	0.67
1:A:800:LYS:NZ	1:A:800:LYS:HB3	2.08	0.67
1:A:68:PRO:HD2	1:A:71:LEU:HD12	1.78	0.66
1:A:16:TYR:CE2	1:A:240:MET:HG3	2.30	0.66
1:A:162:SER:HB3	1:A:169:ASP:HB3	1.76	0.65
1:A:286:THR:CG2	1:A:291:ARG:HG3	2.26	0.65
1:A:286:THR:HG22	1:A:292:ILE:O	1.95	0.65
1:A:404:LEU:HD22	1:A:534:LEU:HD11	1.78	0.65
1:A:612:GLN:NE2	1:A:692:GLN:HG3	2.13	0.64
1:A:395:THR:HG22	1:A:588:VAL:HG22	1.78	0.64
1:A:243:VAL:HG22	1:A:244:ASN:N	2.12	0.64
1:A:27:SER:CA	1:A:28:VAL:O	2.45	0.64
1:A:285:LEU:HB3	1:A:307:MET:CE	2.26	0.64
1:A:635:ASP:O	1:A:659:PHE:HA	1.98	0.64
1:A:23:LYS:C	1:A:474:PRO:HG3	2.23	0.64
1:A:371:ILE:HD11	1:A:376:LYS:HA	1.79	0.63
1:A:1021:CYS:SG	1:A:1023:VAL:HG13	2.38	0.63
1:A:404:LEU:HB2	1:A:573:LEU:HD11	1.80	0.63
1:A:473:SER:HB3	1:A:474:PRO:HD3	1.80	0.63
1:A:23:LYS:HA	1:A:23:LYS:HZ3	1.63	0.63
1:A:23:LYS:O	1:A:474:PRO:CG	2.39	0.63
1:A:254:LEU:HB3	1:A:333:PHE:HB2	1.80	0.63
1:A:551:ARG:HB3	1:A:551:ARG:NH1	2.13	0.63
1:A:760:TYR:CE1	1:A:939:MET:HE2	2.30	0.62
1:A:6:TYR:HB2	1:A:56:TYR:O	1.98	0.62
1:A:25:LEU:H	1:A:474:PRO:HD3	1.65	0.62
1:A:267:PHE:HA	1:A:301:THR:O	1.98	0.62
1:A:676:PHE:HB2	1:A:694:TYR:CE1	2.34	0.62
1:A:229:LYS:HA	1:A:234:PHE:HD2	1.64	0.62
1:A:181:CYS:SG	1:A:186:LEU:HD13	2.39	0.62
1:A:285:LEU:HB3	1:A:307:MET:HE2	1.81	0.62
1:A:374:PHE:CE1	1:A:691:LYS:HD3	2.35	0.62
1:A:222:SER:C	1:A:224:PRO:HD3	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:HB2	1:A:306:TYR:HB3	1.82	0.61
1:A:166:ALA:O	1:A:170:ILE:HG13	2.00	0.61
1:A:107:TYR:HE1	1:A:112:GLU:HG3	1.65	0.61
1:A:585:PRO:O	1:A:587:GLN:N	2.33	0.61
1:A:913:ASP:O	1:A:917:LYS:HD3	2.00	0.61
1:A:617:MET:SD	1:A:623:VAL:HG21	2.40	0.61
1:A:763:VAL:HG13	1:A:874:LEU:HG	1.83	0.61
1:A:604:MET:HE2	1:A:690:MET:HG2	1.83	0.60
1:A:261:ARG:HG3	1:A:261:ARG:HH11	1.64	0.60
1:A:583:THR:HG22	1:A:583:THR:O	2.01	0.60
1:A:256:MET:HE1	1:A:333:PHE:HD2	1.66	0.60
1:A:71:LEU:HD22	1:A:74:LEU:HB2	1.83	0.60
1:A:882:ARG:HG3	1:A:882:ARG:HH11	1.65	0.60
1:A:50:LYS:HG3	1:A:52:LEU:HD23	1.84	0.59
1:A:110:GLU:CG	1:A:124:GLN:HG2	2.32	0.59
1:A:51:ALA:H	1:A:212:TYR:HE2	1.48	0.59
1:A:371:ILE:HG13	1:A:377:GLU:O	2.03	0.59
1:A:520:TYR:HB3	1:A:538:MET:CE	2.32	0.59
1:A:574:LEU:O	1:A:578:ILE:HG12	2.02	0.59
1:A:625:TRP:HB2	1:A:666:LEU:HB2	1.85	0.58
1:A:16:TYR:HD1	1:A:245:GLY:O	1.86	0.58
1:A:26:ILE:HD11	1:A:248:PHE:C	2.29	0.58
1:A:25:LEU:O	1:A:472:TYR:HA	2.04	0.58
1:A:258:ALA:HB2	1:A:312:PRO:HG3	1.86	0.58
1:A:680:CYS:SG	1:A:682:THR:HG23	2.44	0.58
1:A:457:GLU:HG3	1:A:523:ALA:CB	2.34	0.58
1:A:882:ARG:HG3	1:A:882:ARG:NH1	2.19	0.58
1:A:201:MET:HE3	1:A:203:SER:CB	2.32	0.57
1:A:562:PHE:HD1	1:A:628:PHE:CD1	2.22	0.57
1:A:241:TYR:O	1:A:247:THR:HG22	2.04	0.57
