Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:48 PM GMT

PDB ID	:	1CK7
Title	:	GELATINASE A (FULL-LENGTH)
Authors	:	Morgunova, E.; Tuuttila, A.; Bergmann, U.; Isupov, M.; Lindqvist, Y.; Schneider, G.; Tryggvason, K.
Deposited on	:	1999-04-28
Resolution	:	2.80 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

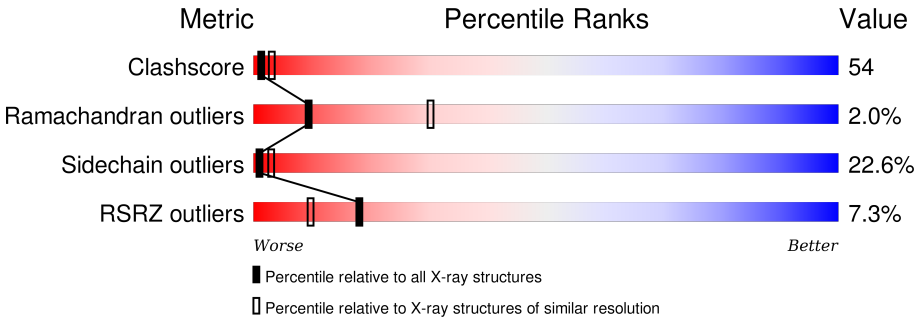
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	631	7%, 35%, 46%, 16%

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
4	CL	A	995	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5051 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 PROTEIN (GELATINASE A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4930	3166	812	925	27			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	ALA	GLU	ENGINEERED	UNP P08253

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		

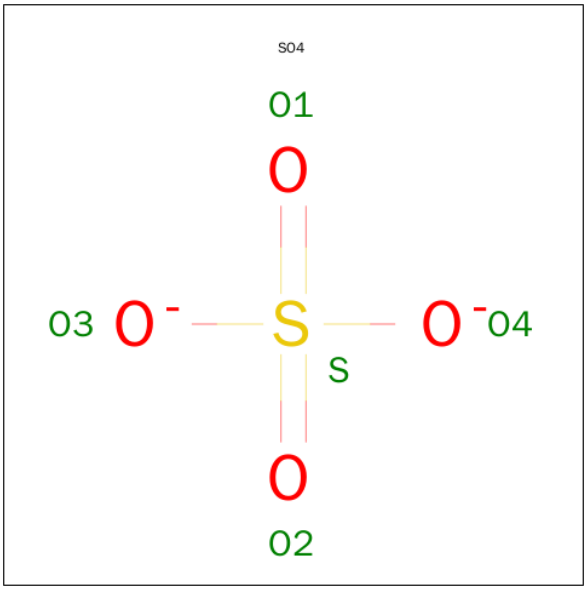
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

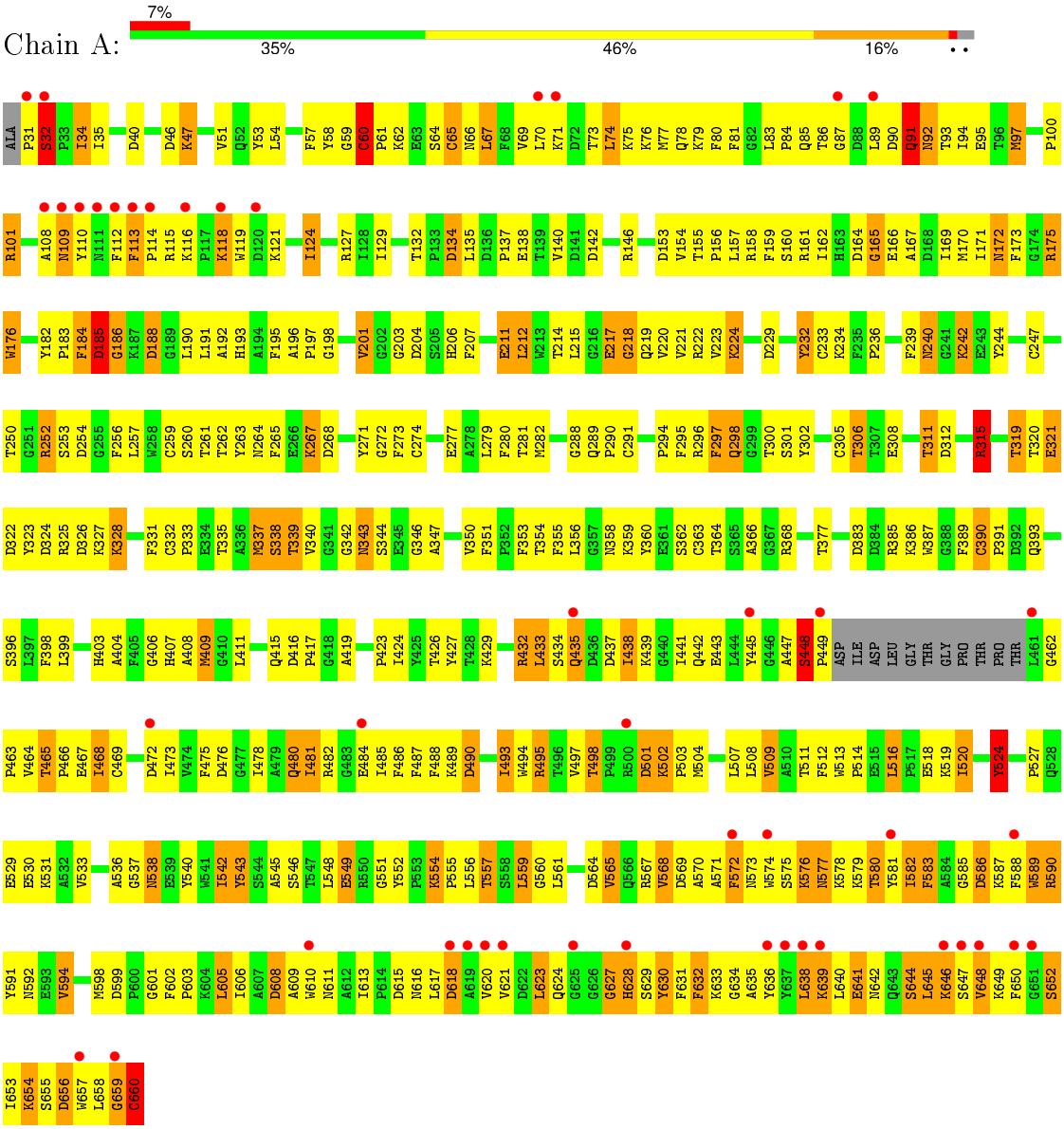
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	104	Total O 104 104	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PROTEIN (GELATINASE A)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	121.32Å 121.32Å 345.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 2.80 34.89 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.00-2.80) 88.5 (34.89-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	0.92 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.286 , 0.327 0.283 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	2 of 33340 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5051	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NA, ZN, CA, CL

