Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:18 PM GMT

PDB ID	:	1EZL
Title	:	CRYSTAL STRUCTURE OF THE DISULPHIDE BOND-DEFICIENT AZURIN MUTANT C3A/C26A: HOW IMPORTANT IS THE S-S BOND FOR FOLDING AND STABILITY?
Authors	:	Bonander, N.; Leckner, J.; Guo, H.; Karlsson, B.G.; Sjolin, L.
Deposited on	:	2000-05-11
Resolution	:	2.00 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
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 (i)) were used in the production of this report:

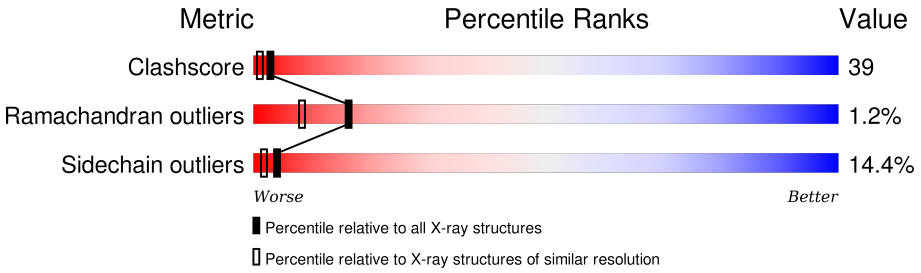
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	48% 40% 12%
1	B	128	50% 41% 9%
1	C	128	47% 45% 7%
1	D	128	37% 47% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4267 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 AZURIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			972	607	164	194	7			
1	B	128	Total	C	N	O	S	0	0	0
			972	607	164	194	7			
1	C	128	Total	C	N	O	S	0	0	0
			972	607	164	194	7			
1	D	128	Total	C	N	O	S	0	0	0
			972	607	164	194	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	CYS	ENGINEERED	UNP P00282
A	26	ALA	CYS	ENGINEERED	UNP P00282
B	133	ALA	CYS	ENGINEERED	UNP P00282
B	156	ALA	CYS	ENGINEERED	UNP P00282
C	263	ALA	CYS	ENGINEERED	UNP P00282
C	286	ALA	CYS	ENGINEERED	UNP P00282
D	393	ALA	CYS	ENGINEERED	UNP P00282
D	416	ALA	CYS	ENGINEERED	UNP P00282

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	93	Total O 93 93	0	0
3	B	97	Total O 97 97	0	0
3	C	97	Total O 97 97	0	0
3	D	88	Total O 88 88	0	0

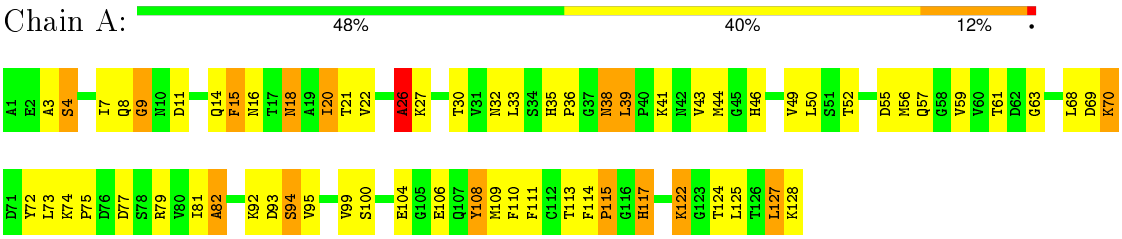
3 Residue-property plots (i)

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.

Note EDS was not executed.

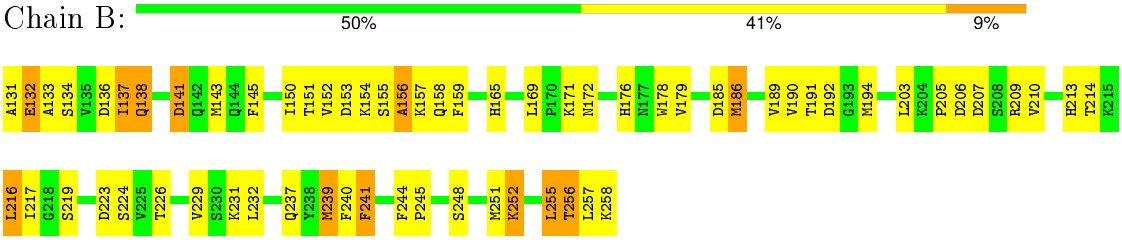
- Molecule 1: AZURIN

Chain A:



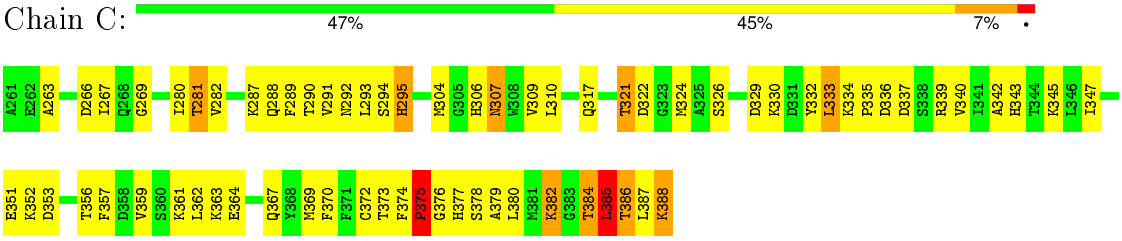
- Molecule 1: AZURIN

Chain B:



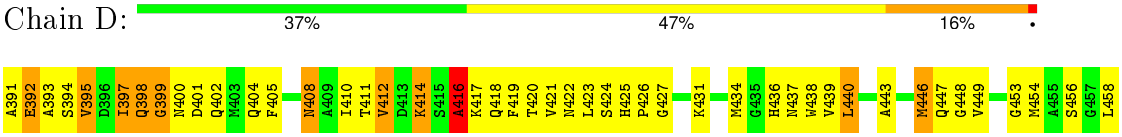
- Molecule 1: AZURIN

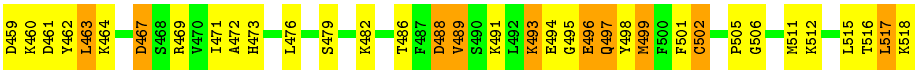
Chain C:



- Molecule 1: AZURIN

Chain D:




D459
K460
D461
Y462
L463
K464
D467
S468
R469
V470
I471
A472
H473
L476
S479
K482
T486
F487
D488
V489
S490
K491
L492
K493
E494
G495
E496
Q497
Y498
N499
F500
F501
G502
P505
G506
H511
K512
L515
T516
L517
K518

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.40Å 80.40Å 110.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4267	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU

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	1.07	1/989 (0.1%)	1.13	4/1333 (0.3%)
1	B	1.06	2/989 (0.2%)	1.18	3/1333 (0.2%)
1	C	1.05	1/989 (0.1%)	1.23	4/1333 (0.3%)
1	D	1.22	3/989 (0.3%)	1.24	5/1333 (0.4%)
All	All	1.10	7/3956 (0.2%)	1.20	16/5332 (0.3%)

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	2
1	C	0	1
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	416	ALA	CA-CB	15.89	1.85	1.52
1	A	26	ALA	CA-CB	9.29	1.72	1.52
1	B	239	MET	CG-SD	-6.10	1.65	1.81
1	C	263	ALA	CA-CB	5.42	1.63	1.52
1	D	438	TRP	CB-CG	5.35	1.59	1.50
1	B	156	ALA	CA-CB	5.25	1.63	1.52
1	D	412	VAL	CB-CG1	-5.02	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	385	LEU	N-CA-C	-7.84	89.84	111.00
1	C	333	LEU	CA-CB-CG	6.80	130.93	115.30
1	D	416	ALA	CB-CA-C	6.78	120.27	110.10
1	D	399	GLY	N-CA-C	-6.66	96.44	113.10
1	A	9	GLY	N-CA-C	-6.27	97.43	113.10
1	B	141	ASP	CB-CG-OD2	6.16	123.85	118.30
1	C	380	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	A	117	HIS	N-CA-C	5.90	126.93	111.00
1	D	467	ASP	N-CA-C	-5.79	95.37	111.00
1	A	15	PHE	N-CA-C	-5.64	95.76	111.00
1	D	517	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	26	ALA	CB-CA-C	5.56	118.44	110.10
1	B	216	LEU	N-CA-C	-5.15	97.10	111.00
1	D	395	VAL	N-CA-C	-5.13	97.14	111.00
1	B	255	LEU	N-CA-C	-5.09	97.25	111.00
1	C	384	THR	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	TYR	Sidechain
1	A	26	ALA	Mainchain
1	C	332	TYR	Sidechain
1	D	416	ALA	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	972	0	954	61	0
1	B	972	0	951	58	0
1	C	972	0	951	72	0
1	D	972	0	951	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	93	0	0	8	0
3	B	97	0	0	6	0
3	C	97	0	0	14	0
3	D	88	0	0	13	0
All	All	4267	0	3807	303	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 39.