1:A:15:ASP:C	1:A:17:ALA:H	2.11	0.57
1:A:50:LYS:HG3	1:A:52:LEU:CD2	2.35	0.56
1:A:316:MET:CE	1:A:330:GLN:HG2	2.34	0.56
1:A:641:PHE:CD1	1:A:678:VAL:HG13	2.40	0.56
1:A:708:PHE:O	1:A:709:TYR:CG	2.58	0.56
1:A:157:THR:HG21	1:A:303:PHE:O	2.04	0.56
1:A:883:ARG:HB2	1:A:884:PRO:HD2	1.87	0.56
1:A:454:LEU:HD13	1:A:534:LEU:HD21	1.88	0.56
1:A:26:ILE:HG23	1:A:330:GLN:NE2	2.20	0.56
1:A:760:TYR:CD2	1:A:906:GLU:HG2	2.41	0.56
1:A:73:PHE:CD1	1:A:73:PHE:C	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:HG3	1:A:1017:TRP:HZ3	1.71	0.56
1:A:250:SER:O	1:A:252:PRO:HD3	2.06	0.56
1:A:256:MET:HE1	1:A:333:PHE:CD2	2.40	0.56
1:A:893:ARG:H	1:A:893:ARG:HD3	1.71	0.56
1:A:405:VAL:HG22	1:A:406:TYR:N	2.21	0.55
1:A:525:ASP:OD2	1:A:528:LYS:HB2	2.06	0.55
1:A:7:ILE:O	1:A:90:LEU:HA	2.06	0.55
1:A:157:THR:HB	1:A:265:TYR:HB3	1.89	0.55
1:A:637:HIS:HB3	1:A:680:CYS:SG	2.47	0.55
1:A:782:GLU:CD	1:A:782:GLU:H	2.14	0.55
1:A:92:ASN:HD21	1:A:94:ALA:HB3	1.71	0.55
1:A:9:ILE:HG23	1:A:174:LEU:HD21	1.89	0.55
1:A:50:LYS:HB2	1:A:172:SER:O	2.07	0.55
1:A:388:VAL:HG13	1:A:389:PHE:CD1	2.41	0.55
1:A:562:PHE:HD1	1:A:628:PHE:CE1	2.24	0.55
1:A:652:ARG:HD3	1:A:845:ARG:C	2.32	0.54
1:A:756:ILE:HD12	1:A:760:TYR:CE2	2.42	0.54
1:A:1039:GLN:NE2	1:A:1040:ASN:N	2.54	0.54
1:A:281:HIS:HE1	1:A:318:SER:OG	1.91	0.54
1:A:988:HIS:O	1:A:989:ARG:HB2	2.07	0.54
1:A:966:MET:HA	1:A:1003:THR:O	2.08	0.54
1:A:23:LYS:HA	1:A:23:LYS:NZ	2.22	0.54
1:A:609:TYR:CE1	1:A:689:GLY:HA3	2.43	0.54
1:A:893:ARG:HH12	1:A:956:HIS:CG	2.25	0.54
1:A:307:MET:HG2	1:A:308:VAL:N	2.23	0.54
1:A:753:GLU:CD	1:A:753:GLU:H	2.14	0.54
1:A:223:GLU:O	1:A:225:GLU:N	2.41	0.54
1:A:985:GLN:HB3	1:A:990:GLY:CA	2.38	0.54
1:A:50:LYS:HB2	1:A:50:LYS:HZ2	1.73	0.53
1:A:426:HIS:CE1	1:A:427:LEU:HD13	2.43	0.53
1:A:73:PHE:C	1:A:73:PHE:HD1	2.16	0.53
1:A:16:TYR:CD2	1:A:240:MET:HE2	2.43	0.53
1:A:107:TYR:HB2	1:A:111:HIS:HB2	1.89	0.53
1:A:447:HIS:CD2	1:A:449:LYS:HG3	2.43	0.53
1:A:401:TYR:CD2	1:A:568:GLU:HG3	2.44	0.53
1:A:388:VAL:HG13	1:A:389:PHE:CE1	2.44	0.53
1:A:157:THR:HG22	1:A:304:ASP:HB3	1.91	0.53
1:A:562:PHE:CD1	1:A:628:PHE:CE1	2.96	0.53
1:A:286:THR:HG21	1:A:291:ARG:HG3	1.91	0.52
1:A:519:MET:HE3	1:A:535:ILE:HD11	1.90	0.52
1:A:42:ASP:HB2	1:A:43:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:HIS:C	1:A:194:ILE:HD12	2.34	0.52
1:A:746:ASN:ND2	1:A:749:LEU:HD23	2.25	0.52
1:A:1005:GLN:HG3	1:A:1006:THR:N	2.25	0.52
1:A:350:LYS:CE	1:A:350:LYS:HA	2.38	0.52
1:A:350:LYS:HA	1:A:350:LYS:NZ	2.25	0.52
1:A:194:ILE:HG21	1:A:197:GLU:HG2	1.92	0.52
1:A:359:ALA:O	1:A:449:LYS:HB2	2.10	0.52
1:A:374:PHE:CD1	1:A:691:LYS:HD3	2.44	0.52
1:A:521:TYR:HB3	1:A:535:ILE:HD13	1.91	0.52
1:A:1033:THR:HG23	1:A:1034:THR:N	2.25	0.52