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	1.32	2/5085 (0.0%)	1.36	40/6891 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	CYS	C-OXT	82.38	2.79	1.23
1	A	220	VAL	CB-CG1	5.94	1.65	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	659	GLY	C-N-CA	10.63	148.28	121.70
1	A	524	TYR	CA-CB-CG	10.03	132.45	113.40
1	A	175	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	252	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	222	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	60	CYS	CA-CB-SG	8.57	129.44	114.00
1	A	641	GLU	N-CA-CB	8.37	125.66	110.60
1	A	385	ARG	CD-NE-CZ	7.61	134.25	123.60
1	A	660	CYS	CA-CB-SG	7.27	127.09	114.00
1	A	185	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	186	GLY	O-C-N	-6.67	112.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ASP	O-C-N	-6.62	111.94	123.20
1	A	182	TYR	N-CA-CB	-6.59	98.74	110.60
1	A	297	PHE	C-N-CA	-6.57	105.27	121.70
1	A	589	TRP	CA-CB-CG	6.47	126.00	113.70
1	A	193	HIS	CA-CB-CG	6.36	124.40	113.60
1	A	184	PHE	CB-CG-CD2	6.29	125.21	120.80
1	A	134	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	383	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	222	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	252	ARG	NH1-CZ-NH2	6.12	126.13	119.40
1	A	240	ASN	C-N-CA	-6.11	109.47	122.30
1	A	315	ARG	CA-CB-CG	6.09	126.79	113.40
1	A	435	GLN	OE1-CD-NE2	-5.91	108.31	121.90
1	A	240	ASN	CA-C-N	5.84	127.88	116.20
1	A	188	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	435	GLN	CG-CD-NE2	5.70	130.37	116.70
1	A	182	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	263	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	60	CYS	CB-CA-C	5.41	121.22	110.40
1	A	113	PHE	CA-CB-CG	-5.40	100.95	113.90
1	A	385	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	242	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	218	GLY	O-C-N	-5.28	114.25	122.70
1	A	432	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	175	ARG	CA-CB-CG	-5.16	102.06	113.40
1	A	211	GLU	C-N-CA	-5.14	108.84	121.70
1	A	543	TYR	O-C-N	5.11	130.87	122.70
1	A	232	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	297	PHE	N-CA-CB	5.05	119.68	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ASP	Mainchain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4930	0	4651	516	1
2	A	2	0	0	0	0
3	A	3	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	10	0	0	0	0
7	A	104	0	0	13	0
All	All	5051	0	4651	516	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 54.

