



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2016 – 05:37 PM EDT

PDB ID : 4WKG
Title : The crystal structure of apo ArnA features an unexpected central binding pocket and provides an explanation for enzymatic coop-erativity
Authors : Grimm, C.
Deposited on : 2014-10-02
Resolution : 2.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

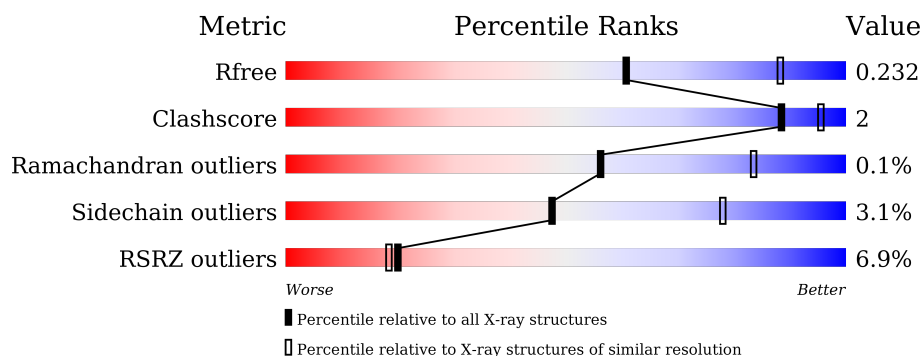
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	660	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>..</div> </div> </div>
1	B	660	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	660	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	660	<div> <div>17%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
1	E	660	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
1	F	660	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	A	701[A]	-	-	-	X
2	DTT	A	701[B]	-	-	-	X
2	DTT	D	701[A]	-	-	-	X
2	DTT	D	701[B]	-	-	-	X
3	ACT	A	702	-	-	-	X
3	ACT	F	701	-	-	-	X

2 Entry composition [i](#)

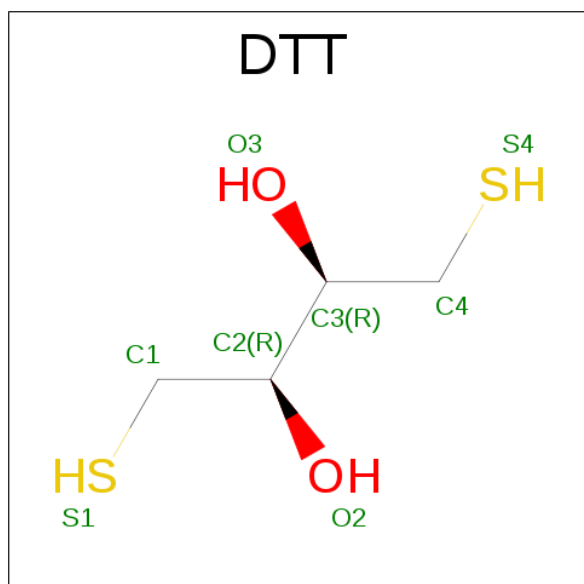
There are 4 unique types of molecules in this entry. The entry contains 60000 atoms, of which 29761 are hydrogens and 0 are deuteriums.

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 Bifunctional polymyxin resistance protein ArnA.

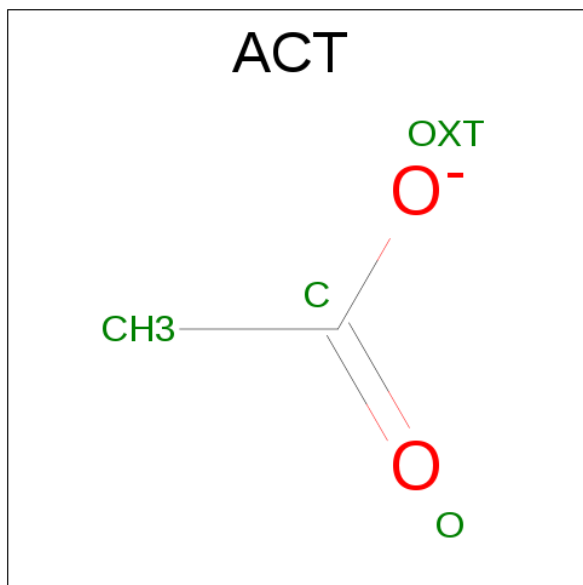
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	636	Total	C	H	N	O	S	0	0	0
			9951	3195	4945	889	903	19			
1	B	643	Total	C	H	N	O	S	0	0	0
			10036	3234	4972	897	914	19			
1	C	637	Total	C	H	N	O	S	0	0	0
			9963	3203	4947	888	906	19			
1	D	641	Total	C	H	N	O	S	0	0	0
			9973	3218	4936	889	911	19			
1	E	643	Total	C	H	N	O	S	0	0	0
			10032	3231	4974	894	914	19			
1	F	637	Total	C	H	N	O	S	0	0	0
			9950	3197	4941	888	905	19			