All (303) 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:D:416:ALA:CB	1:D:416:ALA:CA	1.85	1.49
1:D:434:MET:SD	1:D:434:MET:CE	2.01	1.48
1:D:391:ALA:HB1	1:D:410:ILE:HG21	1.34	1.09
1:D:391:ALA:N	1:D:419:PHE:HB3	1.74	1.01
1:D:412:VAL:HG13	1:D:419:PHE:CD2	1.96	1.00
1:D:412:VAL:HG13	1:D:419:PHE:CE2	2.01	0.95
1:D:416:ALA:HB3	1:D:419:PHE:CZ	2.02	0.94
1:D:424:SER:HB3	1:D:482:LYS:HD3	1.48	0.94
1:B:151:THR:HG23	1:B:258:LYS:HD3	1.50	0.93
1:D:397:ILE:HD11	1:D:405:PHE:CD2	2.04	0.92
1:A:61:THR:HG21	1:B:237:GLN:HE22	1.39	0.88
1:A:32:ASN:HB3	1:A:92:LYS:NZ	1.88	0.88
1:D:496:GLU:HG2	1:D:498:TYR:CZ	2.09	0.86
1:A:61:THR:HG21	1:B:237:GLN:NE2	1.94	0.81
1:D:395:VAL:HG12	1:D:421:VAL:HG22	1.61	0.81
1:A:108:TYR:HB2	1:A:125:LEU:HB3	1.63	0.80
1:D:458:LEU:HD12	3:D:775:HOH:O	1.85	0.77
1:D:440:LEU:HD23	1:D:471:ILE:HB	1.67	0.76
1:D:395:VAL:CG1	1:D:421:VAL:HG22	2.14	0.76
1:D:416:ALA:HB3	1:D:419:PHE:CE1	2.22	0.75
1:A:8:GLN:HG2	1:A:36:PRO:HD3	1.67	0.75
1:C:307:ASN:HD21	1:C:373:THR:H	1.32	0.75
1:D:411:THR:HG23	1:D:518:LYS:HE2	1.69	0.74
1:D:454:MET:HB2	3:D:575:HOH:O	1.87	0.74
1:A:32:ASN:HB3	1:A:92:LYS:HZ2	1.50	0.74
1:B:194:MET:SD	3:B:796:HOH:O	2.44	0.74
1:D:412:VAL:HA	1:D:419:PHE:HE2	1.51	0.74
1:C:367:GLN:HG2	1:C:388:LYS:HB3	1.70	0.74
1:D:458:LEU:HB2	3:D:775:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:MET:HG3	1:D:505:PRO:HG3	1.68	0.73
1:C:367:GLN:HA	1:C:388:LYS:HB3	1.71	0.72
1:D:392:GLU:N	1:D:419:PHE:CD2	2.58	0.71
1:D:392:GLU:H	1:D:412:VAL:HG22	1.54	0.71
1:B:137:ILE:HD12	1:B:138:GLN:N	2.04	0.71
1:D:391:ALA:HA	1:D:412:VAL:HG22	1.72	0.71
1:B:185:ASP:O	1:B:189:VAL:HG23	1.90	0.71
1:A:55:ASP:O	1:A:59:VAL:HG23	1.91	0.70
1:D:391:ALA:HB1	1:D:410:ILE:CG2	2.17	0.69
1:B:186:MET:O	1:B:190:VAL:HG23	1.93	0.69
1:C:329:ASP:HB3	3:C:837:HOH:O	1.93	0.69
1:A:22:VAL:O	1:A:128:LYS:HG2	1.93	0.68
1:D:431:LYS:HE2	3:D:775:HOH:O	1.95	0.67
1:D:392:GLU:N	1:D:419:PHE:HD2	1.93	0.67
1:B:171:LYS:HE3	1:B:216:LEU:HD23	1.76	0.67
1:D:456:SER:O	1:D:460:LYS:HG3	1.95	0.67
1:C:386:THR:C	1:C:388:LYS:N	2.43	0.66
1:B:232:LEU:CB	1:B:257:LEU:HD11	2.25	0.66
1:D:412:VAL:HA	1:D:419:PHE:CE2	2.30	0.65
1:A:20:ILE:HD12	1:A:110:PHE:CE1	2.31	0.65
1:B:245:PRO:HA	3:B:796:HOH:O	1.95	0.65
1:C:386:THR:C	1:C:388:LYS:H	1.98	0.65
1:B:151:THR:CG2	1:B:258:LYS:HD3	2.24	0.65
1:A:124:THR:HG23	3:A:687:HOH:O	1.95	0.65
1:D:425:HIS:CD2	1:D:436:HIS:CD2	2.85	0.65
1:D:419:PHE:O	1:D:486:THR:HA	1.97	0.65
1:A:3:ALA:HB1	1:A:26:ALA:HB1	1.79	0.64
1:D:422:ASN:HB3	1:D:482:LYS:HE3	1.79	0.64
1:C:317:GLN:HB2	3:C:771:HOH:O	1.97	0.64
1:D:461:ASP:HB2	3:D:732:HOH:O	1.97	0.64
1:A:32:ASN:HB3	1:A:92:LYS:HZ1	1.60	0.64
1:C:387:LEU:HD13	1:C:387:LEU:O	1.97	0.64
1:A:111:PHE:HE2	1:A:113:THR:HG22	1.62	0.64