All (516) 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:224:LYS:HA	1:A:224:LYS:HE2	1.33	1.09
1:A:65:CYS:HA	1:A:69:VAL:HG21	1.29	1.06
1:A:109:ASN:ND2	1:A:113:PHE:CE1	2.23	1.06
1:A:319:THR:HG22	1:A:328:LYS:HB3	1.36	1.06
1:A:172:ASN:HD22	1:A:173:PHE:N	1.55	1.02
1:A:602:PHE:HB3	1:A:603:PRO:HA	1.40	1.02
1:A:73:THR:HA	1:A:76:LYS:HD2	1.39	0.99
1:A:315:ARG:HG3	1:A:315:ARG:HH11	1.28	0.98
1:A:482:ARG:HG2	1:A:530:GLU:OE2	1.64	0.98
1:A:223:VAL:CG1	1:A:272:GLY:HA3	1.96	0.96
1:A:185:ASP:HB3	7:A:1017:HOH:O	1.67	0.95
1:A:172:ASN:ND2	1:A:173:PHE:H	1.64	0.95
1:A:640:LEU:HA	1:A:647:SER:O	1.66	0.95
1:A:320:THR:HG22	7:A:1030:HOH:O	1.67	0.94
1:A:91:GLN:N	1:A:91:GLN:HE21	1.63	0.94
1:A:108:ALA:HB1	1:A:110:TYR:CD1	2.02	0.94
1:A:489:LYS:HG3	1:A:490:ASP:H	1.32	0.94
1:A:570:ALA:HB3	1:A:583:PHE:HB2	1.51	0.93
1:A:172:ASN:HD22	1:A:173:PHE:H	1.03	0.92
1:A:617:LEU:HA	1:A:633:LYS:HD3	1.51	0.92
1:A:66:ASN:H	1:A:69:VAL:HG22	1.36	0.90
1:A:224:LYS:CE	1:A:224:LYS:HA	1.98	0.89
1:A:118:LYS:HG2	1:A:118:LYS:O	1.69	0.89
1:A:343:ASN:HD21	1:A:387:TRP:H	1.22	0.88
1:A:66:ASN:H	1:A:69:VAL:CG2	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:LYS:O	1:A:648:VAL:HG22	1.73	0.88
1:A:611:ASN:HB2	1:A:645:LEU:CD1	2.05	0.87
1:A:108:ALA:HB1	1:A:110:TYR:HD1	1.39	0.87
1:A:579:LYS:HG2	1:A:590:ARG:NE	1.89	0.87
1:A:639:LYS:NZ	1:A:649:LYS:HB2	1.89	0.86
1:A:640:LEU:HD11	1:A:645:LEU:HA	1.56	0.85
1:A:70:LEU:HG	1:A:74:LEU:HD12	1.58	0.85
1:A:57:PHE:CZ	1:A:101:ARG:HD2	2.12	0.85
1:A:320:THR:HG21	1:A:326:ASP:HB2	1.58	0.85
1:A:91:GLN:HE21	1:A:91:GLN:H	1.21	0.85
1:A:467:GLU:HA	7:A:1006:HOH:O	1.77	0.85
1:A:70:LEU:O	1:A:74:LEU:HB2	1.77	0.85
1:A:645:LEU:HD13	1:A:645:LEU:C	1.98	0.84
1:A:91:GLN:NE2	1:A:91:GLN:H	1.77	0.83
1:A:74:LEU:HD13	1:A:87:GLY:O	1.79	0.83
1:A:65:CYS:HA	1:A:69:VAL:CG2	2.08	0.82
1:A:648:VAL:O	1:A:649:LYS:HG3	1.79	0.82
1:A:611:ASN:HB2	1:A:645:LEU:HD11	1.62	0.81
1:A:162:ILE:HD11	1:A:167:ALA:HB2	1.63	0.81
1:A:53:TYR:CG	1:A:97:MET:HE2	2.15	0.81
1:A:224:LYS:HG3	1:A:280:PHE:CE2	2.16	0.80
1:A:260:SER:HB3	1:A:265:PHE:CD1	2.17	0.80
1:A:74:LEU:HD21	1:A:89:LEU:HD23	1.64	0.80
1:A:155:THR:HB	1:A:156:PRO:CD	2.11	0.79
1:A:114:PRO:HG2	1:A:198:GLY:CA	2.13	0.79
1:A:113:PHE:CB	1:A:196:ALA:HB3	2.13	0.79
1:A:319:THR:CG2	1:A:328:LYS:HB3	2.12	0.79
1:A:233:CYS:CB	1:A:259:CYS:SG	2.71	0.79
1:A:109:ASN:ND2	1:A:113:PHE:CZ	2.51	0.79
1:A:481:ILE:HG22	1:A:482:ARG:H	1.46	0.79
1:A:433:LEU:HD22	1:A:437:ASP:HB2	1.64	0.78
1:A:641:GLU:HG3	1:A:647:SER:OG	1.84	0.78
1:A:579:LYS:HG2	1:A:590:ARG:HE	1.48	0.77
1:A:260:SER:HB3	1:A:265:PHE:HD1	1.48	0.77
1:A:641:GLU:CG	1:A:647:SER:OG	2.32	0.77
1:A:475:PHE:HB2	1:A:478:ILE:HD11	1.66	0.77
1:A:502:LYS:HE2	1:A:503:PRO:HD2	1.66	0.77
1:A:531:LYS:NZ	1:A:549:GLU:OE2	2.15	0.77
1:A:549:GLU:HB3	1:A:552:TYR:CD2	2.18	0.77
1:A:641:GLU:CB	1:A:647:SER:OG	2.33	0.76
1:A:169:ILE:HG23	1:A:203:GLY:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LYS:CE	1:A:642:ASN:HB3	2.16	0.76
1:A:646:LYS:C	1:A:646:LYS:HD3	2.06	0.76
1:A:542:ILE:O	1:A:549:GLU:HB2	1.86	0.76
1:A:339:THR:HG22	1:A:346:GLY:HA2	1.65	0.75
1:A:61:PRO:HD2	1:A:64:SER:OG	1.86	0.75
1:A:590:ARG:NH1	1:A:602:PHE:HZ	1.84	0.75
1:A:109:ASN:CG	1:A:113:PHE:CZ	2.59	0.75
1:A:639:LYS:HG2	1:A:649:LYS:O	1.87	0.75
1:A:645:LEU:O	1:A:645:LEU:HD22	1.87	0.74
1:A:154:VAL:HG11	1:A:438:ILE:HG23	1.69	0.74
1:A:481:ILE:HG22	1:A:482:ARG:N	2.01	0.74
1:A:311:THR:HB	7:A:1013:HOH:O	1.88	0.74
1:A:155:THR:HB	1:A:156:PRO:HD2	1.68	0.74
1:A:398:PHE:CE2	1:A:399:LEU:HD23	2.22	0.73
1:A:635:ALA:O	7:A:1094:HOH:O	2.06	0.73
1:A:112:PHE:O	1:A:112:PHE:CD1	2.41	0.73
1:A:201:VAL:O	1:A:204:ASP:HB2	1.89	0.72
1:A:646:LYS:O	1:A:648:VAL:CG2	2.36	0.72
1:A:195:PHE:CD2	1:A:201:VAL:HG13	2.25	0.72
1:A:480:GLN:HG3	1:A:485:ILE:HD13	1.72	0.72
1:A:158:ARG:NH2	1:A:449:PRO:HD2	2.05	0.72
1:A:639:LYS:HE3	1:A:649:LYS:O	1.90	0.71
1:A:611:ASN:CB	1:A:645:LEU:HD11	2.19	0.71
1:A:65:CYS:CA	1:A:69:VAL:HG21	2.15	0.71
1:A:113:PHE:CG	1:A:196:ALA:HB3	2.25	0.71
1:A:644:SER:O	1:A:647:SER:HB3	1.89	0.71
1:A:239:PHE:CE2	1:A:240:ASN:ND2	2.58	0.71
1:A:185:ASP:O	1:A:185:ASP:OD1	2.07	0.71
1:A:658:LEU:O	1:A:660:CYS:HB2	1.91	0.71
1:A:641:GLU:HB2	1:A:647:SER:CB	2.21	0.71
1:A:233:CYS:CB	1:A:259:CYS:HG	2.03	0.71
1:A:157:LEU:O	1:A:158:ARG:HD3	1.91	0.70
1:A:172:ASN:ND2	1:A:173:PHE:N	2.30	0.70
1:A:157:LEU:HD11	1:A:445:TYR:CD2	2.26	0.70
1:A:364:THR:HG23	1:A:366:ALA:H	1.56	0.70
1:A:129:ILE:CD1	1:A:170:MET:HB3	2.23	0.69
1:A:549:GLU:HB3	1:A:552:TYR:HD2	1.58	0.69
1:A:114:PRO:HG2	1:A:198:GLY:HA3	1.74	0.68
1:A:40:ASP:OD2	1:A:368:ARG:NH2	2.25	0.68
1:A:574:TRP:HB3	1:A:577:ASN:OD1	1.94	0.68
1:A:513:TRP:HB3	1:A:516:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:TYR:CE1	1:A:580:THR:HG21	2.29	0.68
1:A:135:LEU:HB2	1:A:140:VAL:HG23	1.75	0.68
1:A:571:ALA:O	1:A:572:PHE:HB3	1.94	0.68
1:A:315:ARG:HH11	1:A:315:ARG:CG	2.04	0.67
1:A:31:PRO:O	1:A:32:SER:OG	2.12	0.67
1:A:119:TRP:N	1:A:445:TYR:OH	2.27	0.67
1:A:223:VAL:HG11	1:A:272:GLY:HA3	1.74	0.67
1:A:247:CYS:CB	1:A:274:CYS:SG	2.83	0.67
1:A:114:PRO:CG	1:A:198:GLY:HA3	2.25	0.67
1:A:579:LYS:HG2	1:A:590:ARG:CD	2.24	0.67
1:A:639:LYS:HZ2	1:A:649:LYS:HB2	1.57	0.67
1:A:242:LYS:HZ1	1:A:351:PHE:HD2	1.43	0.67
1:A:224:LYS:HG3	1:A:280:PHE:HE2	1.58	0.66
1:A:224:LYS:O	1:A:224:LYS:HD3	1.95	0.66
1:A:613:ILE:HD12	1:A:631:PHE:CD2	2.30	0.66
1:A:53:TYR:CB	1:A:97:MET:HE2	2.24	0.66
1:A:533:VAL:HG22	1:A:542:ILE:HG23	1.78	0.66
1:A:615:ASP:O	1:A:616:ASN:HB2	1.96	0.66
1:A:518:GLU:CD	1:A:518:GLU:H	2.00	0.66
1:A:119:TRP:CE2	1:A:197:PRO:HB3	2.31	0.66
1:A:606:ILE:HB	1:A:615:ASP:OD1	1.94	0.66
