Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:02 PM EDT

PDB ID	:	3HHD
Title	:	Structure of the Human Fatty Acid Synthase KS-MAT Didomain as a Framework for Inhibitor Design.
Authors	:	Pappenberger, G.M.; Benz, J.; Thoma, R.; Rudolph, M.G.
Deposited on	:	2009-05-15
Resolution	:	2.15 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:

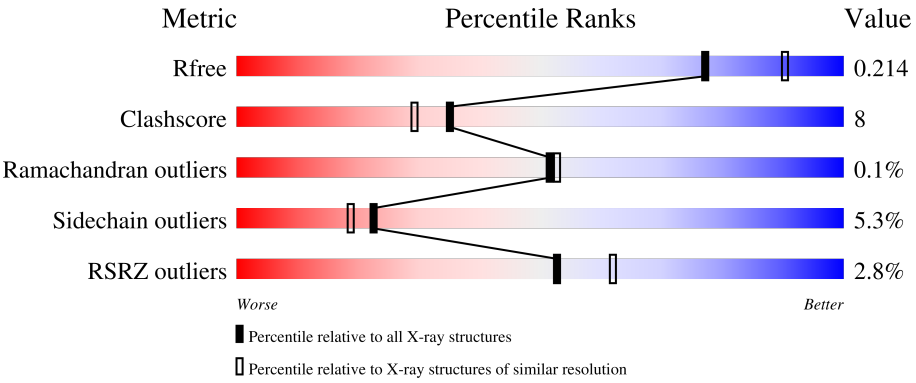
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	965	2% 72% 15% • 12%
1	B	965	4% 71% 15% • 12%
1	C	965	2% 73% 14% • 11%
1	D	965	3% 72% 14% • 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27836 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	852	Total	C	N	O	S	0	2	0
			6497	4119	1144	1200	34			
1	B	852	Total	C	N	O	S	0	3	0
			6505	4125	1147	1199	34			
1	C	855	Total	C	N	O	S	0	1	0
			6512	4127	1147	1204	34			
1	D	854	Total	C	N	O	S	0	2	0
			6512	4129	1146	1203	34			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P49327
A	0	THR	-	expression tag	UNP P49327
A	1	GLY	-	expression tag	UNP P49327
B	-1	SER	-	expression tag	UNP P49327
B	0	THR	-	expression tag	UNP P49327
B	1	GLY	-	expression tag	UNP P49327
C	-1	SER	-	expression tag	UNP P49327
C	0	THR	-	expression tag	UNP P49327
C	1	GLY	-	expression tag	UNP P49327
D	-1	SER	-	expression tag	UNP P49327
D	0	THR	-	expression tag	UNP P49327
D	1	GLY	-	expression tag	UNP P49327

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

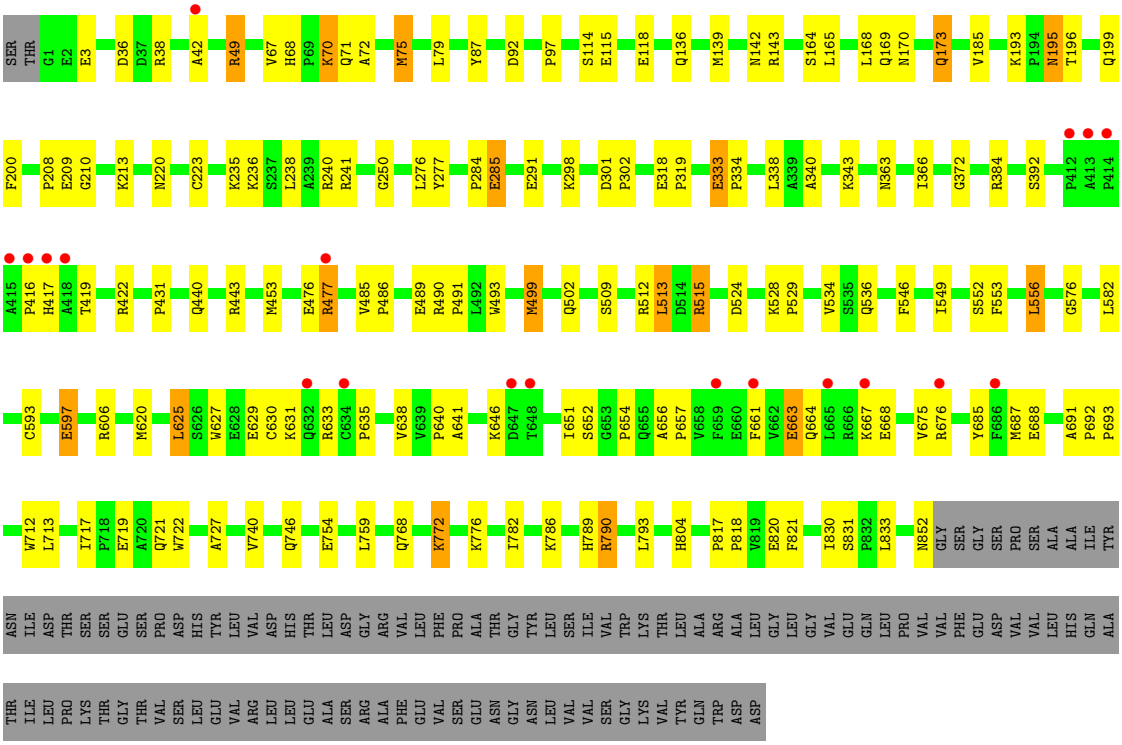
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	561	Total O 561 561	0	0
3	B	371	Total O 371 371	0	0
3	C	437	Total O 437 437	0	0
3	D	439	Total O 439 439	0	0

3 Residue-property plots (i)

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.

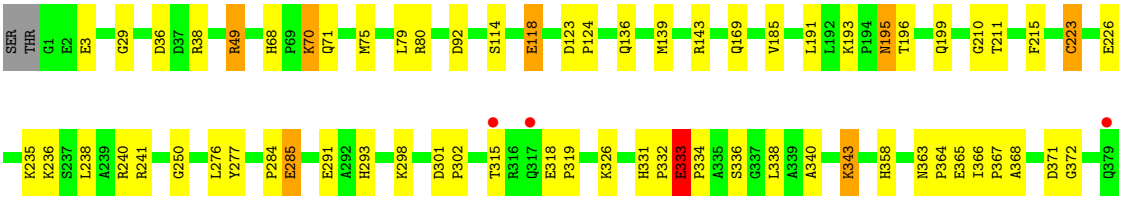
• Molecule 1: Fatty acid synthase

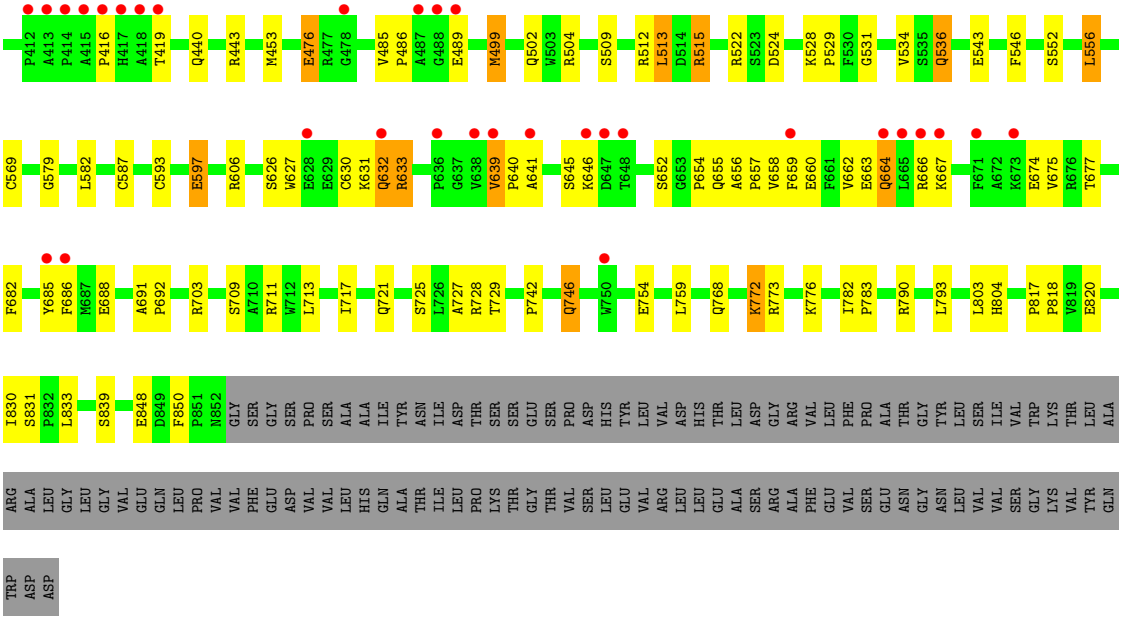
Chain A:



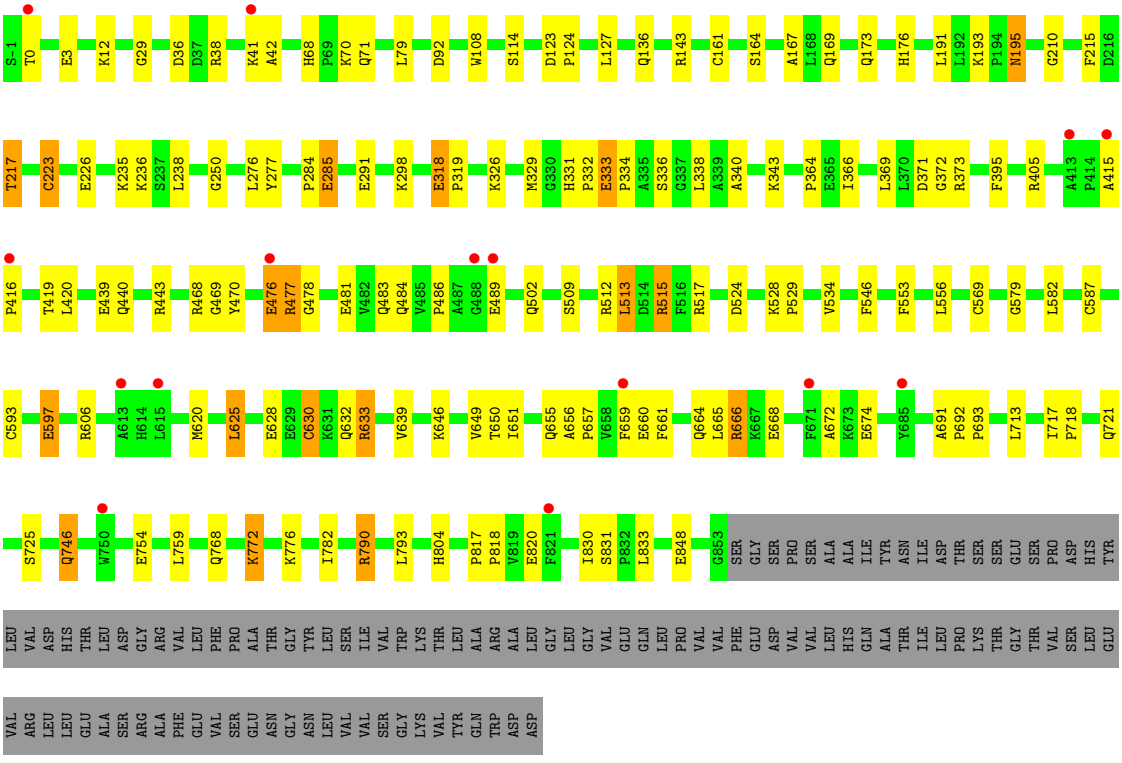
• Molecule 1: Fatty acid synthase

Chain B:

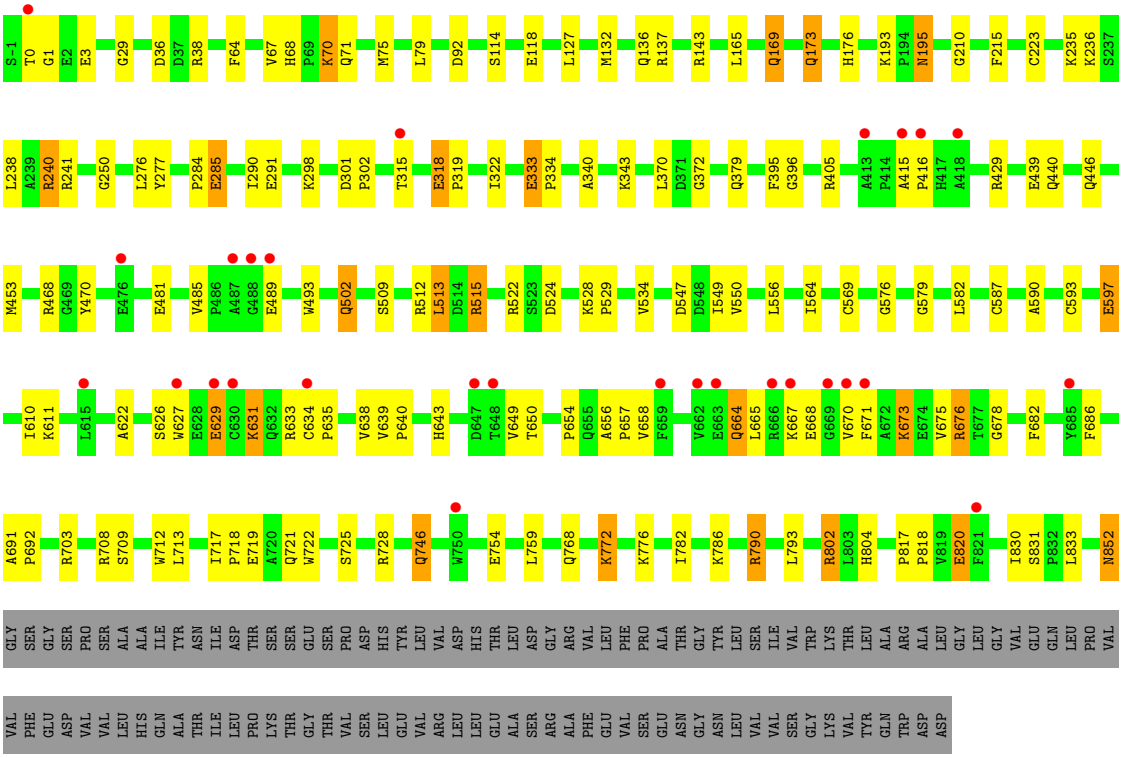




• Molecule 1: Fatty acid synthase



• Molecule 1: Fatty acid synthase


S-1 T0 G1 E2 E3 G29 D36 D37 R38 F64 V67 H68 P69 K70 Q71 M75 L79 D92 S114 E118 L127 M132 Q136 R137 R143 L165 Q169 Q173 H176 K193 P194 N195 G210 F215 C223 K235 S237
L238 A239 R240 R241 G250 L276 Y277 P284 E285 I290 E291 K298 D301 P302 T315 E318 P319 I322 E333 P334 A340 K343 L370 D371 G372 Q379 F395 G396 R405 A413 P414 A415 P416 H417 A418 R429 E439 Q440 Q446
M453 R468 G469 Y470 E476 E481 V485 P486 A487 G488 E489 W493 Q502 S509 R512 L513 D514 R515 R522 S523 D524 K528 P529 V534 D547 D548 I549 V550 L556 I564 C569 G576 G579 L582 C587 A590 C593 E597
I610 K611 L615 A622 S626 W627 E628 E629 C630 K631 Q632 R633 C634 P635 V638 V639 P640 H643 D647 T648 V649 T650 P654 Q655 A656 P657 V658 F659 V662 E663 Q664 L665 R666 K667 E668 G669 V670 F671 A672 K673 E674 V675 R676 T677 G678 F682 Y685 F686
A691 P692 R703 R708 S709 W712 L713 I717 P718 E719 A720 Q721 W722 S725 R728 Q746 W750 E754 L759 Q768 K772 K776 I782 K786 R790 L793 R802 L803 H804 P817 P818 V819 E820 F821 I830 S831 P832 L833 N852
GLY SER GLY SER PRO SER ALA ALA ILE TYR ASN ILE ASP THR SER SER GLU SER PRO ASP HIS TYR LEU VAL ASP HIS THR LEU ASP GLY ARG VAL LEU PHE PRO ALA THR GLY TYR LEU SER ILE VAL TRP LYS THR LEU ALA ARG ALA LEU GLY LEU GLY VAL GLU GLN LEU PRO VAL
VAL PHE GLU ASP VAL VAL LEU HIS GLN ALA THR ILE LEU PRO LYS THR GLY THR VAL SER LEU GLU VAL ARG LEU LEU GLU ALA SER ARG ALA PHE GLU VAL SER GLU ASN GLY ASN LEU VAL VAL SER GLY LYS VAL TYR GLN TRP ASP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.62Å 91.16Å 132.11Å 73.84° 86.83° 62.54°	Depositor
Resolution (Å)	45.64 – 2.15 45.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.64-2.15) 97.5 (45.64-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.14Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.169 , 0.211 0.171 , 0.214	Depositor DCC
R_{free} test set	9152 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27836	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% 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, 0.333 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: 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	0.68	1/6662 (0.0%)	0.68	0/9058
1	B	0.61	1/6673 (0.0%)	0.66	1/9074 (0.0%)
1	C	0.63	2/6674 (0.0%)	0.67	1/9075 (0.0%)
1	D	0.62	1/6678 (0.0%)	0.68	2/9083 (0.0%)
All	All	0.64	5/26687 (0.0%)	0.67	4/36290 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	593	CYS	CB-SG	-7.10	1.70	1.82
1	A	593	CYS	CB-SG	-5.64	1.72	1.81
1	D	223	CYS	CB-SG	-5.36	1.73	1.81
1	B	593	CYS	CB-SG	-5.31	1.73	1.81
1	C	161	CYS	CB-SG	-5.06	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	137	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	333	GLU	C-N-CD	5.47	139.88	128.40
1	C	468	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	802	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6497	0	6477	106	0
1	B	6505	0	6491	119	0
1	C	6512	0	6491	94	0
1	D	6512	0	6487	117	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	561	0	0	8	0
3	B	371	0	0	11	0
3	C	437	0	0	13	0
3	D	439	0	0	15	0
All	All	27836	0	25946	427	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 8.