1:C:326:SER:HB3	1:C:330:LYS:HB2	1.79	0.64
1:C:266:ASP:OD2	1:C:292:ASN:HB2	1.98	0.64
1:D:476:LEU:HD23	3:D:775:HOH:O	1.96	0.63
1:A:68:LEU:HD12	3:A:521:HOH:O	1.98	0.63
1:A:99:VAL:O	1:A:99:VAL:HG12	1.98	0.63
1:D:397:ILE:HD11	1:D:405:PHE:CG	2.35	0.62
1:C:339:ARG:NH2	3:C:663:HOH:O	2.31	0.62
1:C:387:LEU:O	1:C:388:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ALA:CB	1:D:416:ALA:HA	2.20	0.62
1:D:493:LYS:NZ	1:D:493:LYS:HB2	2.14	0.62
1:B:154:LYS:HG3	1:B:257:LEU:HD23	1.81	0.62
1:D:495:GLY:HA2	3:D:577:HOH:O	2.00	0.62
1:D:398:GLN:OE1	1:D:426:PRO:HD3	1.99	0.61
1:D:443:ALA:HA	1:D:499:MET:HG3	1.82	0.61
1:C:306:HIS:HA	1:C:372:CYS:SG	2.40	0.61
1:D:392:GLU:HG2	1:D:394:SER:O	2.00	0.61
1:C:282:VAL:CG2	1:C:385:LEU:HD11	2.31	0.61
1:B:232:LEU:HB2	1:B:257:LEU:HD11	1.82	0.61
1:D:416:ALA:CB	1:D:419:PHE:CE1	2.83	0.61
1:A:4:SER:HA	1:A:30:THR:O	1.99	0.61
1:A:61:THR:CG2	1:B:237:GLN:HE22	2.13	0.61
1:A:57:GLN:HG2	1:B:239:MET:SD	2.41	0.60
1:C:307:ASN:C	1:C:307:ASN:HD22	2.04	0.60
1:D:392:GLU:O	1:D:419:PHE:CD2	2.55	0.60
1:B:154:LYS:CG	1:B:257:LEU:HD23	2.30	0.60
1:B:159:PHE:O	1:B:226:THR:HA	2.01	0.60
1:A:92:LYS:HG3	1:A:93:ASP:N	2.16	0.60
1:B:165:HIS:CG	1:B:219:SER:HA	2.37	0.60
1:D:464:LYS:O	1:D:467:ASP:HB2	2.02	0.60
1:A:111:PHE:CE2	1:A:113:THR:HG22	2.37	0.59
1:D:497:GLN:HE21	1:D:497:GLN:HA	1.67	0.59
1:D:392:GLU:HG3	3:D:733:HOH:O	2.02	0.59
1:D:398:GLN:O	1:D:405:PHE:HA	2.03	0.59
1:C:352:LYS:NZ	3:C:862:HOH:O	2.34	0.59
1:D:394:SER:HA	1:D:420:THR:O	2.02	0.59
1:A:63:GLY:O	1:A:72:TYR:HA	2.02	0.59
1:C:317:GLN:O	1:C:321:THR:HB	2.03	0.59
1:A:18:ASN:ND2	3:A:834:HOH:O	2.36	0.59
1:D:401:ASP:HA	1:D:434:MET:HG2	1.85	0.59
1:B:179:VAL:O	1:B:240:PHE:HA	2.03	0.58
1:B:217:ILE:HG22	3:B:553:HOH:O	2.03	0.58
1:C:367:GLN:CA	1:C:388:LYS:HB3	2.34	0.58
1:D:498:TYR:C	1:D:499:MET:HG2	2.23	0.57
1:A:74:LYS:O	1:A:77:ASP:HB2	2.04	0.57
1:D:417:LYS:O	1:D:418:GLN:HG2	2.05	0.57
1:C:385:LEU:O	1:C:387:LEU:N	2.37	0.57
1:A:4:SER:HB2	1:A:30:THR:HB	1.86	0.57
1:D:489:VAL:O	1:D:489:VAL:HG13	2.04	0.57
1:A:82:ALA:HA	3:A:594:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLN:HA	1:C:357:PHE:O	2.05	0.57
1:C:374:PHE:HB3	1:C:377:HIS:ND1	2.20	0.57
1:D:424:SER:HB3	1:D:482:LYS:CD	2.30	0.56
1:D:425:HIS:HB3	1:D:479:SER:HA	1.86	0.56
1:D:440:LEU:CD1	1:D:515:LEU:HD13	2.35	0.56
1:C:367:GLN:HA	1:C:388:LYS:C	2.26	0.56
1:C:367:GLN:HA	1:C:388:LYS:CB	2.36	0.56
1:B:133:ALA:CB	1:B:156:ALA:HB1	2.36	0.55
1:A:74:LYS:HG2	1:A:75:PRO:HD2	1.87	0.55
1:C:290:THR:HA	1:C:356:THR:HA	1.88	0.55
1:B:153:ASP:OD1	1:B:155:SER:HB3	2.07	0.55
1:D:493:LYS:NZ	1:D:494:GLU:O	2.40	0.55
1:D:399:GLY:HA2	1:D:404:GLN:O	2.06	0.55
1:A:50:LEU:HD11	1:A:108:TYR:HB3	1.87	0.55
1:D:463:LEU:HD12	3:D:728:HOH:O	2.05	0.55