1:A:628:HIS:HA	1:A:640:LEU:O	1.95	0.65
1:A:617:LEU:HD23	1:A:617:LEU:H	1.60	0.65
1:A:489:LYS:HG3	1:A:490:ASP:N	2.09	0.65
1:A:618:ASP:OD1	1:A:633:LYS:HA	1.96	0.65
1:A:513:TRP:CB	1:A:516:LEU:HD22	2.27	0.64
1:A:219:GLN:HE22	1:A:337:MET:H	1.44	0.64
1:A:113:PHE:HB2	1:A:196:ALA:HB3	1.78	0.64
1:A:53:TYR:CD2	1:A:97:MET:HB2	2.33	0.64
1:A:57:PHE:HZ	1:A:190:LEU:HD22	1.62	0.64
1:A:552:TYR:CE1	1:A:554:LYS:HE3	2.32	0.64
1:A:247:CYS:HB3	1:A:274:CYS:SG	2.38	0.64
1:A:652:SER:O	1:A:656:ASP:HB2	1.97	0.64
1:A:129:ILE:HD12	1:A:170:MET:HB3	1.80	0.63
1:A:90:ASP:O	1:A:93:THR:N	2.31	0.63
1:A:493:ILE:HG13	1:A:493:ILE:O	1.98	0.63
1:A:164:ASP:OD1	1:A:165:GLY:N	2.32	0.63
1:A:627:GLY:HA2	1:A:642:ASN:ND2	2.13	0.63
1:A:71:LYS:HB3	1:A:87:GLY:HA3	1.81	0.62
1:A:545:ALA:O	1:A:546:SER:HB3	1.98	0.62
1:A:114:PRO:HG2	1:A:198:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG13	1:A:552:TYR:CZ	2.34	0.62
1:A:572:PHE:CE1	1:A:620:VAL:HG11	2.34	0.62
1:A:119:TRP:CD2	1:A:197:PRO:HB3	2.35	0.62
1:A:433:LEU:HD22	1:A:437:ASP:CB	2.29	0.62
1:A:576:LYS:HE3	1:A:642:ASN:HB3	1.82	0.62
1:A:639:LYS:CG	1:A:649:LYS:O	2.48	0.61
1:A:628:HIS:HE1	1:A:639:LYS:HD2	1.65	0.61
1:A:592:ASN:OD1	1:A:594:VAL:HG23	2.00	0.61
1:A:224:LYS:HG3	1:A:280:PHE:CZ	2.35	0.61
1:A:233:CYS:HB3	1:A:259:CYS:SG	2.39	0.61
1:A:552:TYR:CZ	1:A:554:LYS:HE3	2.35	0.61
1:A:555:PRO:HB2	1:A:557:THR:HG23	1.82	0.61
1:A:590:ARG:NH1	1:A:602:PHE:CZ	2.68	0.61
1:A:611:ASN:HB2	1:A:645:LEU:CG	2.31	0.61
1:A:469:CYS:HA	1:A:660:CYS:SG	2.41	0.61
1:A:142:ASP:OD1	1:A:146:ARG:NH1	2.34	0.61
1:A:90:ASP:O	1:A:92:ASN:N	2.35	0.60
1:A:109:ASN:O	1:A:113:PHE:HZ	1.84	0.60
1:A:398:PHE:CD2	1:A:399:LEU:HD23	2.36	0.60
1:A:247:CYS:CB	1:A:274:CYS:HG	2.11	0.60
1:A:581:TYR:HA	1:A:589:TRP:O	2.02	0.60
1:A:289:GLN:HB3	1:A:290:PRO:HD2	1.82	0.60
1:A:108:ALA:CB	1:A:110:TYR:HD1	2.14	0.60
1:A:114:PRO:HG3	7:A:1007:HOH:O	2.02	0.60
1:A:639:LYS:NZ	1:A:649:LYS:CB	2.63	0.60
1:A:315:ARG:NH1	1:A:332:CYS:O	2.34	0.60
1:A:260:SER:CB	1:A:265:PHE:HD1	2.12	0.60
1:A:520:ILE:HD13	1:A:520:ILE:H	1.66	0.59
1:A:277:GLU:HB2	1:A:291:CYS:SG	2.42	0.59
1:A:617:LEU:CD2	1:A:617:LEU:H	2.14	0.59
1:A:233:CYS:HB3	1:A:259:CYS:HB2	1.84	0.59
1:A:565:VAL:HG23	1:A:567:ARG:H	1.67	0.59
1:A:66:ASN:OD1	1:A:69:VAL:HG13	2.03	0.59
1:A:221:VAL:O	1:A:232:TYR:HA	2.03	0.59
1:A:224:LYS:HG3	1:A:282:MET:HE1	1.84	0.59
1:A:475:PHE:HB2	1:A:478:ILE:CD1	2.32	0.59
1:A:574:TRP:CZ2	1:A:576:LYS:NZ	2.70	0.58
1:A:645:LEU:HD13	1:A:646:LYS:N	2.18	0.58
1:A:214:THR:HG22	1:A:219:GLN:HA	1.86	0.58
1:A:426:THR:OG1	1:A:511:THR:HG22	2.02	0.58
1:A:588:PHE:HE2	1:A:609:ALA:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LEU:HD13	1:A:623:LEU:H	1.67	0.58
1:A:653:ILE:O	1:A:657:TRP:HB2	2.04	0.58
1:A:488:PHE:CB	1:A:520:ILE:HD11	2.32	0.58
1:A:100:PRO:HB3	1:A:191:LEU:HD21	1.84	0.58
1:A:480:GLN:HG3	1:A:485:ILE:CD1	2.33	0.58
1:A:153:ASP:HB2	7:A:1059:HOH:O	2.04	0.58
1:A:466:PRO:HB2	1:A:494:TRP:CH2	2.37	0.58
1:A:624:GLN:HG3	1:A:624:GLN:O	2.02	0.58
1:A:113:PHE:CD2	1:A:114:PRO:O	2.57	0.57
1:A:368:ARG:NH1	1:A:389:PHE:HZ	2.03	0.57
1:A:576:LYS:NZ	1:A:642:ASN:HA	2.20	0.57
1:A:78:GLN:OE1	1:A:86:THR:O	2.23	0.57
1:A:404:ALA:O	1:A:407:HIS:HB2	2.05	0.57
1:A:590:ARG:O	1:A:598:MET:SD	2.63	0.57
1:A:639:LYS:CE	1:A:649:LYS:HB2	2.34	0.57
1:A:67:LEU:O	1:A:71:LYS:HG2	2.03	0.57
1:A:176:TRP:HA	1:A:184:PHE:O	2.04	0.57
1:A:233:CYS:HB3	1:A:259:CYS:CB	2.35	0.56
1:A:214:THR:HB	1:A:218:GLY:O	2.05	0.56
1:A:363:CYS:CB	1:A:390:CYS:SG	2.93	0.56
1:A:114:PRO:HD2	1:A:197:PRO:O	2.06	0.56
1:A:355:PHE:HB3	1:A:360:TYR:CE1	2.40	0.56
1:A:343:ASN:H	1:A:343:ASN:ND2	2.02	0.56
1:A:297:PHE:HB3	1:A:302:TYR:HE2	1.70	0.56
1:A:265:PHE:HE1	1:A:271:TYR:HB3	1.71	0.56
1:A:576:LYS:HZ2	1:A:642:ASN:CB	2.19	0.56
1:A:223:VAL:CG1	1:A:272:GLY:CA	2.80	0.56
1:A:545:ALA:O	1:A:546:SER:CB	2.51	0.56
1:A:113:PHE:CD2	1:A:113:PHE:C	2.79	0.56
1:A:480:GLN:CG	1:A:485:ILE:HD13	2.34	0.56
1:A:623:LEU:HD21	1:A:630:TYR:HE1	1.71	0.56
1:A:124:ILE:O	1:A:159:PHE:HA	2.07	0.55
1:A:252:ARG:NH2	1:A:254:ASP:OD2	2.39	0.55
1:A:590:ARG:HH11	1:A:602:PHE:HZ	1.54	0.55
1:A:360:TYR:CE2	1:A:364:THR:HG21	2.42	0.55
1:A:256:PHE:HA	1:A:279:LEU:HD13	1.88	0.55
1:A:644:SER:OG	1:A:647:SER:HB2	2.06	0.55
1:A:621:VAL:HG12	1:A:632:PHE:CE1	2.41	0.55
1:A:576:LYS:NZ	1:A:642:ASN:HB3	2.21	0.54
1:A:434:SER:O	1:A:438:ILE:HG12	2.07	0.54
1:A:611:ASN:HB2	1:A:645:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HH21	1:A:449:PRO:HD2	1.72	0.54
1:A:484:GLU:HB2	1:A:486:PHE:HE1	1.72	0.54
1:A:478:ILE:HG12	1:A:487:PHE:CD2	2.42	0.54
1:A:223:VAL:HG13	1:A:272:GLY:HA3	1.88	0.54
1:A:641:GLU:H	1:A:647:SER:CB	2.21	0.54
1:A:533:VAL:HG22	1:A:542:ILE:HD13	1.89	0.54
1:A:653:ILE:N	7:A:1094:HOH:O	2.39	0.54
1:A:53:TYR:HB3	1:A:97:MET:HE2	1.89	0.54
1:A:132:THR:O	1:A:132:THR:HG23	2.07	0.54
1:A:623:LEU:HD22	1:A:623:LEU:N	2.23	0.54
1:A:464:VAL:HG22	1:A:465:THR:N	2.22	0.54
1:A:342:GLY:HA2	1:A:387:TRP:CZ2	2.43	0.54
1:A:127:ARG:HH21	1:A:311:THR:HG22	1.73	0.54
1:A:473:ILE:HD12	1:A:489:LYS:HD3	1.89	0.53
1:A:605:LEU:CB	1:A:608:ASP:HB2	2.37	0.53
1:A:214:THR:O	1:A:396:SER:HA	2.09	0.53
1:A:638:LEU:HD21	1:A:650:PHE:CE1	2.43	0.53
1:A:158:ARG:HH21	1:A:449:PRO:CD	2.20	0.53
1:A:574:TRP:NE1	1:A:576:LYS:NZ	2.57	0.53
1:A:621:VAL:HG12	1:A:632:PHE:CZ	2.44	0.53
1:A:339:THR:HG22	1:A:346:GLY:CA	2.37	0.53
1:A:339:THR:HB	1:A:347:ALA:O	2.08	0.53
1:A:192:ALA:HB1	1:A:206:HIS:O	2.08	0.53
1:A:468:ILE:HD13	1:A:503:PRO:HG2	1.90	0.53
1:A:630:TYR:CD2	1:A:639:LYS:HB3	2.44	0.52
1:A:617:LEU:N	1:A:617:LEU:HD23	2.24	0.52
1:A:466:PRO:HB2	1:A:494:TRP:HH2	1.73	0.52
1:A:118:LYS:O	1:A:119:TRP:C	2.48	0.52