All (427) 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:656:ALA:HB3	1:B:657:PRO:HD3	1.45	0.95
1:D:656:ALA:HB3	1:D:657:PRO:HD3	1.50	0.94
1:A:42:ALA:HB1	1:A:49:ARG:HD2	1.56	0.87
1:A:67:VAL:HG11	1:A:75:MET:HE1	1.56	0.85
1:D:556:LEU:HD23	1:D:582:LEU:HD23	1.62	0.81
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.68	0.75
1:C:333:GLU:HB2	1:C:334:PRO:HD2	1.68	0.75
1:B:639:VAL:HG22	1:B:640:PRO:HD2	1.70	0.72
1:D:626:SER:OG	1:D:629:GLU:HB2	1.88	0.72
1:A:790:ARG:CD	1:A:790:ARG:H	2.01	0.72
1:C:790:ARG:H	1:C:790:ARG:CD	2.03	0.69
1:B:728:ARG:HG2	1:B:729:THR:HG23	1.73	0.69
1:D:633:ARG:NH2	1:D:668:GLU:OE1	2.25	0.69
1:B:368:ALA:HA	1:B:371:ASP:OD1	1.92	0.69
1:D:790:ARG:CD	1:D:790:ARG:H	2.03	0.69
1:C:848:GLU:HG2	3:C:1008:HOH:O	1.93	0.69
1:B:440:GLN:OE1	1:B:443:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLN:OE1	1:A:443:ARG:NH1	2.26	0.69
1:D:786:LYS:NZ	3:D:1096:HOH:O	2.24	0.68
1:A:477:ARG:NH1	1:A:789:HIS:HE2	1.91	0.68
1:C:440:GLN:HG3	1:C:833:LEU:HD22	1.76	0.68
1:D:440:GLN:HG3	1:D:833:LEU:HD22	1.76	0.68
1:B:655:GLN:HG3	1:B:659:PHE:CE2	2.30	0.67
1:D:291:GLU:HG2	1:D:340:ALA:HB1	1.78	0.66
1:A:209:GLU:OE2	1:A:213:LYS:NZ	2.27	0.66
1:C:3:GLU:OE2	1:C:236:LYS:HD2	1.96	0.66
1:D:515:ARG:HB2	3:D:1250:HOH:O	1.95	0.65
1:C:477:ARG:HG3	1:C:478:GLY:H	1.61	0.65
3:A:1712:HOH:O	1:C:41:LYS:HD3	1.96	0.65
1:C:193:LYS:HE3	1:C:195:ASN:HB2	1.79	0.65
1:D:656:ALA:CB	1:D:657:PRO:HD3	2.25	0.65
1:B:656:ALA:O	1:B:660:GLU:HG2	1.97	0.64
1:D:68[A]:HIS:HB3	1:D:71:GLN:OE1	1.97	0.64
1:A:3:GLU:OE2	1:A:236:LYS:HD2	1.98	0.64
1:A:663:GLU:OE1	1:A:663:GLU:HA	1.96	0.64
1:D:768:GLN:O	1:D:772:LYS:HD2	1.98	0.63
1:A:768:GLN:O	1:A:772:LYS:HD2	1.98	0.63
1:B:68:HIS:CE1	1:B:70:LYS:HG3	2.33	0.63
1:A:68:HIS:CE1	1:A:70:LYS:HG3	2.33	0.63
1:C:333:GLU:HB2	1:C:334:PRO:CD	2.29	0.63
1:D:290:ILE:HG23	1:D:322:ILE:HG22	1.80	0.63
1:A:363:ASN:HB3	1:A:366:ILE:HD12	1.80	0.63
1:A:515:ARG:HB2	3:A:1251:HOH:O	1.99	0.62
1:B:768:GLN:O	1:B:772:LYS:HD2	1.99	0.62
1:C:217:THR:HG23	1:C:364:PRO:CD	2.28	0.62
1:C:666:ARG:NH1	1:C:672:ALA:O	2.32	0.62
1:C:318:GLU:HG2	3:C:1794:HOH:O	1.98	0.62
1:A:786:LYS:NZ	3:A:1091:HOH:O	2.29	0.62
1:D:71:GLN:HB3	3:D:1519:HOH:O	2.00	0.62
1:A:664:GLN:O	1:A:667:LYS:HB2	1.99	0.62
1:C:768:GLN:O	1:C:772:LYS:HD2	1.99	0.62
1:D:691:ALA:HB3	1:D:692:PRO:HD3	1.82	0.62
1:A:139:MET:HE3	1:D:395:PHE:CE1	2.34	0.61
1:B:645:SER:HA	1:B:746:GLN:CG	2.29	0.61
1:B:703:ARG:NH2	3:B:1065:HOH:O	2.29	0.61
1:C:285:GLU:HB3	3:C:1536:HOH:O	1.99	0.61
1:D:285:GLU:O	1:D:285:GLU:HG3	2.00	0.61
1:D:547:ASP:OD1	1:D:676:ARG:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:HB2	1:D:334:PRO:HD2	1.82	0.61
1:D:804:HIS:HB2	3:D:1053:HOH:O	2.00	0.61
1:A:68:HIS:HE1	1:A:70:LYS:HG3	1.65	0.61
1:B:645:SER:HA	1:B:746:GLN:HG2	1.81	0.61
1:C:556:LEU:HD23	1:C:582:LEU:HD23	1.82	0.61
1:B:333:GLU:HB2	1:B:334:PRO:HD2	1.83	0.61
1:D:67:VAL:HG11	1:D:75:MET:HE1	1.83	0.61
1:B:3:GLU:OE2	1:B:236:LYS:HD2	2.01	0.61
1:A:790:ARG:H	1:A:790:ARG:NE	1.98	0.61
1:B:68:HIS:HE1	1:B:70:LYS:HG3	1.64	0.61
1:C:691:ALA:HB3	1:C:692:PRO:HD3	1.83	0.60
1:B:691:ALA:HB3	1:B:692:PRO:HD3	1.82	0.60
1:D:3:GLU:OE2	1:D:236:LYS:HD2	2.01	0.60
1:A:333:GLU:HB2	1:A:334:PRO:HD2	1.82	0.60
1:D:193:LYS:HE3	1:D:195:ASN:HB2	1.82	0.60
1:C:661:PHE:O	1:C:665:LEU:HG	2.02	0.60
1:B:641:ALA:HB2	1:B:652:SER:HB2	1.84	0.60
1:B:746:GLN:HE21	1:B:746:GLN:CA	2.15	0.60
1:D:790:ARG:H	1:D:790:ARG:NE	1.99	0.60
1:A:193:LYS:HE3	1:A:195:ASN:HB2	1.84	0.60
1:A:417:HIS:ND1	1:A:422:ARG:NH2	2.49	0.60
1:B:285:GLU:O	1:B:285:GLU:HG3	1.99	0.60
1:D:754:GLU:HG2	1:D:776:LYS:HD3	1.84	0.60
1:B:531:GLY:HA2	3:B:1230:HOH:O	2.02	0.59
1:C:790:ARG:H	1:C:790:ARG:NE	2.00	0.59
1:B:476:GLU:HB2	3:B:1353:HOH:O	2.01	0.59
1:B:75:MET:HE1	1:B:79:LEU:HG	1.85	0.59
1:B:664:GLN:O	1:B:667:LYS:HB2	2.03	0.59
1:C:285:GLU:O	1:C:285:GLU:HG3	2.00	0.59
1:B:193:LYS:HE3	1:B:195:ASN:HB2	1.84	0.58
1:B:627:TRP:CD1	1:B:631:LYS:HE2	2.37	0.58
1:B:632:GLN:HG3	1:B:633:ARG:HG2	1.84	0.58
1:C:754:GLU:HG2	1:C:776:LYS:HD3	1.84	0.58
1:A:633:ARG:NH2	1:A:668:GLU:OE1	2.36	0.58
1:B:79:LEU:HD21	1:B:143[A]:ARG:HG3	1.86	0.58
1:C:42:ALA:HA	3:C:1704:HOH:O	2.04	0.58
1:D:290:ILE:CG2	1:D:322:ILE:HG22	2.34	0.58
1:A:499:MET:HE2	1:A:553:PHE:HE1	1.68	0.58
1:D:470:TYR:CZ	1:D:481:GLU:HG3	2.39	0.58
1:A:691:ALA:HB3	1:A:692:PRO:HD3	1.85	0.58
1:A:301:ASP:HB2	1:A:302:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:TRP:CD1	1:A:631:LYS:HE2	2.38	0.57
1:C:405:ARG:NH1	3:C:1194:HOH:O	2.34	0.57
1:B:685:TYR:O	1:B:688:GLU:HB2	2.03	0.57
1:C:0:THR:HG23	1:C:176:HIS:HE1	1.69	0.57
1:C:477:ARG:CG	1:C:478:GLY:H	2.15	0.57
1:B:504[B]:ARG:NH2	1:B:543:GLU:OE1	2.38	0.57
1:D:703:ARG:NH1	3:D:1142:HOH:O	2.38	0.57
1:A:625:LEU:HD12	1:A:629:GLU:HB3	1.87	0.56
1:C:291:GLU:HG2	1:C:340:ALA:HB1	1.86	0.56
1:B:139:MET:HE3	1:C:395:PHE:CE1	2.39	0.56
1:B:293:HIS:O	1:B:326:LYS:HE2	2.04	0.56
1:A:285:GLU:O	1:A:285:GLU:HG3	2.06	0.56
1:B:363:ASN:HB3	1:B:366:ILE:HD12	1.88	0.56
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.86	0.56
1:B:658:VAL:O	1:B:662:VAL:HG23	2.06	0.55
1:C:502:GLN:HG3	1:C:546:PHE:HB3	1.88	0.55
1:D:639:VAL:HG22	1:D:640:PRO:N	2.21	0.55
1:D:440:GLN:HG3	1:D:833:LEU:CD2	2.36	0.55
1:A:754:GLU:HG2	1:A:776:LYS:HD3	1.89	0.54
1:D:509:SER:O	1:D:512:ARG:HD3	2.06	0.54
1:B:440:GLN:HG2	1:B:833:LEU:HD11	1.89	0.54
1:C:217:THR:HG23	1:C:364:PRO:HD2	1.88	0.54
1:B:235:LYS:HE2	1:B:238:LEU:HD13	1.89	0.54
1:C:440:GLN:HG3	1:C:833:LEU:CD2	2.37	0.54
1:D:627:TRP:HA	1:D:649:VAL:HG21	1.89	0.54
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.89	0.54
1:D:319:PRO:HB3	1:D:372:GLY:O	2.08	0.54
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.89	0.54
1:D:333:GLU:CB	1:D:334:PRO:CD	2.85	0.54
1:B:502:GLN:HG3	1:B:546:PHE:HB3	1.90	0.54
1:B:556:LEU:HD22	1:B:582:LEU:HD23	1.90	0.54
1:A:685:TYR:O	1:A:688:GLU:HB2	2.08	0.53
1:C:332:PRO:HG2	1:C:336:SER:HA	1.89	0.53
1:A:499:MET:CE	1:A:553:PHE:CE1	2.91	0.53
1:A:285:GLU:HB3	3:A:1073:HOH:O	2.07	0.53
1:B:509:SER:O	1:B:512:ARG:HD3	2.09	0.53
1:C:333:GLU:CB	1:C:334:PRO:CD	2.87	0.53
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.90	0.53
1:A:440:GLN:HG2	1:A:833:LEU:HD11	1.91	0.53
1:B:746:GLN:HE21	1:B:746:GLN:C	2.11	0.53
1:A:502:GLN:HG3	1:A:546:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:SER:O	1:A:512:ARG:HD3	2.09	0.52
1:A:556:LEU:HD22	1:A:582:LEU:HD23	1.89	0.52
1:B:333:GLU:HB2	1:B:334:PRO:CD	2.38	0.52
1:D:550:VAL:HG23	1:D:611:LYS:HD2	1.92	0.52
1:A:240:ARG:NH1	1:A:821:PHE:CE2	2.78	0.52
1:A:319:PRO:HB3	1:A:372:GLY:O	2.09	0.52