1:D:425:HIS:CG	1:D:479:SER:HA	2.42	0.55
1:C:282:VAL:HG21	1:C:385:LEU:HD11	1.88	0.54
1:B:133:ALA:HB2	1:B:156:ALA:CB	2.37	0.54
1:D:398:GLN:HG2	1:D:426:PRO:HD3	1.89	0.54
1:B:150:ILE:O	1:B:255:LEU:HA	2.07	0.54
1:A:8:GLN:HG2	1:A:36:PRO:CD	2.36	0.54
1:A:61:THR:HG23	3:A:693:HOH:O	2.07	0.54
1:B:232:LEU:HB3	1:B:257:LEU:HD11	1.88	0.54
1:A:20:ILE:HB	1:A:125:LEU:HD12	1.90	0.54
1:A:114:PHE:CD2	1:A:117:HIS:NE2	2.75	0.54
1:D:425:HIS:CD2	1:D:436:HIS:HD2	2.25	0.54
1:B:223:ASP:OD1	1:B:224:SER:N	2.41	0.53
1:A:81:ILE:O	1:A:82:ALA:HB2	2.08	0.53
1:D:488:ASP:O	1:D:491:LYS:HB2	2.09	0.53
1:D:412:VAL:CG1	1:D:419:PHE:CE2	2.85	0.53
1:A:33:LEU:O	1:A:92:LYS:HD2	2.08	0.53
1:C:267:ILE:O	1:C:293:LEU:HA	2.09	0.53
1:D:423:LEU:O	1:D:482:LYS:HA	2.08	0.53
1:A:117:HIS:CD2	1:A:117:HIS:N	2.75	0.53
1:A:35:HIS:CD2	1:A:46:HIS:CD2	2.97	0.52
1:D:391:ALA:HA	1:D:412:VAL:CG2	2.37	0.52
1:C:374:PHE:CD2	1:C:377:HIS:CE1	2.97	0.52
1:D:392:GLU:N	1:D:412:VAL:HG22	2.22	0.52
1:D:416:ALA:HB3	1:D:419:PHE:HZ	1.70	0.52
1:C:388:LYS:HD2	3:C:878:HOH:O	2.08	0.52
1:D:402:GLN:HG3	3:D:921:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:HD12	1:C:369:MET:O	2.10	0.52
1:C:385:LEU:C	1:C:387:LEU:H	2.12	0.52
1:C:326:SER:HB3	1:C:330:LYS:CB	2.39	0.52
1:B:214:THR:HB	1:B:223:ASP:OD2	2.10	0.52
1:D:418:GLN:C	1:D:419:PHE:HD1	2.14	0.51
1:C:307:ASN:ND2	1:C:373:THR:H	2.04	0.51
1:A:57:GLN:HG2	1:B:186:MET:HE1	1.93	0.51
1:D:400:ASN:OD1	1:D:402:GLN:N	2.43	0.51
1:D:391:ALA:O	1:D:392:GLU:HB3	2.11	0.51
1:D:434:MET:CE	1:D:434:MET:CG	2.86	0.51
1:C:293:LEU:O	1:C:352:LYS:HG3	2.11	0.51
1:B:143:MET:HE3	1:D:506:GLY:HA3	1.93	0.51
1:B:217:ILE:HG13	1:B:217:ILE:O	2.10	0.51
1:D:392:GLU:HB3	1:D:394:SER:O	2.11	0.51
1:A:8:GLN:O	1:A:15:PHE:HA	2.12	0.50
1:B:205:PRO:O	1:B:206:ASP:C	2.50	0.50
1:D:414:LYS:HB2	1:D:518:LYS:OXT	2.11	0.50
1:C:367:GLN:HG2	1:C:388:LYS:CB	2.41	0.50
1:A:18:ASN:HB2	1:D:404:GLN:OE1	2.12	0.50
1:A:49:VAL:O	1:A:110:PHE:HA	2.11	0.50
1:B:150:ILE:HG13	1:B:240:PHE:CE1	2.47	0.49
1:B:133:ALA:HB2	1:B:156:ALA:HB2	1.94	0.49
1:D:392:GLU:O	1:D:393:ALA:C	2.49	0.49
1:C:322:ASP:OD1	1:C:339:ARG:NH1	2.46	0.49
1:C:347:ILE:HB	1:C:351:GLU:HB2	1.94	0.49
1:D:408:ASN:HA	3:D:567:HOH:O	2.12	0.49
1:B:131:ALA:O	1:B:132:GLU:HG3	2.12	0.49
1:D:410:ILE:HG22	1:D:412:VAL:HG23	1.95	0.49
1:C:364:GLU:HA	1:C:387:LEU:HD11	1.94	0.48
3:C:738:HOH:O	1:D:446:MET:SD	2.60	0.48
1:B:237:GLN:NE2	3:B:686:HOH:O	2.46	0.48
1:A:122:LYS:HD3	1:A:122:LYS:N	2.27	0.48
1:C:307:ASN:HD21	1:C:373:THR:N	2.04	0.48
1:B:207:ASP:OD1	1:B:209:ARG:HB2	2.13	0.48
1:D:437:ASN:OD1	1:D:502:CYS:HA	2.13	0.48
1:C:376:GLY:O	1:C:379:ALA:HB2	2.13	0.48
1:C:363:LYS:O	1:C:387:LEU:HD11	2.13	0.48
1:C:307:ASN:ND2	1:C:372:CYS:HA	2.28	0.48
1:B:133:ALA:HB1	1:B:156:ALA:HB1	1.94	0.48