1:A:281:THR:HG23	1:A:289:GLN:O	2.10	0.52
1:A:579:LYS:HB3	1:A:590:ARG:HD2	1.90	0.52
1:A:175:ARG:O	1:A:176:TRP:C	2.46	0.52
1:A:236:PRO:HA	1:A:244:TYR:O	2.09	0.52
1:A:435:GLN:HA	1:A:438:ILE:HG13	1.92	0.52
1:A:129:ILE:HD11	1:A:170:MET:HB3	1.91	0.52
1:A:628:HIS:HB3	1:A:630:TYR:CZ	2.45	0.52
1:A:475:PHE:CB	1:A:478:ILE:HD11	2.37	0.52
1:A:640:LEU:CD1	1:A:645:LEU:HA	2.34	0.52
1:A:498:THR:O	1:A:501:ASP:OD1	2.26	0.52
1:A:588:PHE:CE2	1:A:609:ALA:HB3	2.45	0.52
1:A:641:GLU:N	1:A:647:SER:OG	2.43	0.52
1:A:529:GLU:HB2	1:A:531:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:TRP:HB2	1:A:445:TYR:OH	2.10	0.52
1:A:576:LYS:HZ1	1:A:642:ASN:HA	1.74	0.51
1:A:57:PHE:CZ	1:A:190:LEU:HD22	2.45	0.51
1:A:252:ARG:HH21	1:A:254:ASP:CG	2.11	0.51
1:A:64:SER:O	1:A:69:VAL:HG11	2.11	0.51
1:A:576:LYS:NZ	1:A:642:ASN:CB	2.73	0.51
1:A:78:GLN:HG2	1:A:83:LEU:HD12	1.92	0.51
1:A:66:ASN:OD1	1:A:69:VAL:HG22	2.11	0.51
1:A:630:TYR:HD2	1:A:639:LYS:HB3	1.76	0.51
1:A:551:GLY:O	1:A:554:LYS:HE2	2.11	0.51
1:A:119:TRP:NE1	1:A:408:ALA:O	2.43	0.51
1:A:576:LYS:NZ	1:A:642:ASN:CA	2.73	0.51
1:A:127:ARG:NH2	1:A:311:THR:HG22	2.25	0.51
1:A:137:PRO:O	1:A:138:GLU:C	2.49	0.51
1:A:623:LEU:HD21	1:A:630:TYR:CE1	2.45	0.51
1:A:472:ASP:OD1	1:A:654:LYS:NZ	2.43	0.51
1:A:224:LYS:CG	1:A:282:MET:HE1	2.41	0.50
1:A:433:LEU:HD13	1:A:438:ILE:HD13	1.93	0.50
1:A:573:ASN:HD21	1:A:578:LYS:HA	1.77	0.50
1:A:628:HIS:CE1	1:A:639:LYS:HD2	2.45	0.50
1:A:641:GLU:HB2	1:A:647:SER:OG	2.09	0.50
1:A:113:PHE:HD2	1:A:114:PRO:O	1.93	0.50
1:A:536:ALA:O	1:A:537:GLY:C	2.47	0.50
1:A:632:PHE:N	1:A:632:PHE:CD1	2.79	0.50
1:A:80:PHE:HA	1:A:415:GLN:NE2	2.26	0.50
1:A:66:ASN:N	1:A:69:VAL:CG2	2.68	0.50
1:A:363:CYS:HB3	1:A:390:CYS:SG	2.51	0.50
1:A:176:TRP:CE3	1:A:185:ASP:HA	2.46	0.50
1:A:513:TRP:HD1	1:A:543:TYR:CE2	2.30	0.50
1:A:114:PRO:HG2	1:A:197:PRO:O	2.12	0.50
1:A:212:LEU:O	1:A:212:LEU:HG	2.12	0.50
1:A:47:LYS:O	1:A:51:VAL:HG23	2.12	0.50
1:A:66:ASN:N	1:A:69:VAL:HG22	2.17	0.50
1:A:639:LYS:O	1:A:648:VAL:CG1	2.60	0.49
1:A:265:PHE:CE1	1:A:271:TYR:HB3	2.47	0.49
1:A:468:ILE:CD1	1:A:503:PRO:HG2	2.42	0.49
1:A:108:ALA:CB	1:A:110:TYR:CD1	2.88	0.49
1:A:108:ALA:O	1:A:110:TYR:N	2.45	0.49
1:A:475:PHE:CE1	1:A:487:PHE:HB3	2.47	0.49
1:A:538:ASN:OD1	1:A:538:ASN:N	2.45	0.49
1:A:217:GLU:HG2	1:A:427:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HB	1:A:233:CYS:SG	2.53	0.49
1:A:529:GLU:OE1	1:A:531:LYS:HE3	2.12	0.49
1:A:415:GLN:O	1:A:417:PRO:HD3	2.12	0.49
1:A:368:ARG:NH1	1:A:389:PHE:CZ	2.80	0.49
1:A:486:PHE:HB3	1:A:488:PHE:CE1	2.48	0.49
1:A:567:ARG:CZ	1:A:567:ARG:CB	2.91	0.49
1:A:53:TYR:CD1	1:A:97:MET:HE2	2.47	0.49
1:A:261:THR:HB	1:A:262:THR:HG23	1.94	0.49
1:A:339:THR:CG2	1:A:346:GLY:HA2	2.38	0.49
1:A:57:PHE:CZ	1:A:101:ARG:CD	2.92	0.49
1:A:142:ASP:OD1	1:A:146:ARG:HG3	2.13	0.49
1:A:321:GLU:HG2	7:A:1078:HOH:O	2.13	0.49
1:A:561:LEU:HD21	1:A:582:ILE:HD12	1.95	0.49
1:A:78:GLN:CG	1:A:83:LEU:HD12	2.42	0.49
1:A:586:ASP:HB3	1:A:615:ASP:OD2	2.13	0.49
1:A:533:VAL:HG22	1:A:542:ILE:CD1	2.43	0.48
1:A:247:CYS:HG	1:A:274:CYS:HG	0.51	0.48
1:A:442:GLN:O	1:A:445:TYR:O	2.30	0.48
1:A:554:LYS:CB	1:A:555:PRO:HD2	2.43	0.48
1:A:513:TRP:O	1:A:516:LEU:HB2	2.13	0.48
1:A:639:LYS:HZ1	1:A:649:LYS:CB	2.26	0.48
1:A:583:PHE:N	1:A:583:PHE:CD1	2.81	0.48
1:A:618:ASP:OD1	1:A:633:LYS:HD2	2.13	0.48
1:A:493:ILE:CG2	1:A:509:VAL:HB	2.44	0.48
1:A:322:ASP:HB3	1:A:325:ARG:HB3	1.96	0.48
1:A:90:ASP:O	1:A:91:GLN:C	2.52	0.48
1:A:623:LEU:HD22	1:A:623:LEU:H	1.76	0.48
1:A:60:CYS:HB2	1:A:73:THR:HG21	1.96	0.48
1:A:54:LEU:HD12	1:A:70:LEU:HD12	1.96	0.48
1:A:91:GLN:N	1:A:91:GLN:NE2	2.39	0.48
1:A:469:CYS:CB	1:A:660:CYS:HG	2.23	0.48
1:A:565:VAL:HG23	1:A:567:ARG:O	2.14	0.48
1:A:71:LYS:HA	1:A:87:GLY:CA	2.44	0.48
1:A:605:LEU:HB3	1:A:608:ASP:HB2	1.94	0.48
1:A:579:LYS:HG2	1:A:590:ARG:CG	2.44	0.48
1:A:218:GLY:O	1:A:219:GLN:C	2.50	0.48
1:A:280:PHE:HE2	1:A:282:MET:HE1	1.78	0.47
1:A:580:THR:O	1:A:591:TYR:N	2.47	0.47
1:A:602:PHE:HB3	1:A:603:PRO:CA	2.26	0.47
1:A:320:THR:HG21	1:A:326:ASP:CB	2.35	0.47
1:A:197:PRO:HG3	1:A:408:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HA	1:A:302:TYR:O	2.14	0.47
1:A:176:TRP:O	1:A:183:PRO:HA	2.14	0.47
1:A:297:PHE:O	1:A:298:GLN:HG2	2.13	0.47
1:A:64:SER:O	1:A:69:VAL:HG21	2.14	0.47
1:A:577:ASN:N	1:A:577:ASN:OD1	2.48	0.47
1:A:646:LYS:O	1:A:646:LYS:HD3	2.14	0.47
1:A:108:ALA:C	1:A:110:TYR:HD1	2.18	0.47
1:A:524:TYR:CE2	1:A:533:VAL:HG11	2.50	0.47
1:A:244:TYR:OH	1:A:250:THR:HG21	2.14	0.47
1:A:289:GLN:HB3	1:A:290:PRO:CD	2.45	0.47
1:A:134:ASP:OD2	1:A:212:LEU:HA	2.15	0.47
1:A:618:ASP:OD1	1:A:618:ASP:N	2.38	0.47
1:A:343:ASN:ND2	1:A:386:LYS:HZ2	2.13	0.47
1:A:484:GLU:HG2	1:A:497:VAL:HG12	1.96	0.47
1:A:567:ARG:NH1	1:A:567:ARG:HB2	2.30	0.47
1:A:315:ARG:NH2	1:A:335:THR:OG1	2.48	0.47
1:A:654:LYS:HG3	1:A:660:CYS:SG	2.55	0.47
1:A:305:CYS:HB2	1:A:315:ARG:HD2	1.98	0.46
1:A:475:PHE:CD2	1:A:478:ILE:HD11	2.50	0.46
1:A:398:PHE:CE2	1:A:399:LEU:CD2	2.96	0.46
1:A:493:ILE:HG23	1:A:509:VAL:HB	1.98	0.46
1:A:488:PHE:HB3	1:A:520:ILE:HD11	1.96	0.46
1:A:78:GLN:HG2	1:A:83:LEU:HB2	1.97	0.46
1:A:281:THR:O	1:A:288:GLY:HA2	2.16	0.46
1:A:71:LYS:CB	1:A:87:GLY:HA3	2.44	0.46
1:A:343:ASN:HD22	1:A:344:SER:N	2.13	0.46
1:A:478:ILE:HG12	1:A:487:PHE:HD2	1.81	0.46
1:A:543:TYR:CD2	1:A:548:LEU:HA	2.50	0.46
1:A:540:TYR:CZ	1:A:559:LEU:HD22	2.51	0.46
1:A:83:LEU:HD13	1:A:93:THR:HA	1.96	0.46
1:A:484:GLU:OE1	1:A:495:ARG:NH1	2.36	0.46
1:A:176:TRP:O	1:A:184:PHE:N	2.38	0.46
1:A:502:LYS:HE2	1:A:503:PRO:CD	2.42	0.46
1:A:646:LYS:HD3	1:A:647:SER:N	2.30	0.46
1:A:224:LYS:CA	1:A:224:LYS:HE2	2.24	0.45
1:A:297:PHE:O	1:A:324:ASP:OD2	2.33	0.45