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	1
			36	8	20	4	4		
2	D	1	Total	C	H	O	S	0	1
			36	8	20	4	4		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	F	1	Total	C	H	O	0	0
			7	2	3	2		

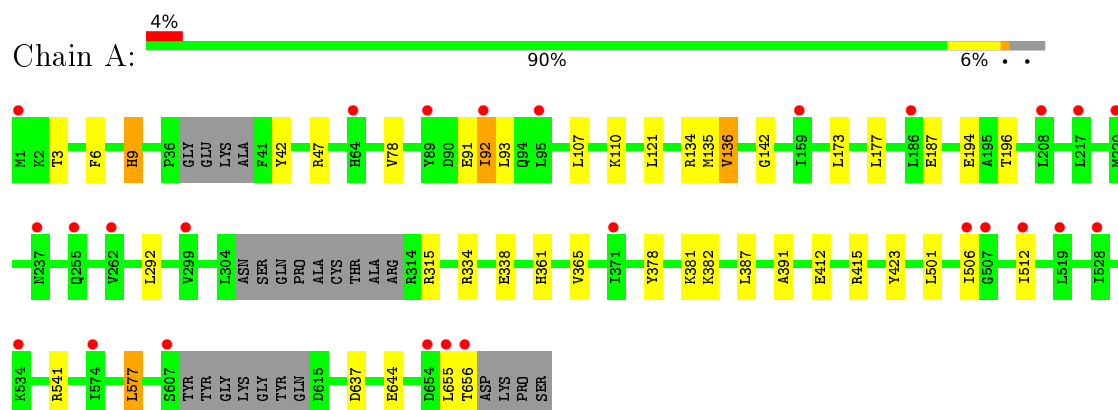
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		

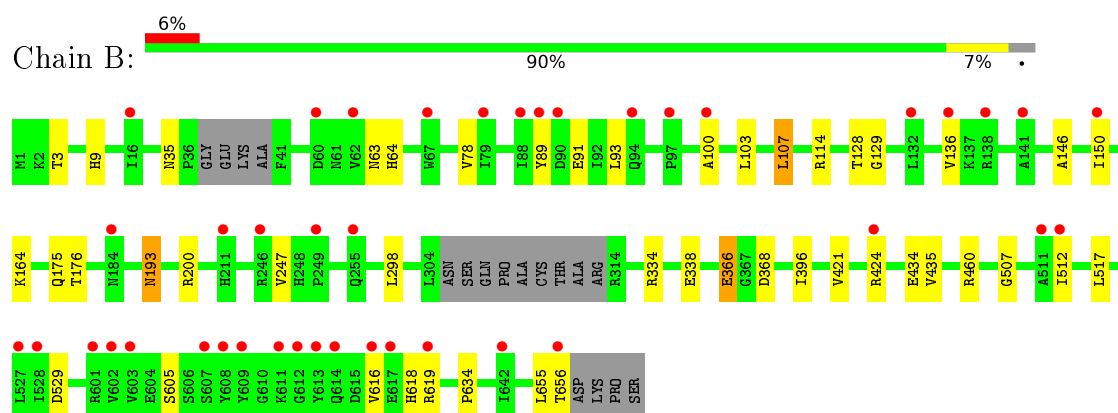
3 Residue-property plots [i](#)

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.