1:A:25:LEU:HD23	1:A:471:TYR:CE2	2.45	0.52
1:A:208:ASN:HD21	1:A:238:ASN:HB2	1.73	0.52
1:A:717:ILE:O	1:A:805:PHE:HA	2.10	0.52
1:A:902:LEU:HD22	1:A:903:VAL:N	2.25	0.52
1:A:756:ILE:HD13	1:A:757:GLY:N	2.23	0.51
1:A:1018:LEU:HA	1:A:1034:THR:HG22	1.91	0.51
1:A:562:PHE:CD1	1:A:628:PHE:HE1	2.29	0.51
1:A:229:LYS:HA	1:A:234:PHE:CE2	2.45	0.51
1:A:459:ILE:HD11	1:A:521:TYR:HE1	1.72	0.51
1:A:397:ILE:HD11	1:A:578:ILE:HD13	1.92	0.51
1:A:129:LYS:O	1:A:129:LYS:HG2	2.11	0.51
1:A:366:TYR:HD1	1:A:606:GLY:O	1.93	0.51
1:A:520:TYR:O	1:A:535:ILE:HD12	2.11	0.51
1:A:637:HIS:HA	1:A:682:THR:HG21	1.92	0.51
1:A:243:VAL:O	1:A:245:GLY:N	2.43	0.50
1:A:167:PRO:HB3	1:A:1024:THR:HG23	1.94	0.50
1:A:433:VAL:HG12	1:A:435:TRP:HD1	1.75	0.50
1:A:96:ARG:CB	1:A:97:PRO:HD2	2.40	0.50
1:A:491:ALA:HB1	1:A:492:PRO:HD2	1.92	0.50
1:A:683:THR:O	1:A:686:TYR:N	2.45	0.50
1:A:470:THR:HG23	1:A:523:ALA:CB	2.29	0.50
1:A:585:PRO:C	1:A:587:GLN:N	2.65	0.50
1:A:405:VAL:HG21	1:A:429:ILE:O	2.12	0.50
1:A:406:TYR:OH	1:A:456:ILE:HG22	2.11	0.50
1:A:366:TYR:CD1	1:A:606:GLY:O	2.64	0.50
1:A:546:LEU:HD23	1:A:552:GLN:HA	1.94	0.50
1:A:177:PRO:CG	1:A:199:VAL:HG11	2.42	0.50
1:A:272:GLU:OE1	1:A:972:ILE:HG23	2.12	0.49
1:A:455:SER:O	1:A:522:SER:HA	2.12	0.49
1:A:491:ALA:HB3	1:A:494:GLU:HG3	1.94	0.49
1:A:963:TRP:HE1	1:A:1009:MET:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:VAL:HG21	1:A:971:GLU:O	2.12	0.49
1:A:592:ASP:O	1:A:596:GLN:HG2	2.11	0.49
1:A:395:THR:HG22	1:A:588:VAL:HA	1.93	0.49
1:A:934:ILE:HG22	1:A:938:LYS:HE3	1.94	0.49
1:A:71:LEU:CD2	1:A:74:LEU:HB2	2.42	0.49
1:A:187:ASP:O	1:A:187:ASP:CG	2.54	0.49
1:A:714:THR:HB	1:A:802:LYS:HB3	1.93	0.49
1:A:108:TYR:N	1:A:108:TYR:CD1	2.80	0.49
1:A:251:LEU:HB3	1:A:331:ALA:HB1	1.94	0.49
1:A:710:LEU:C	1:A:710:LEU:HD12	2.37	0.49
1:A:966:MET:CB	1:A:1004:TYR:HD1	2.25	0.49
1:A:196:ARG:HB3	1:A:198:PHE:CE1	2.47	0.49
1:A:966:MET:HB3	1:A:1004:TYR:HD1	1.77	0.49
1:A:15:ASP:HA	1:A:46:ARG:O	2.13	0.48
1:A:42:ASP:O	1:A:221:CYS:SG	2.67	0.48
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.29	0.48
1:A:285:LEU:HB3	1:A:307:MET:HE3	1.95	0.48
1:A:565:VAL:HG22	1:A:602:HIS:HD2	1.77	0.48
1:A:659:PHE:HB3	1:A:660:PRO:CD	2.42	0.48
1:A:905:ASP:O	1:A:907:ASN:N	2.46	0.48
1:A:22:GLU:C	1:A:24:LYS:N	2.68	0.48
1:A:155:CYS:SG	1:A:179:ILE:CG2	3.02	0.48
1:A:411:ASP:C	1:A:413:SER:N	2.71	0.48
1:A:984:PHE:CD2	1:A:1007:LEU:HD13	2.49	0.48
1:A:22:GLU:C	1:A:24:LYS:H	2.20	0.48
1:A:395:THR:HG22	1:A:588:VAL:CG2	2.43	0.48
1:A:10:ILE:HD12	1:A:10:ILE:O	2.14	0.48
1:A:560:TYR:CE1	1:A:626:TYR:CD2	3.02	0.48
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.68	0.47
1:A:562:PHE:HB2	1:A:628:PHE:CE1	2.49	0.47