1:C:656:ALA:HB3	1:C:657:PRO:CD	2.40	0.52
1:A:79:LEU:HD21	1:A:143[A]:ARG:HG3	1.92	0.52
1:B:365:GLU:O	1:B:367:PRO:HD3	2.09	0.52
1:B:663:GLU:HA	1:B:663:GLU:OE1	2.09	0.52
1:D:649:VAL:CG1	1:D:650:THR:N	2.73	0.52
1:B:68:HIS:HE1	1:B:70:LYS:CG	2.22	0.52
1:D:622:ALA:HB3	1:D:673:LYS:HG2	1.92	0.52
1:C:579:GLY:HA3	1:C:587:CYS:SG	2.50	0.52
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.92	0.51
1:B:717:ILE:HD13	1:B:727:ALA:HB2	1.90	0.51
1:C:92:ASP:HB2	1:C:831:SER:HB3	1.91	0.51
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.92	0.51
1:B:522:ARG:HD2	3:B:1105:HOH:O	2.10	0.51
1:C:509:SER:O	1:C:512:ARG:HD3	2.10	0.51
1:C:524:ASP:OD1	1:C:534:VAL:N	2.43	0.51
1:A:549:ILE:HD11	1:A:553:PHE:CZ	2.45	0.51
1:B:639:VAL:CG2	1:B:640:PRO:HD2	2.41	0.51
1:C:486:PRO:HD2	3:C:1576:HOH:O	2.11	0.51
1:A:235:LYS:HE2	1:A:238:LEU:HD13	1.92	0.51
1:B:656:ALA:CB	1:B:657:PRO:HD3	2.28	0.51
1:C:235:LYS:HE2	1:C:238:LEU:HD13	1.92	0.51
1:D:333:GLU:CB	1:D:334:PRO:HD2	2.41	0.51
1:A:68:HIS:HE1	1:A:70:LYS:CG	2.24	0.50
1:D:671:PHE:CZ	1:D:673:LYS:HB3	2.45	0.50
1:B:92:ASP:HB2	1:B:831:SER:HB3	1.93	0.50
1:B:331:HIS:CD2	1:B:333:GLU:H	2.29	0.50
1:A:524:ASP:OD1	1:A:534:VAL:N	2.44	0.50
1:B:319:PRO:HB3	1:B:372:GLY:O	2.11	0.50
1:D:405:ARG:NH1	3:D:1100:HOH:O	2.35	0.50
1:C:173:GLN:HG3	3:C:992:HOH:O	2.11	0.50
1:D:92:ASP:HB2	1:D:831:SER:HB3	1.92	0.50
1:D:852:ASN:HD22	1:D:852:ASN:C	2.15	0.50
1:D:493:TRP:CD2	1:D:576:GLY:HA3	2.46	0.50
1:C:0:THR:HG23	1:C:176:HIS:CE1	2.46	0.49
1:D:639:VAL:CG2	1:D:640:PRO:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ARG:NH1	1:A:668:GLU:OE1	2.45	0.49
1:D:675:VAL:HG12	1:D:676:ARG:N	2.28	0.49
1:C:484:GLN:OE1	3:C:1480:HOH:O	2.19	0.49
1:B:499:MET:HE3	1:B:682:PHE:CD2	2.47	0.49
1:B:597:GLU:CD	1:B:597:GLU:H	2.16	0.49
1:D:524:ASP:OD1	1:D:534:VAL:N	2.46	0.49
1:A:499:MET:HE1	1:A:553:PHE:CE1	2.47	0.49
1:A:92:ASP:HB2	1:A:831:SER:HB3	1.93	0.49
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.95	0.49
1:A:333:GLU:CB	1:A:334:PRO:CD	2.90	0.49
1:A:200:PHE:CZ	1:D:132:MET:HE1	2.48	0.48
1:D:627:TRP:CA	1:D:649:VAL:HG21	2.43	0.48
1:A:71:GLN:HB2	3:A:1037:HOH:O	2.12	0.48
1:D:719:GLU:HG3	1:D:722:TRP:CE3	2.48	0.48
1:B:139:MET:CE	1:C:395:PHE:CE1	2.96	0.48
1:A:139:MET:CE	1:D:395:PHE:CE1	2.95	0.48
1:A:416:PRO:O	1:A:419:THR:OG1	2.31	0.48
1:D:235:LYS:HE2	1:D:238:LEU:HD13	1.94	0.48
1:B:524:ASP:OD1	1:B:534:VAL:N	2.46	0.48
1:B:656:ALA:HB3	1:B:657:PRO:CD	2.29	0.48
1:B:754:GLU:HG2	1:B:776:LYS:HD2	1.94	0.48
1:D:597:GLU:H	1:D:597:GLU:CD	2.17	0.48
1:D:627:TRP:CE3	1:D:643:HIS:HB2	2.48	0.48
1:D:627:TRP:HE1	1:D:631:LYS:NZ	2.12	0.48
1:A:417:HIS:HE1	3:A:1365:HOH:O	1.97	0.48
1:C:29:GLY:HA2	3:C:1031:HOH:O	2.14	0.48
1:D:549:ILE:HG23	1:D:678:GLY:HA3	1.95	0.48
1:B:75:MET:HE3	1:B:79:LEU:HD23	1.95	0.48
1:A:675:VAL:HG12	1:A:676:ARG:N	2.29	0.48
1:A:597:GLU:H	1:A:597:GLU:CD	2.17	0.48
1:D:515:ARG:CB	3:D:1250:HOH:O	2.56	0.47
1:D:79:LEU:HD21	1:D:143:ARG:HG3	1.97	0.47
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.43	0.47
1:A:170:ASN:HA	1:A:173:GLN:HG3	1.96	0.47
1:B:804:HIS:HB2	3:B:1104:HOH:O	2.14	0.47
1:C:319:PRO:HB3	1:C:372:GLY:O	2.13	0.47
1:A:493:TRP:CD2	1:A:576:GLY:HA3	2.50	0.47
1:A:499:MET:CE	1:A:553:PHE:HE1	2.28	0.47
1:B:675:VAL:HG12	1:B:677:THR:HG23	1.96	0.47
1:C:513:LEU:HD22	1:C:793:LEU:HD13	1.97	0.47
1:D:664:GLN:O	1:D:664:GLN:HG2	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:HIS:HB2	1:C:71:GLN:OE1	2.15	0.47
1:C:597:GLU:CD	1:C:597:GLU:H	2.18	0.47
1:C:759:LEU:HD23	1:C:782:ILE:HB	1.97	0.47
1:D:318:GLU:HG2	3:D:984:HOH:O	2.15	0.47
1:D:0:THR:HG23	1:D:176:HIS:HE1	1.80	0.47
1:D:634:CYS:SG	1:D:638:VAL:HG12	2.55	0.47
1:A:75:MET:HE2	1:A:75:MET:HB2	1.76	0.46
1:B:36:ASP:OD1	1:B:38:ARG:HB2	2.15	0.46
1:B:711:ARG:NE	3:B:1120:HOH:O	2.47	0.46
1:B:515:ARG:HB2	3:B:988:HOH:O	2.15	0.46
1:B:536:GLN:NE2	3:B:1011:HOH:O	2.47	0.46
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.50	0.46
1:D:0:THR:HG23	1:D:176:HIS:CE1	2.50	0.46
1:B:250:GLY:HA3	1:B:276:LEU:HD21	1.98	0.46
1:B:645:SER:HA	1:B:746:GLN:HG3	1.97	0.46
1:B:675:VAL:HG12	1:B:677:THR:CG2	2.45	0.46
1:D:240:ARG:NE	3:D:1005:HOH:O	2.47	0.46
1:D:241:ARG:HB2	1:D:453:MET:HE1	1.97	0.46
1:A:67:VAL:HG11	1:A:75:MET:CE	2.38	0.46
1:B:759:LEU:HD23	1:B:782:ILE:HB	1.97	0.46
1:D:68[A]:HIS:CE1	1:D:70:LYS:HG3	2.51	0.46
1:A:241:ARG:HB2	1:A:453:MET:HE1	1.96	0.46
1:A:68:HIS:CE1	1:A:70:LYS:CG	2.98	0.46
1:D:36:ASP:OD1	1:D:38:ARG:HB2	2.16	0.46
1:A:528:LYS:N	1:A:529:PRO:CD	2.79	0.46
1:C:470:TYR:CZ	1:C:481:GLU:HG3	2.50	0.46
1:C:477:ARG:HA	1:C:477:ARG:HD3	1.48	0.46
1:A:513:LEU:HD22	1:A:793:LEU:HD13	1.97	0.46
1:B:68:HIS:CE1	1:B:70:LYS:CG	2.96	0.46
1:B:75:MET:HE2	1:B:80:ARG:HG2	1.98	0.46
1:B:210:GLY:C	1:B:223:CYS:HB2	2.36	0.46
1:B:315:THR:HG23	1:B:315:THR:O	2.15	0.46
1:C:692:PRO:HB2	1:C:693:PRO:HD3	1.98	0.46
1:A:72:ALA:HA	1:A:75:MET:HE3	1.97	0.46
1:C:371:ASP:OD2	1:C:373:ARG:NH2	2.47	0.46
1:D:627:TRP:CD1	1:D:627:TRP:C	2.90	0.46
1:A:208:PRO:HD2	1:A:220:ASN:ND2	2.31	0.45
1:B:333:GLU:CB	1:B:334:PRO:CD	2.94	0.45
1:C:664:GLN:O	1:C:668:GLU:HG3	2.16	0.45
1:A:485:VAL:HA	1:A:486:PRO:HD3	1.83	0.45
1:C:439:GLU:HB2	3:C:1046:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:LEU:CD1	1:C:630:CYS:SG	3.04	0.45
1:C:649:VAL:CG1	1:C:650:THR:N	2.79	0.45
1:C:660:GLU:O	1:C:664:GLN:HG3	2.17	0.45
1:D:502[A]:GLN:CG	1:D:676:ARG:NH2	2.80	0.45
1:D:654:PRO:O	1:D:658:VAL:HG23	2.16	0.45
1:D:708:ARG:HG2	1:D:712:TRP:CZ3	2.52	0.45
1:C:36:ASP:OD1	1:C:38:ARG:HB2	2.17	0.45
1:D:513:LEU:HD22	1:D:793:LEU:HD13	1.99	0.45
1:A:200:PHE:CE2	1:D:132:MET:HE1	2.52	0.45
1:D:717:ILE:HA	1:D:718:PRO:HD3	1.87	0.45
1:B:332:PRO:HG2	1:B:336:SER:HA	1.99	0.45
1:B:528:LYS:N	1:B:529:PRO:CD	2.79	0.45
1:C:528:LYS:HB3	1:C:529:PRO:HD3	1.99	0.45
1:C:655:GLN:HG3	1:C:659:PHE:CE2	2.52	0.45
1:A:200:PHE:CZ	1:D:132:MET:CE	3.00	0.45
1:C:329:MET:HE2	1:C:332:PRO:HD3	1.98	0.45
1:C:79:LEU:HD21	1:C:143:ARG:HG3	1.99	0.45
1:D:127:LEU:HD12	1:D:127:LEU:C	2.37	0.45
1:D:528:LYS:N	1:D:529:PRO:CD	2.80	0.45
1:C:633:ARG:HE	1:C:633:ARG:HB3	1.70	0.45
1:D:169:GLN:O	1:D:173:GLN:HG2	2.16	0.45
1:D:556:LEU:HD23	1:D:582:LEU:CD2	2.40	0.45
1:D:708:ARG:HD2	1:D:712:TRP:CZ3	2.52	0.45
1:B:817:PRO:HA	1:B:818:PRO:HD3	1.88	0.44
1:C:528:LYS:N	1:C:529:PRO:CD	2.80	0.44
1:C:553:PHE:CD1	1:C:582:LEU:HD22	2.52	0.44
1:D:759:LEU:HD23	1:D:782:ILE:HB	1.99	0.44
1:A:115:GLU:HA	1:A:118:GLU:HG3	1.98	0.44
1:A:620:MET:HA	1:A:651:ILE:O	2.18	0.44
1:A:641:ALA:HB2	1:A:652:SER:HB2	1.99	0.44
1:B:92:ASP:HA	1:B:830:ILE:HB	1.99	0.44
1:C:476:GLU:O	1:C:477:ARG:HB2	2.17	0.44
1:C:579:GLY:CA	1:C:587:CYS:SG	3.05	0.44