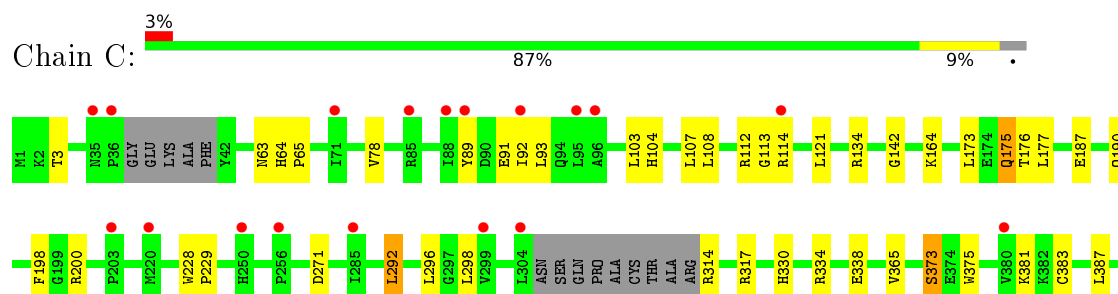
- Molecule 1: Bifunctional polymyxin resistance protein ArnA

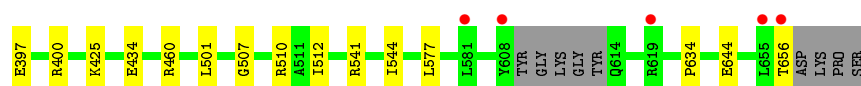


- Molecule 1: Bifunctional polymyxin resistance protein ArnA

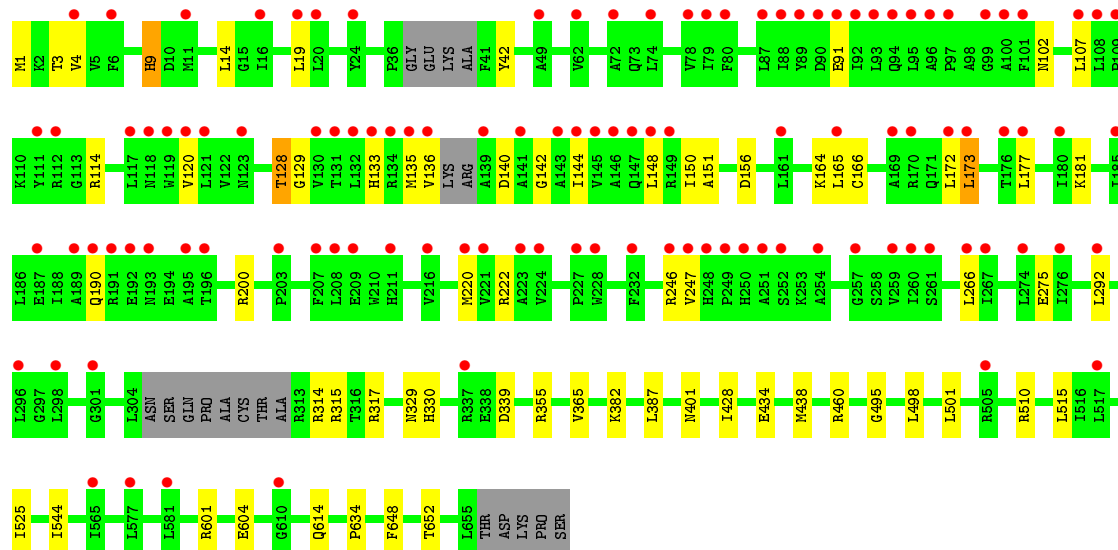
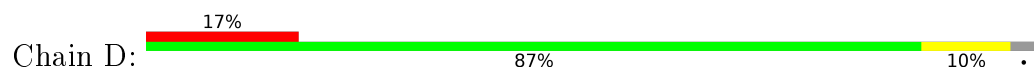