1:A:636:VAL:HG23	1:A:636:VAL:O	2.14	0.47
1:A:30:THR:O	1:A:31:GLU:HB2	2.15	0.47
1:A:97:PRO:HA	1:A:130:VAL:O	2.14	0.47
1:A:320:GLN:HG3	1:A:661:GLN:OE1	2.14	0.47
1:A:403:LYS:HE3	1:A:532:THR:O	2.14	0.47
1:A:491:ALA:O	1:A:493:THR:N	2.47	0.47
1:A:671:ASP:OD1	1:A:672:THR:HG22	2.14	0.47
1:A:728:PRO:HD2	1:A:949:ASN:OD1	2.14	0.47
1:A:418:LYS:HE3	1:A:418:LYS:HB3	1.78	0.47
1:A:641:PHE:CE1	1:A:678:VAL:CG1	2.97	0.47
1:A:832:PRO:C	1:A:834:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:LEU:HB3	1:A:658:LEU:HD11	1.96	0.47
1:A:44:ILE:HG23	1:A:220:TYR:HB2	1.96	0.47
1:A:807:ASN:ND2	1:A:809:ALA:H	2.13	0.47
1:A:114:ALA:HA	1:A:163:HIS:HB3	1.97	0.47
1:A:295:ILE:HD13	1:A:303:PHE:CE1	2.50	0.47
1:A:618:CYS:O	1:A:621:ASP:HB2	2.15	0.47
1:A:644:ASN:OD1	1:A:670:PRO:HA	2.13	0.47
1:A:115:ILE:HG23	1:A:115:ILE:O	2.14	0.47
1:A:223:GLU:C	1:A:225:GLU:N	2.70	0.47
1:A:25:LEU:HD23	1:A:471:TYR:HE2	1.79	0.47
1:A:522:SER:HB3	1:A:529:ASP:HB3	1.97	0.47
1:A:155:CYS:O	1:A:265:TYR:HE1	1.98	0.47
1:A:18:SER:HB3	1:A:46:ARG:NH2	2.30	0.46
1:A:965:LEU:HB3	1:A:999:ILE:CD1	2.46	0.46
1:A:316:MET:HG3	1:A:317:LEU:N	2.29	0.46
1:A:636:VAL:O	1:A:682:THR:HG21	2.15	0.46
1:A:18:SER:C	1:A:20:HIS:N	2.71	0.46
1:A:50:LYS:CB	1:A:50:LYS:NZ	2.77	0.46
1:A:16:TYR:CD1	1:A:245:GLY:O	2.68	0.46
1:A:539:LYS:C	1:A:540:ILE:HD12	2.40	0.46
1:A:463:PHE:CD1	1:A:463:PHE:C	2.93	0.46
1:A:735:GLU:O	1:A:739:LEU:HG	2.15	0.46
1:A:406:TYR:CZ	1:A:456:ILE:HG22	2.51	0.46
1:A:100:PHE:O	1:A:100:PHE:CD1	2.69	0.46
1:A:683:THR:O	1:A:684:ASP:C	2.59	0.46
1:A:899:LEU:HB2	1:A:965:LEU:HD23	1.96	0.46
1:A:520:TYR:HB3	1:A:538:MET:HE1	1.98	0.46
1:A:631:GLY:HA3	1:A:635:ASP:OD2	2.16	0.46
1:A:12:THR:OG1	1:A:13:THR:N	2.49	0.45
1:A:455:SER:HB2	1:A:498:TYR:OH	2.16	0.45
1:A:957:VAL:HG23	1:A:1038:LEU:O	2.16	0.45
1:A:985:GLN:HA	1:A:992:TYR:O	2.15	0.45
1:A:366:TYR:CE2	1:A:601:MET:HG3	2.51	0.45
1:A:200:VAL:HG13	1:A:243:VAL:CG2	2.46	0.45
1:A:287:ASN:CB	1:A:306:TYR:HB3	2.47	0.45
1:A:350:LYS:CA	1:A:350:LYS:HE2	2.46	0.45
1:A:447:HIS:HD2	1:A:449:LYS:HG3	1.81	0.45
1:A:746:ASN:HD21	1:A:947:PHE:HE2	1.64	0.45
1:A:945:ARG:HE	1:A:945:ARG:HB3	1.53	0.45
1:A:154:ASN:O	1:A:181:CYS:HA	2.17	0.45
1:A:71:LEU:HD11	1:A:77:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PRO:HG3	1:A:199:VAL:HG11	1.98	0.45
1:A:677:ASN:HD21	1:A:693:LYS:NZ	2.14	0.45
1:A:708:PHE:O	1:A:709:TYR:CD2	2.70	0.45
1:A:829:PRO:HB3	1:A:864:VAL:HG22	1.99	0.45
1:A:849:GLY:H	1:A:852:ASP:HB2	1.81	0.45
1:A:251:LEU:HD12	1:A:252:PRO:HD2	1.97	0.45
1:A:350:LYS:HA	1:A:350:LYS:HE2	1.99	0.45
1:A:912:LEU:HD12	1:A:912:LEU:O	2.16	0.45
1:A:50:LYS:HZ2	1:A:50:LYS:CB	2.30	0.45
1:A:361:GLU:HA	1:A:404:LEU:HA	1.99	0.45