1:D:564:ILE:HD13	1:D:590:ALA:HB2	1.99	0.44
1:A:168:LEU:HD12	1:A:185:VAL:HG21	1.99	0.44
1:A:582:LEU:HD13	1:A:606:ARG:HD3	1.99	0.44
1:B:343:LYS:HD3	1:B:343:LYS:C	2.38	0.44
1:B:641:ALA:O	1:B:742:PRO:HA	2.18	0.44
1:D:301:ASP:HB2	1:D:302:PRO:HD3	1.99	0.44
1:B:499:MET:CE	1:B:682:PHE:CD2	3.01	0.44
1:D:626:SER:HG	1:D:629:GLU:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:OD1	1:A:38:ARG:HB2	2.17	0.44
1:B:79:LEU:HD21	1:B:143[B]:ARG:HG2	1.99	0.44
1:B:301:ASP:HB2	1:B:302:PRO:HD3	1.99	0.44
1:A:490:ARG:HA	1:A:491:PRO:HD2	1.90	0.44
1:C:620:MET:HA	1:C:651:ILE:O	2.17	0.43
1:D:468:ARG:HD2	1:D:485:VAL:HG21	2.00	0.43
1:D:654:PRO:HB2	1:D:657:PRO:HD2	2.00	0.43
1:A:301:ASP:CB	1:A:302:PRO:HD3	2.49	0.43
1:A:638:VAL:HG11	1:A:651:ILE:HD12	2.00	0.43
1:C:210:GLY:C	1:C:223:CYS:HB2	2.37	0.43
1:C:804:HIS:HB2	3:C:1176:HOH:O	2.18	0.43
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.53	0.43
1:B:343:LYS:HD3	1:B:343:LYS:O	2.18	0.43
1:C:582:LEU:HD13	1:C:606:ARG:HD3	2.00	0.43
1:D:649:VAL:HG12	1:D:650:THR:N	2.33	0.43
1:B:29:GLY:HA2	3:B:1085:HOH:O	2.18	0.43
1:C:250:GLY:HA3	1:C:276:LEU:HD21	2.01	0.43
1:C:515:ARG:HD3	1:C:569:CYS:SG	2.59	0.43
1:C:416:PRO:O	1:C:419:THR:OG1	2.36	0.43
1:B:416:PRO:O	1:B:419:THR:OG1	2.35	0.43
1:B:513:LEU:HD22	1:B:793:LEU:HD13	2.00	0.43
1:B:582:LEU:HD13	1:B:606:ARG:HD3	1.99	0.43
1:B:633:ARG:HE	1:B:633:ARG:HB3	1.49	0.43
1:A:210:GLY:C	1:A:223:CYS:HB2	2.38	0.43
1:B:49:ARG:H	1:B:49:ARG:HG2	1.68	0.43
1:D:502[A]:GLN:HG2	1:D:676:ARG:NH2	2.34	0.43
1:B:75:MET:CE	1:B:79:LEU:HG	2.48	0.43
1:C:517:ARG:HD2	3:C:1631:HOH:O	2.17	0.43
1:B:191:LEU:HG	1:B:226:GLU:HG2	2.01	0.43
1:C:326:LYS:HE3	1:C:331:HIS:CD2	2.54	0.43
1:C:477:ARG:CG	1:C:478:GLY:N	2.80	0.43
1:D:29:GLY:HA2	3:D:1089:HOH:O	2.18	0.43
1:C:108:TRP:HB3	1:C:167:ALA:HB1	2.01	0.42
1:C:692:PRO:HB2	1:C:693:PRO:CD	2.48	0.42
1:D:439:GLU:HB2	3:D:1126:HOH:O	2.19	0.42
1:A:804:HIS:HB2	3:A:1291:HOH:O	2.19	0.42
1:B:196:THR:HA	1:B:199:GLN:HE21	1.84	0.42
1:C:123:ASP:HA	1:C:124:PRO:HD2	1.94	0.42
1:C:127:LEU:C	1:C:127:LEU:HD12	2.39	0.42
1:C:164:SER:HB2	1:C:338:LEU:HG	2.01	0.42
1:D:92:ASP:HA	1:D:830:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:THR:O	1:D:315:THR:HG23	2.18	0.42
1:B:211:THR:CG2	1:B:358:HIS:CD2	3.02	0.42
1:C:469:GLY:HA2	1:C:481:GLU:O	2.19	0.42
1:D:633:ARG:O	1:D:635:PRO:HD3	2.20	0.42
1:B:803:LEU:HD12	1:B:803:LEU:HA	1.82	0.42
1:C:277:TYR:CZ	1:C:284:PRO:HG3	2.55	0.42
1:C:420:LEU:HD21	1:C:512:ARG:HB3	2.00	0.42
1:C:746:GLN:HE21	1:C:746:GLN:HB3	1.61	0.42
1:A:528:LYS:HB3	1:A:529:PRO:HD3	2.01	0.42
1:D:0:THR:HG23	1:D:1:GLY:N	2.35	0.42
1:A:431:PRO:HG2	1:B:839:SER:HB2	2.01	0.42
1:A:633:ARG:HH12	1:A:668:GLU:CD	2.23	0.42
1:B:240:ARG:HA	1:B:240:ARG:HD2	1.86	0.42
1:D:528:LYS:HB3	1:D:529:PRO:HD3	2.02	0.42
1:A:165:LEU:HD22	1:A:392:SER:HB2	2.02	0.42
1:B:241:ARG:HB2	1:B:453:MET:HE1	2.01	0.42
1:D:550:VAL:HG23	1:D:611:LYS:CD	2.49	0.42
1:D:665:LEU:HD23	1:D:665:LEU:HA	1.82	0.42
1:B:185:VAL:HG12	1:B:338:LEU:HD11	2.01	0.41
1:B:579:GLY:HA3	1:B:587:CYS:SG	2.60	0.41
1:B:782:ILE:HA	1:B:783:PRO:HD2	1.93	0.41
1:C:191:LEU:HG	1:C:226:GLU:HG2	2.02	0.41
1:C:817:PRO:HA	1:C:818:PRO:HD3	1.91	0.41
1:D:75:MET:HE2	1:D:75:MET:HB2	1.82	0.41
1:D:277:TYR:CZ	1:D:284:PRO:HG3	2.55	0.41
1:A:92:ASP:HA	1:A:830:ILE:HB	2.02	0.41
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.55	0.41
1:A:692:PRO:HB2	1:A:693:PRO:HD3	2.02	0.41
1:D:165:LEU:HD12	1:D:165:LEU:HA	1.90	0.41
1:C:12:LYS:HE3	3:C:1180:HOH:O	2.19	0.41
1:A:196:THR:HA	1:A:199:GLN:HE21	1.85	0.41
1:B:71:GLN:O	1:B:75:MET:HG3	2.21	0.41
1:B:75:MET:HE2	1:B:80:ARG:CG	2.50	0.41
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.55	0.41
3:A:1238:HOH:O	1:B:839:SER:HA	2.18	0.41
1:B:499:MET:HE1	1:B:682:PHE:CG	2.56	0.41
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.86	0.41
1:D:379:GLN:HG3	3:D:1343:HOH:O	2.19	0.41
1:D:493:TRP:CE2	1:D:576:GLY:HA3	2.56	0.41
1:D:746:GLN:HE21	1:D:746:GLN:HB3	1.64	0.41
1:D:817:PRO:HA	1:D:818:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:TYR:CZ	1:B:284:PRO:HG3	2.56	0.41
1:B:656:ALA:CB	1:B:657:PRO:CD	2.96	0.41
1:B:848:GLU:OE2	3:B:1055:HOH:O	2.22	0.41
1:D:415:ALA:HB1	1:D:416:PRO:HD2	2.03	0.41
1:B:682:PHE:HB3	3:B:1187:HOH:O	2.20	0.41
1:D:64:PHE:CD1	1:D:429:ARG:HD3	2.56	0.41
1:A:277:TYR:CZ	1:A:284:PRO:HG3	2.55	0.41
1:A:717:ILE:HD13	1:A:727:ALA:HB2	2.02	0.41
1:B:118:GLU:HG2	1:B:850:PHE:CE1	2.56	0.41
1:D:210:GLY:HA2	3:D:1012:HOH:O	2.20	0.41
1:D:671:PHE:HZ	1:D:673:LYS:HD2	1.86	0.41
1:A:169:GLN:O	1:A:173:GLN:HG2	2.20	0.41
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.84	0.41
1:D:67:VAL:HG11	1:D:75:MET:CE	2.49	0.41
1:D:250:GLY:HA3	1:D:276:LEU:HD21	2.02	0.41
1:D:579:GLY:HA3	1:D:587:CYS:SG	2.61	0.41
1:A:552:SER:O	1:A:556:LEU:HB2	2.21	0.40
1:B:123:ASP:HA	1:B:124:PRO:HD2	1.93	0.40
1:B:552:SER:O	1:B:556:LEU:HB2	2.20	0.40
1:B:746:GLN:HE21	1:B:746:GLN:HA	1.84	0.40
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.98	0.40
1:A:417:HIS:CD2	1:A:417:HIS:H	2.39	0.40
1:A:712:TRP:CD1	1:A:712:TRP:C	2.94	0.40
1:B:363:ASN:OD1	1:B:364:PRO:HD2	2.22	0.40
1:C:92:ASP:HA	1:C:830:ILE:HB	2.02	0.40
1:C:415:ALA:HB1	1:C:416:PRO:HD2	2.03	0.40
1:C:717:ILE:HA	1:C:718:PRO:HD3	1.92	0.40
1:D:240:ARG:CD	3:D:1005:HOH:O	2.69	0.40
1:D:654:PRO:HG3	1:D:686:PHE:CZ	2.56	0.40
1:A:142:ASN:HD22	1:D:396:GLY:HA3	1.85	0.40
1:A:164:SER:HB2	1:A:338:LEU:HG	2.03	0.40
1:A:185:VAL:HG12	1:A:338:LEU:HD11	2.03	0.40
1:B:579:GLY:CA	1:B:587:CYS:SG	3.09	0.40
1:C:754:GLU:HG2	1:C:776:LYS:CD	2.50	0.40
1:D:820:GLU:HB2	3:D:1042:HOH:O	2.20	0.40
1:A:817:PRO:HA	1:A:818:PRO:HD3	1.91	0.40
1:A:87:TYR:CE2	1:A:97:PRO:HG2	2.57	0.40
1:A:687:MET:HB2	1:A:740:VAL:HG12	2.04	0.40
1:B:499:MET:H	1:B:499:MET:HG2	1.70	0.40
1:D:610:ILE:HD13	1:D:682:PHE:HE1	1.87	0.40
1:D:670:VAL:HG12	1:D:671:PHE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	852/965 (88%)	837 (98%)	14 (2%)	1 (0%)	51	53
1	B	853/965 (88%)	836 (98%)	16 (2%)	1 (0%)	51	53
1	C	854/965 (88%)	840 (98%)	13 (2%)	1 (0%)	51	53
1	D	854/965 (88%)	837 (98%)	16 (2%)	1 (0%)	51	53
All	All	3413/3860 (88%)	3350 (98%)	59 (2%)	4 (0%)	51	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	GLU
1	B	333	GLU
1	C	333	GLU
1	D	333	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	698/792 (88%)	666 (95%)	32 (5%)	27	23
1	B	698/792 (88%)	658 (94%)	40 (6%)	20	16
1	C	699/792 (88%)	663 (95%)	36 (5%)	23	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	699/792 (88%)	658 (94%)	41 (6%)	19 15
All	All	2794/3168 (88%)	2645 (95%)	149 (5%)	22 19