1:D:391:ALA:CA	1:D:412:VAL:HG22	2.40	0.48
1:D:412:VAL:HG21	1:D:515:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:HIS:HB3	1:B:219:SER:HA	1.95	0.48
1:A:106:GLU:HB3	1:A:108:TYR:OH	2.14	0.48
1:B:241:PHE:CD1	1:B:241:PHE:N	2.81	0.48
1:D:423:LEU:O	1:D:482:LYS:HD2	2.14	0.47
1:D:397:ILE:HG13	1:D:398:GLN:N	2.28	0.47
1:C:326:SER:OG	1:C:334:LYS:HA	2.13	0.47
1:D:392:GLU:C	1:D:394:SER:N	2.66	0.47
1:A:20:ILE:CD1	1:A:110:PHE:CE1	2.97	0.47
1:C:367:GLN:CG	1:C:388:LYS:HB3	2.40	0.47
1:A:18:ASN:HB3	3:A:616:HOH:O	2.13	0.47
1:D:412:VAL:O	1:D:518:LYS:N	2.40	0.47
1:D:391:ALA:CA	1:D:419:PHE:HD2	2.27	0.47
1:A:32:ASN:HA	1:A:94:SER:HB3	1.97	0.47
1:D:496:GLU:HG2	1:D:498:TYR:OH	2.15	0.47
1:A:3:ALA:CB	1:A:26:ALA:HB1	2.45	0.47
1:D:392:GLU:HB3	1:D:395:VAL:HB	1.97	0.47
1:C:367:GLN:HB3	1:C:388:LYS:OXT	2.15	0.47
1:D:427:GLY:O	1:D:479:SER:HB2	2.15	0.47
1:D:458:LEU:HB3	1:D:462:TYR:CE2	2.49	0.46
1:A:38:ASN:ND2	3:A:784:HOH:O	2.48	0.46
1:D:411:THR:CG2	1:D:518:LYS:HB2	2.46	0.46
1:B:241:PHE:HA	1:B:251:MET:O	2.16	0.46
1:D:448:GLY:HA3	1:D:469:ARG:HH22	1.81	0.46
1:B:256:THR:HB	1:B:258:LYS:HD2	1.97	0.46
1:B:143:MET:HB2	1:B:143:MET:HE2	1.76	0.46
1:C:376:GLY:O	1:C:379:ALA:CB	2.63	0.46
1:C:317:GLN:HG2	1:D:443:ALA:HB1	1.98	0.46
1:D:460:LYS:O	1:D:461:ASP:HB2	2.16	0.46
1:D:458:LEU:C	1:D:461:ASP:H	2.19	0.46
1:A:56:MET:HE2	1:A:109:MET:HG3	1.97	0.46
1:D:391:ALA:C	1:D:392:GLU:O	2.52	0.46
1:C:329:ASP:CB	3:C:837:HOH:O	2.57	0.46
1:A:11:ASP:OD2	1:A:39:LEU:HB2	2.17	0.45
1:A:9:GLY:O	1:A:35:HIS:HA	2.16	0.45
1:B:203:LEU:HD11	1:B:213:HIS:ND1	2.32	0.45
1:D:418:GLN:O	1:D:419:PHE:CD1	2.70	0.45
1:C:388:LYS:HE2	3:C:879:HOH:O	2.16	0.45
1:A:39:LEU:HD12	1:A:43:VAL:CG1	2.45	0.45
1:A:49:VAL:HG21	1:A:113:THR:HG23	1.99	0.45
1:C:294:SER:HB3	3:C:783:HOH:O	2.16	0.45
1:D:412:VAL:O	1:D:517:LEU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:MET:SD	1:C:306:HIS:HE1	2.39	0.45
1:D:440:LEU:HD13	1:D:515:LEU:HD13	1.99	0.45
1:C:280:ILE:HA	3:C:726:HOH:O	2.17	0.45
1:B:141:ASP:OD1	1:B:169:LEU:HG	2.17	0.44
1:D:493:LYS:HB2	1:D:493:LYS:HZ2	1.82	0.44
1:B:159:PHE:HB2	1:B:229:VAL:CG2	2.46	0.44
1:B:157:LYS:HG2	3:B:683:HOH:O	2.16	0.44
1:A:79:ARG:HE	1:A:79:ARG:HB2	1.45	0.44
1:C:385:LEU:C	1:C:387:LEU:N	2.71	0.44
1:A:35:HIS:CD2	1:A:46:HIS:HD2	2.34	0.44
1:D:473:HIS:HD2	3:D:658:HOH:O	2.01	0.44
1:C:281:THR:HG23	3:C:867:HOH:O	2.18	0.44
1:D:471:ILE:O	1:D:471:ILE:HG22	2.16	0.44
1:B:152:VAL:O	1:B:257:LEU:HA	2.18	0.44
1:C:388:LYS:HB2	3:C:878:HOH:O	2.18	0.44
1:B:240:PHE:O	1:B:252:LYS:HA	2.17	0.44
1:B:176:HIS:CE1	1:B:251:MET:SD	3.11	0.43
1:D:471:ILE:O	1:D:472:ALA:HB2	2.19	0.43
1:B:169:LEU:C	1:B:219:SER:HG	2.21	0.43
1:D:437:ASN:O	1:D:502:CYS:HB2	2.18	0.43
1:D:411:THR:HA	1:D:516:THR:O	2.19	0.43