1:A:821:GLN:HG2	1:A:822:THR:N	2.31	0.45
1:A:935:GLU:HA	1:A:938:LYS:HG2	1.98	0.45
1:A:374:PHE:CZ	1:A:691:LYS:HB2	2.53	0.44
1:A:406:TYR:CE1	1:A:456:ILE:HG22	2.52	0.44
1:A:634:ALA:HB1	1:A:971:GLU:OE2	2.16	0.44
1:A:155:CYS:HA	1:A:180:ILE:O	2.17	0.44
1:A:288:LYS:HG3	1:A:303:PHE:CE1	2.48	0.44
1:A:627:LEU:N	1:A:627:LEU:HD23	2.33	0.44
2:A:1048:NAG:O7	2:A:1048:NAG:H3	2.16	0.44
1:A:611:ASN:O	1:A:613:PRO:HD3	2.18	0.44
1:A:972:ILE:O	1:A:974:LEU:HD12	2.18	0.44
1:A:286:THR:HA	1:A:292:ILE:HD12	1.99	0.44
1:A:389:PHE:CD1	1:A:389:PHE:N	2.86	0.44
1:A:596:GLN:HG2	1:A:596:GLN:H	1.68	0.44
1:A:126:ALA:HB3	1:A:136:TYR:HE2	1.82	0.44
1:A:196:ARG:HB3	1:A:198:PHE:HE1	1.82	0.44
1:A:316:MET:SD	1:A:330:GLN:HB3	2.58	0.44
1:A:369:SER:HG	1:A:611:ASN:HD21	1.64	0.44
1:A:371:ILE:HD11	1:A:376:LYS:CA	2.45	0.44
1:A:18:SER:O	1:A:20:HIS:N	2.51	0.43
1:A:266:LEU:O	1:A:267:PHE:HB3	2.18	0.43
1:A:756:ILE:HD13	1:A:756:ILE:C	2.43	0.43
1:A:568:GLU:HB2	1:A:599:ASN:HB3	1.99	0.43
1:A:720:VAL:O	1:A:763:VAL:HA	2.18	0.43
1:A:28:VAL:HG12	1:A:325:LEU:HD21	2.00	0.43
1:A:972:ILE:N	1:A:972:ILE:HD13	2.32	0.43
1:A:419:GLU:HA	1:A:419:GLU:OE1	2.18	0.43
1:A:470:THR:CG2	1:A:523:ALA:O	2.66	0.43
1:A:742:GLN:HB3	1:A:744:VAL:HG23	2.00	0.43
1:A:283:GLN:HB2	1:A:284:ALA:H	1.49	0.43
1:A:426:HIS:HA	1:A:613:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLU:CD	1:A:544:GLY:H	2.25	0.43
1:A:564:THR:CG2	1:A:565:VAL:H	2.29	0.43
1:A:580:MET:HE2	1:A:580:MET:HB3	1.94	0.43
1:A:744:VAL:HG12	1:A:745:SER:N	2.33	0.43
1:A:639:ILE:O	1:A:655:THR:HA	2.18	0.43
1:A:652:ARG:HD2	1:A:847:GLY:O	2.18	0.43
1:A:801:VAL:HG12	1:A:803:ILE:HD12	2.00	0.43
1:A:350:LYS:CE	1:A:350:LYS:CA	2.96	0.43
1:A:18:SER:C	1:A:20:HIS:H	2.27	0.43
1:A:217:ILE:HD13	1:A:227:VAL:HG21	2.01	0.43
1:A:411:ASP:CG	1:A:412:ALA:H	2.27	0.43
1:A:736:LEU:HD22	1:A:736:LEU:O	2.19	0.43
1:A:882:ARG:HH11	1:A:882:ARG:CG	2.31	0.43
1:A:280:PHE:CD1	1:A:285:LEU:HD13	2.54	0.43
1:A:285:LEU:O	1:A:285:LEU:CG	2.64	0.43
1:A:371:ILE:HG12	1:A:372:ASP:N	2.33	0.43
1:A:256:MET:HB3	1:A:260:ASP:OD2	2.19	0.42
1:A:444:VAL:HG11	1:A:456:ILE:CD1	2.49	0.42
1:A:565:VAL:HG22	1:A:602:HIS:CD2	2.53	0.42
1:A:723:GLU:HG3	1:A:919:TYR:OH	2.19	0.42
1:A:945:ARG:HD3	1:A:949:ASN:O	2.20	0.42
1:A:658:LEU:CD2	1:A:662:THR:HB	2.50	0.42
1:A:800:LYS:HB3	1:A:800:LYS:HZ3	1.80	0.42
1:A:861:TYR:CD1	1:A:861:TYR:N	2.87	0.42
1:A:659:PHE:HB3	1:A:660:PRO:HD2	2.01	0.42
1:A:951:GLN:H	1:A:951:GLN:HG2	1.65	0.42
1:A:42:ASP:HA	1:A:227:VAL:HG12	2.02	0.42
1:A:590:LYS:NZ	1:A:590:LYS:HB3	2.34	0.42
1:A:89:HIS:ND1	1:A:137:THR:HB	2.35	0.42
1:A:870:LEU:C	1:A:870:LEU:CD2	2.93	0.42
1:A:69:VAL:HG23	1:A:70:TRP:N	2.34	0.42
1:A:407:ARG:HD3	1:A:407:ARG:HA	1.78	0.42