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	70	LYS
1	A	75	MET
1	A	114	SER
1	A	136	GLN
1	A	173	GLN
1	A	195	ASN
1	A	285	GLU
1	A	298	LYS
1	A	318	GLU
1	A	343	LYS
1	A	384	ARG
1	A	476	GLU
1	A	477	ARG
1	A	489	GLU
1	A	499	MET
1	A	513	LEU
1	A	515	ARG
1	A	536	GLN
1	A	556	LEU
1	A	597	GLU
1	A	625	LEU
1	A	630	CYS
1	A	646	LYS
1	A	663	GLU
1	A	713	LEU
1	A	721	GLN
1	A	746	GLN
1	A	772	LYS
1	A	790	ARG
1	A	820	GLU
1	A	852	ASN
1	B	49	ARG
1	B	70	LYS
1	B	114	SER
1	B	118	GLU

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	169	GLN
1	B	195	ASN
1	B	215	PHE
1	B	223	CYS
1	B	285	GLU
1	B	298	LYS
1	B	318	GLU
1	B	343	LYS
1	B	476	GLU
1	B	489	GLU
1	B	499	MET
1	B	513	LEU
1	B	515	ARG
1	B	536	GLN
1	B	556	LEU
1	B	569	CYS
1	B	597	GLU
1	B	626	SER
1	B	630	CYS
1	B	632	GLN
1	B	633	ARG
1	B	639	VAL
1	B	646	LYS
1	B	664	GLN
1	B	666	ARG
1	B	674	GLU
1	B	709	SER
1	B	713	LEU
1	B	721	GLN
1	B	725	SER
1	B	746	GLN
1	B	772	LYS
1	B	773	ARG
1	B	790	ARG
1	B	820	GLU
1	C	70	LYS
1	C	114	SER
1	C	136	GLN
1	C	169	GLN
1	C	195	ASN
1	C	215	PHE