1:A:129:ILE:HD11	1:A:170:MET:CE	2.46	0.45
1:A:438:ILE:HG12	1:A:438:ILE:H	1.51	0.45
1:A:574:TRP:CE2	1:A:576:LYS:NZ	2.76	0.45
1:A:576:LYS:HZ1	1:A:642:ASN:CA	2.29	0.45
1:A:60:CYS:HA	1:A:61:PRO:HD3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:TRP:O	1:A:578:LYS:N	2.49	0.45
1:A:538:ASN:O	1:A:556:LEU:HG	2.17	0.45
1:A:591:TYR:OH	7:A:1016:HOH:O	1.99	0.45
1:A:527:PRO:HG3	1:A:573:ASN:ND2	2.31	0.45
1:A:295:PHE:CE2	1:A:302:TYR:HB2	2.52	0.45
1:A:481:ILE:CG2	1:A:482:ARG:N	2.73	0.45
1:A:81:PHE:HZ	1:A:101:ARG:NH2	2.15	0.45
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.65	0.45
1:A:79:LYS:HD2	1:A:85:GLN:NE2	2.32	0.45
1:A:403:HIS:CD2	1:A:403:HIS:O	2.69	0.45
1:A:611:ASN:CB	1:A:645:LEU:CD1	2.82	0.45
1:A:46:ASP:CG	1:A:94:ILE:HD13	2.37	0.45
1:A:306:THR:HB	1:A:308:GLU:H	1.82	0.45
1:A:118:LYS:CG	1:A:118:LYS:O	2.51	0.45
1:A:513:TRP:N	1:A:514:PRO:HD3	2.32	0.45
1:A:464:VAL:HG22	1:A:465:THR:H	1.80	0.45
1:A:280:PHE:CE2	1:A:282:MET:HE1	2.52	0.45
1:A:315:ARG:CG	1:A:315:ARG:NH1	2.74	0.44
1:A:524:TYR:CZ	1:A:580:THR:HG21	2.52	0.44
1:A:93:THR:O	1:A:97:MET:HG2	2.17	0.44
1:A:513:TRP:HD1	1:A:543:TYR:CD2	2.34	0.44
1:A:447:ALA:O	1:A:448:SER:OG	2.30	0.44
1:A:568:VAL:HG21	1:A:582:ILE:HG22	2.00	0.44
1:A:188:ASP:N	1:A:211:GLU:OE2	2.50	0.44
1:A:344:SER:HB3	1:A:347:ALA:HB3	2.00	0.44
1:A:81:PHE:CE1	1:A:423:PRO:HG2	2.53	0.44
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.86	0.44
1:A:512:PHE:HB2	1:A:513:TRP:CE3	2.53	0.44
1:A:406:GLY:O	1:A:411:LEU:HB2	2.17	0.44
1:A:581:TYR:CE2	1:A:590:ARG:HD3	2.52	0.44
1:A:633:LYS:O	1:A:634:GLY:C	2.56	0.44
1:A:344:SER:CB	1:A:377:THR:HG21	2.48	0.44
1:A:195:PHE:O	1:A:203:GLY:N	2.48	0.44
1:A:641:GLU:H	1:A:647:SER:HB3	1.83	0.44
1:A:83:LEU:CD1	1:A:93:THR:HA	2.47	0.44
1:A:331:PHE:C	1:A:333:PRO:HD3	2.38	0.44
1:A:233:CYS:SG	1:A:259:CYS:CB	3.07	0.43
1:A:579:LYS:HE3	1:A:599:ASP:OD2	2.18	0.43
1:A:53:TYR:HB3	1:A:97:MET:CE	2.48	0.43
1:A:654:LYS:HB3	1:A:654:LYS:HE3	1.52	0.43
1:A:224:LYS:HB2	1:A:273:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LYS:HE3	1:A:649:LYS:C	2.38	0.43
1:A:605:LEU:HB2	1:A:608:ASP:HB2	2.00	0.43
1:A:641:GLU:CA	1:A:647:SER:OG	2.65	0.43
1:A:300:THR:HG22	1:A:301:SER:N	2.33	0.43
1:A:34:ILE:O	1:A:34:ILE:HG22	2.17	0.43
1:A:69:VAL:HG23	1:A:70:LEU:N	2.34	0.43
1:A:574:TRP:HE3	1:A:581:TYR:HE1	1.66	0.43
1:A:239:PHE:HB3	1:A:244:TYR:CE1	2.53	0.43
1:A:411:LEU:HD11	1:A:441:ILE:HD12	1.99	0.43
1:A:79:LYS:HB2	1:A:85:GLN:NE2	2.33	0.43
1:A:113:PHE:HB2	1:A:114:PRO:HD2	2.00	0.43
1:A:586:ASP:O	1:A:605:LEU:HD22	2.18	0.43
1:A:403:HIS:C	1:A:403:HIS:CD2	2.92	0.43
1:A:354:THR:HG21	7:A:1042:HOH:O	2.18	0.43
1:A:108:ALA:C	1:A:110:TYR:CD1	2.92	0.43
1:A:159:PHE:CE2	1:A:409:MET:HE1	2.54	0.43
1:A:267:LYS:HG3	1:A:268:ASP:N	2.34	0.43
1:A:70:LEU:HG	1:A:74:LEU:CD1	2.38	0.43
1:A:127:ARG:HH11	1:A:127:ARG:HD3	1.70	0.43
1:A:338:SER:O	1:A:391:PRO:HD3	2.19	0.43
1:A:576:LYS:H	1:A:576:LYS:HG2	1.43	0.43
1:A:557:THR:O	1:A:560:GLY:N	2.47	0.43
1:A:572:PHE:CD1	1:A:620:VAL:HG11	2.54	0.43
1:A:416:ASP:HB3	1:A:419:ALA:HB2	2.01	0.43
1:A:113:PHE:N	1:A:113:PHE:CD1	2.84	0.42
1:A:644:SER:OG	1:A:647:SER:CB	2.67	0.42
1:A:488:PHE:CD2	1:A:493:ILE:HG22	2.54	0.42
1:A:416:ASP:OD1	1:A:465:THR:HG21	2.18	0.42
1:A:638:LEU:CD2	1:A:650:PHE:CE1	3.02	0.42
1:A:433:LEU:HB3	1:A:438:ILE:HD13	2.01	0.42
1:A:355:PHE:CZ	1:A:356:LEU:HG	2.54	0.42
1:A:340:VAL:O	1:A:389:PHE:HB2	2.20	0.42
1:A:196:ALA:HB1	1:A:197:PRO:HD2	2.00	0.42
1:A:480:GLN:OE1	1:A:623:LEU:HA	2.19	0.42
1:A:585:GLY:HA2	1:A:616:ASN:OD1	2.19	0.42
1:A:211:GLU:OE1	1:A:211:GLU:HA	2.18	0.42
1:A:75:LYS:HA	1:A:78:GLN:OE1	2.20	0.42
1:A:154:VAL:HG11	1:A:438:ILE:CG2	2.43	0.42
1:A:323:TYR:HA	7:A:1030:HOH:O	2.20	0.42
1:A:113:PHE:HB2	1:A:114:PRO:CD	2.50	0.42
1:A:568:VAL:HG21	1:A:582:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:O	1:A:69:VAL:HG22	2.19	0.42
1:A:112:PHE:O	1:A:112:PHE:CG	2.71	0.42
1:A:567:ARG:CZ	1:A:567:ARG:HB3	2.50	0.42
1:A:462:GLY:HA2	1:A:463:PRO:HD3	1.80	0.42
1:A:556:LEU:O	1:A:557:THR:C	2.58	0.42
1:A:57:PHE:CE2	1:A:101:ARG:HD2	2.53	0.41
1:A:617:LEU:HA	1:A:633:LYS:CD	2.36	0.41
1:A:343:ASN:ND2	1:A:343:ASN:N	2.64	0.41
1:A:513:TRP:HB2	1:A:516:LEU:HD22	2.01	0.41
1:A:564:ASP:OD1	1:A:565:VAL:N	2.52	0.41
1:A:279:LEU:HD12	7:A:1067:HOH:O	2.20	0.41
1:A:59:GLY:O	1:A:60:CYS:C	2.57	0.41
1:A:438:ILE:O	1:A:442:GLN:HG3	2.20	0.41
1:A:73:THR:HA	1:A:76:LYS:CD	2.29	0.41
1:A:223:VAL:HG13	1:A:272:GLY:CA	2.48	0.41
1:A:350:VAL:O	1:A:353:PHE:HB3	2.19	0.41
1:A:155:THR:OG1	1:A:157:LEU:HD12	2.21	0.41
1:A:613:ILE:HG23	1:A:617:LEU:HD13	2.03	0.41
1:A:654:LYS:O	1:A:660:CYS:HB2	2.20	0.41
1:A:109:ASN:HA	1:A:109:ASN:HD22	1.62	0.41
1:A:58:TYR:CZ	1:A:77:MET:HA	2.55	0.41
1:A:613:ILE:CG2	1:A:617:LEU:HD13	2.51	0.41
1:A:239:PHE:HB3	1:A:244:TYR:HE1	1.85	0.41
1:A:583:PHE:N	1:A:583:PHE:HD1	2.19	0.41
1:A:81:PHE:HE1	1:A:423:PRO:HG2	1.86	0.41
1:A:524:TYR:CD2	1:A:533:VAL:HB	2.56	0.41
1:A:652:SER:H	1:A:656:ASP:CG	2.24	0.41
1:A:207:PHE:N	1:A:207:PHE:CD1	2.89	0.41
1:A:171:ILE:HG23	1:A:207:PHE:HE1	1.85	0.41
1:A:588:PHE:CE2	1:A:610:TRP:NE1	2.88	0.41
1:A:47:LYS:HE3	1:A:89:LEU:CD1	2.50	0.40
1:A:47:LYS:HE3	1:A:70:LEU:HD21	2.02	0.40
1:A:109:ASN:O	1:A:113:PHE:CZ	2.71	0.40
1:A:83:LEU:HB3	1:A:84:PRO:CD	2.51	0.40
1:A:297:PHE:HB3	1:A:302:TYR:CE2	2.54	0.40
1:A:623:LEU:CD2	1:A:630:TYR:HE1	2.34	0.40
1:A:574:TRP:CD1	1:A:576:LYS:HG2	2.57	0.40
1:A:645:LEU:C	1:A:645:LEU:CD1	2.72	0.40
1:A:646:LYS:C	1:A:646:LYS:CD	2.80	0.40
1:A:162:ILE:HD12	1:A:164:ASP:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:ND2	1:A:240:ASN:ND2[10_675]	1.61	0.59