1:A:411:ASP:CG	1:A:412:ALA:N	2.77	0.42
1:A:561:LEU:HB2	1:A:627:LEU:HD22	2.01	0.42
1:A:251:LEU:HD21	1:A:254:LEU:CD1	2.50	0.42
1:A:955:MET:HG3	1:A:1011:PRO:HG2	2.01	0.42
1:A:50:LYS:NZ	1:A:207:GLU:OE2	2.53	0.42
1:A:420:ARG:HG2	1:A:424:GLU:HG3	2.02	0.42
1:A:433:VAL:HA	1:A:537:PRO:HG2	2.01	0.42
1:A:79:LYS:HG2	1:A:179:ILE:HB	2.02	0.42
1:A:213:LEU:HA	1:A:213:LEU:HD12	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB3	1:A:409:TYR:HE2	1.85	0.42
1:A:251:LEU:HD21	1:A:254:LEU:HD11	2.01	0.41
1:A:372:ASP:O	1:A:376:LYS:N	2.53	0.41
1:A:373:ILE:HB	1:A:610:GLY:HA3	2.02	0.41
1:A:509:THR:O	1:A:512:ASP:HB2	2.20	0.41
1:A:578:ILE:O	1:A:582:THR:OG1	2.34	0.41
1:A:604:MET:HE3	1:A:604:MET:HB2	1.87	0.41
1:A:10:ILE:HD12	1:A:10:ILE:C	2.44	0.41
1:A:394:THR:HA	1:A:583:THR:HB	2.03	0.41
1:A:411:ASP:HB3	1:A:413:SER:OG	2.20	0.41
1:A:865:ASP:O	1:A:866:GLN:C	2.62	0.41
1:A:228:ASP:HB3	1:A:231:ASN:HB2	2.01	0.41
1:A:386:SER:O	1:A:387:ALA:C	2.63	0.41
1:A:103:HIS:HB2	1:A:159:ILE:O	2.20	0.41
1:A:243:VAL:C	1:A:245:GLY:H	2.29	0.41
1:A:434:ILE:O	1:A:538:MET:HA	2.21	0.41
1:A:15:ASP:C	1:A:17:ALA:N	2.77	0.41
1:A:204:VAL:O	1:A:206:ASP:N	2.53	0.41
1:A:350:LYS:HE2	1:A:350:LYS:N	2.35	0.41
1:A:7:ILE:HD12	1:A:7:ILE:N	2.35	0.41
1:A:136:TYR:CD1	1:A:136:TYR:C	2.98	0.41
1:A:534:LEU:N	1:A:534:LEU:HD12	2.36	0.41
1:A:736:LEU:HD13	1:A:736:LEU:C	2.45	0.41
1:A:883:ARG:HB2	1:A:884:PRO:CD	2.50	0.41
1:A:50:LYS:HB2	1:A:50:LYS:NZ	2.36	0.41
1:A:58:ASP:C	1:A:60:THR:N	2.79	0.41
1:A:183:LYS:HE2	1:A:183:LYS:HB3	1.81	0.41
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.71	0.41
1:A:516:LEU:HA	1:A:516:LEU:HD23	1.79	0.41
1:A:67:LYS:HA	1:A:68:PRO:HD3	1.95	0.41
1:A:448:ASN:OD1	1:A:449:LYS:N	2.54	0.41
1:A:448:ASN:HB2	1:A:490:VAL:HG12	2.03	0.41
1:A:626:TYR:C	1:A:627:LEU:HD23	2.46	0.41
1:A:669:TRP:O	1:A:670:PRO:C	2.61	0.41
1:A:820:VAL:HG22	1:A:842:ILE:CD1	2.51	0.41
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.85	0.41
1:A:165:ASP:OD1	1:A:167:PRO:HD2	2.22	0.40
1:A:401:TYR:O	1:A:403:LYS:HG3	2.21	0.40
1:A:458:PRO:HG2	1:A:458:PRO:O	2.21	0.40
1:A:288:LYS:HE2	1:A:303:PHE:CE2	2.56	0.40
1:A:416:ASN:H	1:A:416:ASN:HD22	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:PRO:O	1:A:588:VAL:N	2.34	0.40
1:A:905:ASP:OD1	1:A:907:ASN:HB2	2.21	0.40
1:A:938:LYS:O	1:A:940:HIS:ND1	2.51	0.40
1:A:384:SER:O	1:A:385:ASP:C	2.65	0.40
1:A:661:GLN:O	1:A:661:GLN:CG	2.69	0.40
1:A:73:PHE:HD1	1:A:73:PHE:O	2.03	0.40
1:A:110:GLU:O	1:A:111:HIS:CD2	2.75	0.40
1:A:288:LYS:HB2	1:A:292:ILE:HG12	2.04	0.40
1:A:298:PHE:HB3	1:A:299:PRO:HD2	2.03	0.40
1:A:309:ALA:HB1	1:A:335:VAL:CG2	2.52	0.40
1:A:368:PRO:C	1:A:370:GLY:N	2.78	0.40
1:A:518:LYS:HD3	1:A:518:LYS:HA	1.86	0.40