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Mol	Chain	Res	Type
1	C	217	THR
1	C	223	CYS
1	C	285	GLU
1	C	298	LYS
1	C	318	GLU
1	C	343	LYS
1	C	443	ARG
1	C	476	GLU
1	C	477	ARG
1	C	483	GLN
1	C	489	GLU
1	C	513	LEU
1	C	515	ARG
1	C	597	GLU
1	C	625	LEU
1	C	628	GLU
1	C	630	CYS
1	C	632	GLN
1	C	633	ARG
1	C	639	VAL
1	C	646	LYS
1	C	666	ARG
1	C	674	GLU
1	C	713	LEU
1	C	721	GLN
1	C	725	SER
1	C	746	GLN
1	C	772	LYS
1	C	790	ARG
1	C	820	GLU
1	D	70	LYS
1	D	114	SER
1	D	118	GLU
1	D	136	GLN
1	D	169	GLN
1	D	173	GLN
1	D	195	ASN
1	D	215	PHE
1	D	240	ARG
1	D	285	GLU
1	D	298	LYS
1	D	318	GLU

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Mol	Chain	Res	Type
1	D	343	LYS
1	D	370	LEU
1	D	446	GLN
1	D	489	GLU
1	D	502[A]	GLN
1	D	502[B]	GLN
1	D	513	LEU
1	D	515	ARG
1	D	522	ARG
1	D	569	CYS
1	D	593	CYS
1	D	597	GLU
1	D	629	GLU
1	D	631	LYS
1	D	664	GLN
1	D	667	LYS
1	D	673	LYS
1	D	676	ARG
1	D	709	SER
1	D	713	LEU
1	D	721	GLN
1	D	725	SER
1	D	728	ARG
1	D	746	GLN
1	D	772	LYS
1	D	790	ARG
1	D	802	ARG
1	D	820	GLU
1	D	852	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	179	GLN
1	A	199	GLN
1	A	271	GLN
1	A	375	GLN
1	A	746	GLN
1	A	852	ASN
1	B	169	GLN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	179	GLN
1	B	199	GLN
1	B	271	GLN
1	B	331	HIS
1	B	375	GLN
1	B	483	GLN
1	B	536	GLN
1	B	723	HIS
1	B	746	GLN
1	C	136	GLN
1	C	169	GLN
1	C	170	ASN
1	C	173	GLN
1	C	199	GLN
1	C	271	GLN
1	C	331	HIS
1	C	375	GLN
1	C	483	GLN
1	C	746	GLN
1	D	199	GLN
1	D	271	GLN
1	D	331	HIS
1	D	746	GLN
1	D	852	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	852/965 (88%)	-0.32	19 (2%)	62	69	8, 22, 56, 78	0
1	B	852/965 (88%)	-0.11	34 (3%)	38	47	15, 31, 63, 91	0
1	C	855/965 (88%)	-0.27	15 (1%)	68	75	13, 28, 60, 78	0
1	D	854/965 (88%)	-0.24	28 (3%)	46	55	10, 27, 60, 85	0
All	All	3413/3860 (88%)	-0.24	96 (2%)	53	62	8, 27, 60, 91	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ALA	7.8
1	B	416	PRO	7.3
1	A	415	ALA	6.8
1	D	415	ALA	6.6
1	A	414	PRO	6.3
1	D	630	CYS	5.4
1	B	478	GLY	5.3
1	B	632	GLN	5.1
1	B	750	TRP	4.8
1	D	627	TRP	4.8
1	C	489	GLU	4.7
1	C	415	ALA	4.7
1	D	416	PRO	4.5
1	D	671	PHE	4.5
1	A	413	ALA	4.5
1	C	488	GLY	4.2
1	C	416	PRO	4.1
1	D	476	GLU	4.1
1	C	476	GLU	4.0
1	B	413	ALA	4.0
1	A	665	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	821	PHE	4.0
1	B	487	ALA	3.9
1	D	750	TRP	3.9
1	C	685	TYR	3.9
1	B	414	PRO	3.7
1	C	750	TRP	3.7
1	D	315	THR	3.7
1	D	659	PHE	3.7
1	B	417	HIS	3.6
1	A	416	PRO	3.6
1	A	417	HIS	3.5
1	A	42	ALA	3.5
1	D	685	TYR	3.5
1	D	418	ALA	3.5
1	B	418	ALA	3.5
1	D	662	VAL	3.5
1	D	821	PHE	3.4
1	D	663	GLU	3.3
1	D	669	GLY	3.3
1	B	671	PHE	3.3
1	D	666	ARG	3.3
1	D	634	CYS	3.3
1	C	0	THR	3.2
1	D	489	GLU	3.2
1	A	418	ALA	3.2
1	B	412	PRO	3.1
1	B	636	PRO	3.1
1	B	317	GLN	3.1
1	D	647	ASP	3.1
1	C	671	PHE	3.0
1	B	648	THR	3.0
1	A	647	ASP	3.0
1	A	412	PRO	2.8
1	C	615	LEU	2.8
1	B	641	ALA	2.8
1	A	659	PHE	2.8
1	D	667	LYS	2.7
1	C	659	PHE	2.7
1	D	487	ALA	2.7
1	B	638	VAL	2.7
1	D	648	THR	2.6
1	B	659	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	628	GLU	2.5
1	A	686	PHE	2.5
1	A	661	PHE	2.5
1	A	648	THR	2.4
1	D	629	GLU	2.4
1	B	315	THR	2.4
1	B	673	LYS	2.3
1	D	670	VAL	2.3
1	B	665	LEU	2.3
1	C	413	ALA	2.3
1	A	632	GLN	2.3
1	B	685	TYR	2.3
1	B	639	VAL	2.3
1	A	634	CYS	2.3
1	B	489	GLU	2.3
1	D	0	THR	2.3
1	C	41	LYS	2.3
1	B	488	GLY	2.3
1	B	666	ARG	2.3
1	B	647	ASP	2.2
1	D	615	LEU	2.2
1	B	686	PHE	2.2
1	D	413	ALA	2.2
1	B	419	THR	2.2
1	B	667	LYS	2.2
1	B	379	GLN	2.1
1	A	676	ARG	2.1
1	C	613	ALA	2.0
1	D	488	GLY	2.0
1	B	664	GLN	2.0
1	A	667	LYS	2.0
1	B	646	LYS	2.0
1	A	477	ARG	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 monosaccharides in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
2	CL	D	964	1/1	0.91	0.11	66,66,66,66	0
2	CL	C	964	1/1	0.94	0.16	76,76,76,76	0

6.5 Other polymers

There are no such residues in this entry.