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	615/631 (98%)	565 (92%)	38 (6%)	12 (2%)	9 30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLY
1	A	448	SER
1	A	490	ASP
1	A	572	PHE
1	A	601	GLY
1	A	627	GLY
1	A	91	GLN
1	A	176	TRP
1	A	481	ILE
1	A	659	GLY
1	A	165	GLY
1	A	32	SER

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	518/527 (98%)	401 (77%)	117 (23%)	1 3

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	34	ILE
1	A	35	ILE
1	A	47	LYS
1	A	60	CYS
1	A	62	LYS
1	A	65	CYS
1	A	67	LEU
1	A	74	LEU
1	A	91	GLN
1	A	92	ASN
1	A	95	GLU
1	A	97	MET
1	A	101	ARG
1	A	109	ASN
1	A	115	ARG
1	A	116	LYS
1	A	118	LYS
1	A	121	LYS
1	A	124	ILE
1	A	160	SER
1	A	161	ARG
1	A	166	GLU
1	A	172	ASN
1	A	201	VAL
1	A	212	LEU
1	A	217	GLU
1	A	224	LYS
1	A	234	LYS
1	A	253	SER
1	A	257	LEU
1	A	264	ASN
1	A	267	LYS
1	A	296	ARG
1	A	298	GLN
1	A	306	THR
1	A	311	THR
1	A	312	ASP