- Molecule 1: Bifunctional polymyxin resistance protein ArnA

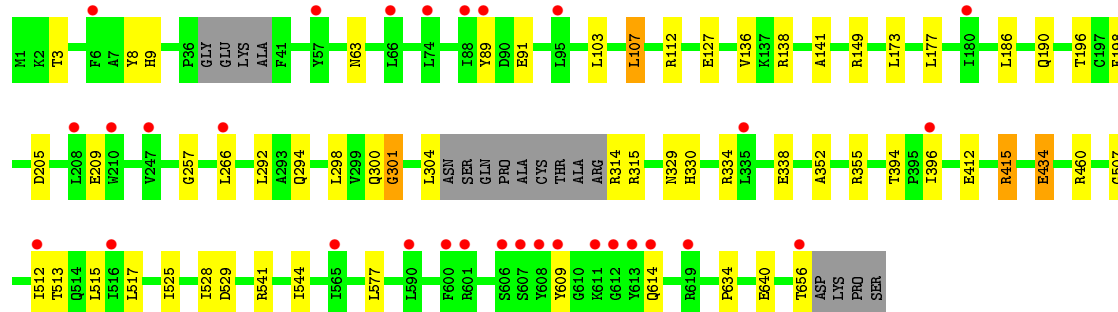
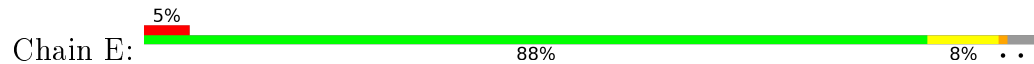




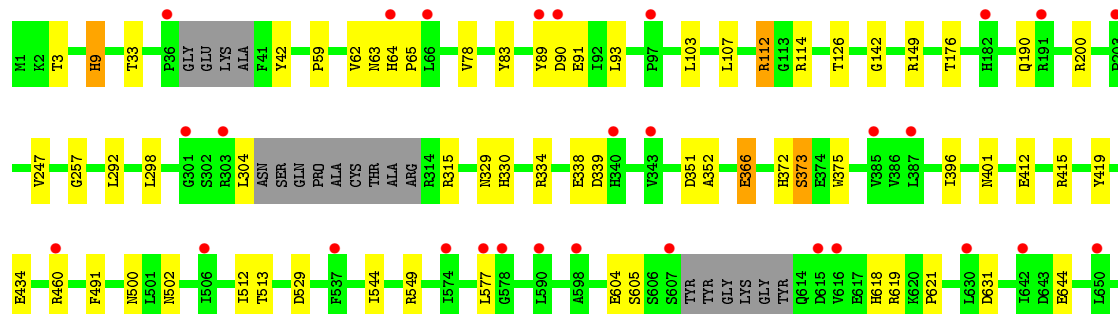
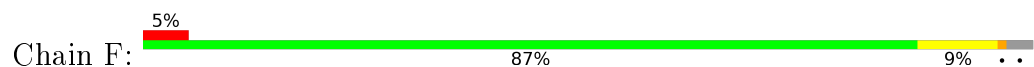
- Molecule 1: Bifunctional polymyxin resistance protein ArnA



- Molecule 1: Bifunctional polymyxin resistance protein ArnA



- Molecule 1: Bifunctional polymyxin resistance protein ArnA



V653	ASP
D654	LYS
L655	PRO
T656	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 112.82Å 113.61Å 81.92° 82.96° 83.80°	Depositor
Resolution (Å)	48.16 – 2.70 48.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.16-2.70) 86.9 (48.16-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.232 0.204 , 0.232	Depositor DCC
R_{free} test set	6443 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	60000	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/5126	0.52	1/6965 (0.0%)
1	B	0.30	0/5188	0.54	1/7051 (0.0%)
1	C	0.27	0/5137	0.51	1/6981 (0.0%)
1	D	0.29	0/5160	0.53	0/7013
1	E	0.29	0/5182	0.53	2/7044 (0.0%)
1	F	0.29	0/5129	0.52	0/6970
All	All	0.29	0/30922	0.53	5/42024 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	301	GLY	C-N-CA	6.51	137.98	121.70
1	B	507	GLY	N-CA-C	5.87	127.77	113.10
1	E	507	GLY	N-CA-C	5.35	126.47	113.10
1	A	577	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	C	507	GLY	N-CA-C	5.10	125.85	113.10