1:A:736:LEU:O	1:A:740:GLN:HG3	2.21	0.40
1:A:847:GLY:O	1:A:848:ALA:C	2.64	0.40
1:A:690:MET:HE3	1:A:690:MET:HB2	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LYS:O	1:A:712:GLU:OE2[2_654]	1.93	0.27

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	1009/1046 (96%)	836 (83%)	142 (14%)	31 (3%)	3 19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP

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Mol	Chain	Res	Type
1	A	27	SER
1	A	243	VAL
1	A	492	PRO
1	A	506	VAL
1	A	683	THR
1	A	703	SER
1	A	17	ALA
1	A	20	HIS
1	A	31	GLU
1	A	35	ILE
1	A	205	VAL
1	A	281	HIS
1	A	348	ARG
1	A	757	GLY
1	A	973	ASP
1	A	28	VAL
1	A	86	VAL
1	A	183	LYS
1	A	351	HIS
1	A	906	GLU
1	A	43	ARG
1	A	267	PHE
1	A	379	LEU
1	A	387	ALA
1	A	458	PRO
1	A	585	PRO
1	A	299	PRO
1	A	613	PRO
1	A	877	PRO
1	A	1001	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	880/921 (96%)	749 (85%)	131 (15%)	3 15

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	TRP
1	A	23	LYS
1	A	30	THR
1	A	32	HIS
1	A	37	LEU
1	A	38	GLN
1	A	42	ASP
1	A	46	ARG
1	A	50	LYS
1	A	52	LEU
1	A	54	LEU
1	A	57	THR
1	A	63	THR
1	A	67	LYS
1	A	71	LEU
1	A	73	PHE
1	A	103	HIS
1	A	106	THR
1	A	110	GLU
1	A	137	THR
1	A	141	LEU
1	A	155	CYS
1	A	157	THR
1	A	181	CYS
1	A	182	LYS
1	A	183	LYS
1	A	185	SER
1	A	186	LEU
1	A	189	GLU
1	A	218	LYS
1	A	223	GLU
1	A	225	GLU
1	A	236	GLU
1	A	247	THR
1	A	256	MET
1	A	259	GLU
1	A	260	ASP
1	A	266	LEU
1	A	283	GLN
1	A	288	LYS
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	291	ARG
1	A	292	ILE
1	A	294	THR
1	A	299	PRO
1	A	312	PRO
1	A	316	MET
1	A	317	LEU
1	A	330	GLN
1	A	334	GLN
1	A	347	ILE
1	A	350	LYS
1	A	351	HIS
1	A	362	ILE
1	A	376	LYS
1	A	388	VAL
1	A	394	THR
1	A	395	THR
1	A	396	ARG
1	A	400	SER
1	A	410	THR
1	A	416	ASN
1	A	417	ARG
1	A	423	GLU
1	A	424	GLU
1	A	427	LEU
1	A	438	VAL
1	A	457	GLU
1	A	470	THR
1	A	488	SER
1	A	490	VAL
1	A	492	PRO
1	A	495	THR
1	A	524	VAL
1	A	527	THR
1	A	549	ASN
1	A	552	GLN
1	A	561	LEU
1	A	590	LYS
1	A	596	GLN
1	A	613	PRO
1	A	627	LEU
1	A	649	ARG

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Mol	Chain	Res	Type
1	A	660	PRO
1	A	662	THR
1	A	672	THR
1	A	678	VAL
1	A	682	THR
1	A	687	THR
1	A	691	LYS
1	A	704	GLU
1	A	714	THR
1	A	720	VAL
1	A	729	GLN
1	A	736	LEU
1	A	749	LEU
1	A	753	GLU
1	A	756	ILE
1	A	771	SER
1	A	779	ARG
1	A	782	GLU
1	A	792	GLN
1	A	794	HIS
1	A	800	LYS
1	A	807	ASN
1	A	820	VAL
1	A	835	THR
1	A	836	LEU
1	A	853	SER
1	A	870	LEU
1	A	882	ARG
1	A	884	PRO
1	A	893	ARG
1	A	895	LEU
1	A	900	LEU
1	A	902	LEU
1	A	942	ILE
1	A	946	MET
1	A	950	LEU
1	A	954	THR
1	A	962	ASN
1	A	966	MET
1	A	972	ILE
1	A	976	THR
1	A	999	ILE

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Mol	Chain	Res	Type