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Mol	Chain	Res	Type
1	A	315	ARG
1	A	319	THR
1	A	321	GLU
1	A	327	LYS
1	A	328	LYS
1	A	337	MET
1	A	338	SER
1	A	339	THR
1	A	343	ASN
1	A	358	ASN
1	A	359	LYS
1	A	362	SER
1	A	390	CYS
1	A	393	GLN
1	A	409	MET
1	A	424	ILE
1	A	429	LYS
1	A	432	ARG
1	A	433	LEU
1	A	438	ILE
1	A	439	LYS
1	A	443	GLU
1	A	448	SER
1	A	465	THR
1	A	468	ILE
1	A	476	ASP
1	A	480	GLN
1	A	493	ILE
1	A	495	ARG
1	A	498	THR
1	A	501	ASP
1	A	502	LYS
1	A	504	MET
1	A	507	LEU
1	A	508	LEU
1	A	509	VAL
1	A	516	LEU
1	A	519	LYS
1	A	520	ILE
1	A	524	TYR
1	A	538	ASN
1	A	542	ILE

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Mol	Chain	Res	Type
1	A	549	GLU
1	A	554	LYS
1	A	557	THR
1	A	559	LEU
1	A	565	VAL
1	A	568	VAL
1	A	569	ASP
1	A	575	SER
1	A	576	LYS
1	A	577	ASN
1	A	580	THR
1	A	582	ILE
1	A	583	PHE
1	A	586	ASP
1	A	587	LYS
1	A	590	ARG
1	A	594	VAL
1	A	605	LEU
1	A	608	ASP
1	A	618	ASP
1	A	623	LEU
1	A	628	HIS
1	A	629	SER
1	A	630	TYR
1	A	632	PHE
1	A	636	TYR
1	A	638	LEU
1	A	639	LYS
1	A	644	SER
1	A	645	LEU
1	A	646	LYS
1	A	648	VAL
1	A	652	SER
1	A	654	LYS
1	A	655	SER
1	A	656	ASP
1	A	660	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN

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Mol	Chain	Res	Type
1	A	85	GLN
1	A	91	GLN
1	A	104	ASN
1	A	109	ASN
1	A	172	ASN
1	A	219	GLN
1	A	240	ASN
1	A	264	ASN
1	A	343	ASN
1	A	415	GLN
1	A	573	ASN
1	A	628	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
6	SO4	A	777	-	4,4,4	0.88	0	6,6,6	0.26	0
6	SO4	A	778	-	4,4,4	1.35	1 (25%)	6,6,6	1.08	1 (16%)

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
6	SO4	A	777	-	-	0/0/0/0	0/0/0/0
6	SO4	A	778	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	778	SO4	O1-S	2.52	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	778	SO4	O4-S-O3	2.24	118.10	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	619/631 (98%)	0.30	45 (7%) 18 10	9, 43, 150, 274	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	PHE	24.9
1	A	109	ASN	17.5
1	A	114	PRO	13.9
1	A	111	ASN	12.4
1	A	112	PHE	10.6
1	A	110	TYR	10.3
1	A	646	LYS	7.0
1	A	116	LYS	6.7
1	A	31	PRO	4.7
1	A	625	GLY	4.7
1	A	650	PHE	4.6
1	A	659	GLY	4.1
1	A	500	ARG	4.0
1	A	639	LYS	4.0
1	A	449	PRO	3.8
1	A	651	GLY	3.7
1	A	70	LEU	3.5
1	A	638	LEU	3.4
1	A	581	TYR	3.4
1	A	32	SER	3.4
1	A	108	ALA	3.1
1	A	621	VAL	3.0
1	A	620	VAL	2.7
1	A	648	VAL	2.7
1	A	118	LYS	2.6
1	A	435	GLN	2.6
1	A	610	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	619	ALA	2.5
1	A	445	TYR	2.4
1	A	588	PHE	2.4
1	A	637	TYR	2.4
1	A	647	SER	2.4
1	A	657	TRP	2.3
1	A	89	LEU	2.3
1	A	87	GLY	2.2
1	A	574	TRP	2.2
1	A	618	ASP	2.2
1	A	461	LEU	2.2
1	A	572	PHE	2.1
1	A	628	HIS	2.1
1	A	71	LYS	2.1
1	A	484	GLU	2.1
1	A	472	ASP	2.0
1	A	120	ASP	2.0
1	A	636	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CL	A	995	1/1	0.89	0.41	1.54	58,58,58,58	0
6	SO4	A	777	5/5	0.89	0.23	1.40	81,82,82,83	0
3	CA	A	992	1/1	0.92	0.19	0.75	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SO4	A	778	5/5	0.94	0.18	0.30	34,41,45,45	0
5	NA	A	996	1/1	0.67	0.34	0.18	61,61,61,61	0
3	CA	A	993	1/1	0.84	0.11	-0.94	108,108,108,108	0
3	CA	A	994	1/1	0.82	0.19	-1.50	63,63,63,63	0
2	ZN	A	991	1/1	0.97	0.09	-2.31	28,28,28,28	0
2	ZN	A	990	1/1	0.99	0.14	-2.35	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.