1:C:359:VAL:C	1:C:361:LYS:H	2.21	0.43
1:A:70:LYS:NZ	3:A:800:HOH:O	2.51	0.43
1:C:335:PRO:O	1:C:336:ASP:C	2.58	0.43
1:C:282:VAL:HG13	1:C:289:PHE:CD1	2.54	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.76	0.42
1:D:473:HIS:CD2	3:D:658:HOH:O	2.71	0.42
1:B:192:ASP:OD1	1:B:209:ARG:NH1	2.46	0.42
1:C:337:ASP:HB3	1:C:340:VAL:HG23	2.02	0.42
1:C:387:LEU:HD13	3:C:563:HOH:O	2.20	0.42
1:A:21:THR:HG21	1:A:128:LYS:HD3	2.00	0.42
1:B:133:ALA:HB2	1:B:156:ALA:HB1	2.01	0.42
1:B:210:VAL:HG11	1:B:213:HIS:CD2	2.55	0.42
1:B:178:TRP:O	1:B:213:HIS:HA	2.19	0.42
1:C:281:THR:CG2	3:C:867:HOH:O	2.68	0.42
1:C:378:SER:O	1:C:382:LYS:HD2	2.20	0.42
1:C:377:HIS:C	1:C:379:ALA:N	2.73	0.42
1:D:501:PHE:HA	1:D:511:MET:O	2.20	0.42
1:B:169:LEU:O	1:B:219:SER:OG	2.29	0.42
1:C:345:LYS:N	1:C:353:ASP:OD2	2.48	0.42
1:B:194:MET:CG	3:B:796:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:ASN:O	1:D:436:HIS:NE2	2.53	0.42
1:D:439:VAL:HG22	1:D:473:HIS:HB2	2.02	0.42
1:C:384:THR:C	1:C:386:THR:N	2.72	0.41
1:A:30:THR:HA	1:A:95:VAL:O	2.20	0.41
1:C:290:THR:HG22	1:C:291:VAL:N	2.35	0.41
1:C:309:VAL:O	1:C:370:PHE:HA	2.20	0.41
1:C:374:PHE:HA	1:C:375:PRO:HD3	1.90	0.41
1:A:114:PHE:CD2	1:A:117:HIS:CE1	3.08	0.41
1:A:110:PHE:O	1:A:122:LYS:HA	2.19	0.41
1:D:437:ASN:ND2	1:D:439:VAL:CG2	2.84	0.41
1:D:391:ALA:O	1:D:395:VAL:HB	2.20	0.41
1:B:154:LYS:HG2	1:B:257:LEU:HD23	2.00	0.41
1:D:425:HIS:CB	1:D:479:SER:HA	2.48	0.41
1:C:357:PHE:HE1	1:C:362:LEU:HD11	1.85	0.41
1:C:370:PHE:O	1:C:382:LYS:HB2	2.21	0.41
1:D:497:GLN:NE2	1:D:497:GLN:HA	2.35	0.41
1:D:518:LYS:HA	1:D:518:LYS:HD3	1.71	0.41
1:C:307:ASN:ND2	1:C:309:VAL:HG23	2.35	0.41
1:C:342:ALA:O	1:C:343:HIS:HB3	2.21	0.41
1:C:269:GLY:O	1:C:295:HIS:HA	2.21	0.41
1:A:41:LYS:HE2	1:A:41:LYS:HB3	1.74	0.41
1:D:449:VAL:O	1:D:453:GLY:N	2.46	0.41
1:A:9:GLY:HA2	1:A:14:GLN:O	2.21	0.40
1:D:412:VAL:CA	1:D:419:PHE:CE2	3.01	0.40
1:D:391:ALA:C	1:D:419:PHE:HD2	2.25	0.40
1:B:203:LEU:HD11	1:B:213:HIS:CG	2.57	0.40
1:D:392:GLU:N	1:D:419:PHE:CE2	2.90	0.40
1:D:398:GLN:OE1	1:D:426:PRO:CD	2.69	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	126/128 (98%)	118 (94%)	6 (5%)	2 (2%)	12 5
1	B	126/128 (98%)	112 (89%)	13 (10%)	1 (1%)	24 15
1	C	126/128 (98%)	112 (89%)	12 (10%)	2 (2%)	12 5
1	D	126/128 (98%)	111 (88%)	14 (11%)	1 (1%)	24 15
All	All	504/512 (98%)	453 (90%)	45 (9%)	6 (1%)	16 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	GLU
1	C	386	THR
1	A	82	ALA
1	D	414	LYS
1	C	375	PRO
1	A	115	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	108/108 (100%)	89 (82%)	19 (18%)	2 1
1	B	108/108 (100%)	93 (86%)	15 (14%)	4 2
1	C	108/108 (100%)	97 (90%)	11 (10%)	9 5
1	D	108/108 (100%)	91 (84%)	17 (16%)	3 1
All	All	432/432 (100%)	370 (86%)	62 (14%)	4 2