1	A	1000	PHE
1	A	1006	THR
1	A	1012	ARG
1	A	1023	VAL
1	A	1039	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	92	ASN
1	A	111	HIS
1	A	281	HIS
1	A	289	ASN
1	A	296	ASN
1	A	320	GLN
1	A	334	GLN
1	A	416	ASN
1	A	489	HIS
1	A	587	GLN
1	A	602	HIS
1	A	611	ASN
1	A	612	GLN
1	A	632	ASN
1	A	657	ASN
1	A	677	ASN
1	A	729	GLN
1	A	740	GLN
1	A	746	ASN
1	A	807	ASN
1	A	980	HIS
1	A	1005	GLN
1	A	1039	GLN
1	A	1040	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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	NAG	A	1047	1	14,14,15	1.04	1 (7%)	17,19,21	1.56	4 (23%)
2	NAG	A	1048	1	14,14,15	0.84	1 (7%)	17,19,21	1.01	1 (5%)

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	NAG	A	1047	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1048	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1047	NAG	C1-C2	3.56	1.57	1.52
2	A	1048	NAG	C1-C2	2.38	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1047	NAG	C1-O5-C5	3.70	117.15	112.19
2	A	1047	NAG	O5-C1-C2	3.20	116.24	111.29
2	A	1048	NAG	O7-C7-C8	-2.71	117.23	122.05
2	A	1047	NAG	C1-C2-N2	-2.49	106.51	110.43
2	A	1047	NAG	O7-C7-C8	-2.02	118.46	122.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1047	NAG	O5-C5-C6-O6
2	A	1047	NAG	C4-C5-C6-O6
2	A	1048	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1048	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1017/1046 (97%)	-0.21	35 (3%) 48 27	6, 39, 108, 241	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	GLY	9.1
1	A	27	SER	6.6
1	A	684	ASP	6.0
1	A	287	ASN	5.5
1	A	704	GLU	4.5
1	A	29	ASP	4.3
1	A	884	PRO	3.9
1	A	183	LYS	3.9
1	A	18	SER	3.8
1	A	63	THR	3.6
1	A	289	ASN	3.5
1	A	22	GLU	3.3
1	A	34	ASN	3.2
1	A	584	ALA	2.9
1	A	473	SER	2.9
1	A	483	VAL	2.9
1	A	17	ALA	2.9
1	A	823	GLU	2.8
1	A	703	SER	2.8
1	A	586	ASP	2.7
1	A	883	ARG	2.7
1	A	38	GLN	2.7
1	A	706	SER	2.6
1	A	288	LYS	2.5
1	A	28	VAL	2.4
1	A	25	LEU	2.4
1	A	21	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	589	ASP	2.3
1	A	593	GLU	2.3
1	A	13	THR	2.3
1	A	413	SER	2.3
1	A	553	LYS	2.3
1	A	23	LYS	2.2
1	A	385	ASP	2.1
1	A	729	GLN	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	NAG	A	1048	14/15	0.62	0.25	284,284,284,284	0
2	NAG	A	1047	14/15	0.74	0.19	143,143,143,143	0
3	CU	A	1054	1/1	0.87	0.24	61,61,61,61	0
3	CU	A	1053	1/1	0.96	0.03	34,34,34,34	0
3	CU	A	1050	1/1	0.97	0.04	46,46,46,46	0
3	CU	A	1049	1/1	0.98	0.03	34,34,34,34	0
3	CU	A	1055	1/1	0.98	0.04	33,33,33,33	0
3	CU	A	1056	1/1	0.98	0.17	27,27,27,27	0
4	O	A	1057	1/1	0.98	0.05	6,6,6,6	0
4	O	A	1058	1/1	0.98	0.23	2,2,2,2	0
3	CU	A	1051	1/1	0.99	0.07	44,44,44,44	0
3	CU	A	1052	1/1	0.99	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.