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	ILE
1	A	16	ASN
1	A	18	ASN
1	A	20	ILE

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	38	ASN
1	A	39	LEU
1	A	44	MET
1	A	52	THR
1	A	69	ASP
1	A	70	LYS
1	A	73	LEU
1	A	94	SER
1	A	100	SER
1	A	104	GLU
1	A	115	PRO
1	A	122	LYS
1	A	127	LEU
1	B	134	SER
1	B	136	ASP
1	B	137	ILE
1	B	138	GLN
1	B	145	PHE
1	B	158	GLN
1	B	172	ASN
1	B	186	MET
1	B	191	THR
1	B	231	LYS
1	B	241	PHE
1	B	244	PHE
1	B	248	SER
1	B	252	LYS
1	B	256	THR
1	C	281	THR
1	C	287	LYS
1	C	295	HIS
1	C	307	ASN
1	C	321	THR
1	C	324	MET
1	C	333	LEU
1	C	375	PRO
1	C	382	LYS
1	C	385	LEU
1	C	388	LYS
1	D	392	GLU
1	D	397	ILE

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Mol	Chain	Res	Type
1	D	398	GLN
1	D	408	ASN
1	D	440	LEU
1	D	446	MET
1	D	447	GLN
1	D	459	ASP
1	D	463	LEU
1	D	488	ASP
1	D	489	VAL
1	D	493	LYS
1	D	496	GLU
1	D	497	GLN
1	D	499	MET
1	D	502	CYS
1	D	512	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	57	GLN
1	B	172	ASN
1	B	237	GLN
1	C	272	GLN
1	C	307	ASN
1	D	418	GLN
1	D	436	HIS
1	D	497	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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