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	5006	4945	4933	20	0
1	B	5064	4972	4977	23	0
1	C	5016	4947	4937	26	0
1	D	5037	4936	4936	33	0
1	E	5058	4974	4966	25	0
1	F	5009	4941	4930	29	0
2	A	16	20	20	0	0
2	D	16	20	20	1	0
3	A	4	3	3	0	0
3	F	4	3	3	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
All	All	30239	29761	29725	150	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 2.

All (150) 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:434:GLU:OE1	1:D:460:ARG:NH2	2.16	0.77
1:A:382:LYS:NZ	1:B:366:GLU:OE2	2.19	0.76
1:B:434:GLU:HG2	1:B:619:ARG:HH22	1.50	0.75
1:F:500:ASN:ND2	1:F:502:ASN:OD1	2.21	0.74
1:F:415:ARG:NH2	1:F:419:TYR:OH	2.21	0.73
1:F:434:GLU:OE1	1:F:460:ARG:NH2	2.22	0.73
1:D:329:ASN:OD1	1:D:355:ARG:NH2	2.21	0.73
1:A:381:LYS:NZ	1:B:368:ASP:OD2	2.22	0.71
1:E:412:GLU:OE1	1:E:415:ARG:NH1	2.23	0.71
1:D:151:ALA:O	1:D:164:LYS:NZ	2.19	0.68
1:F:329:ASN:ND2	1:F:352:ALA:O	2.26	0.67
1:C:383:CYS:O	1:C:425:LYS:NZ	2.25	0.65
1:A:541:ARG:NH2	1:A:644:GLU:OE1	2.28	0.65
1:A:655:LEU:O	1:A:656:THR:OG1	2.08	0.65
1:C:381:LYS:O	1:C:425:LYS:NZ	2.29	0.63
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.33	0.61
1:D:128:THR:OG1	1:D:129:GLY:N	2.34	0.60
1:F:529:ASP:OD2	1:F:605:SER:OG	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:NH1	1:B:338:GLU:OE2	2.35	0.59
1:B:529:ASP:OD2	1:B:605:SER:OG	2.20	0.59
1:C:134:ARG:NH2	1:C:187:GLU:OE2	2.36	0.58
1:D:501:LEU:O	1:D:510:ARG:NH1	2.33	0.58
1:F:351:ASP:OD1	1:F:352:ALA:N	2.38	0.57
1:B:434:GLU:OE1	1:B:460:ARG:NH2	2.39	0.56
1:F:112:ARG:NH1	1:F:190:GLN:OE1	2.38	0.56
1:D:107:LEU:HD13	1:D:129:GLY:HA3	1.89	0.55
1:D:102:ASN:HB2	1:D:135:MET:SD	2.47	0.55
1:E:512:ILE:HG22	1:E:577:LEU:HD21	1.89	0.55
1:F:64:HIS:HD2	1:F:65:PRO:HD2	1.71	0.55
1:A:3:THR:HG22	1:A:78:VAL:HG13	1.89	0.54
1:C:501:LEU:O	1:C:510:ARG:NH1	2.37	0.54
1:F:3:THR:HG22	1:F:78:VAL:HG13	1.88	0.54
1:E:541:ARG:NH1	1:E:640:GLU:OE2	2.41	0.53
1:D:135:MET:O	1:D:136:VAL:HG22	2.08	0.53
1:C:373:SER:HB3	1:C:375:TRP:CZ3	2.44	0.53
1:E:334:ARG:NH1	1:E:338:GLU:OE2	2.41	0.52
1:C:434:GLU:OE1	1:C:460:ARG:NH2	2.43	0.52
1:F:512:ILE:HG22	1:F:577:LEU:HD21	1.92	0.52
1:C:3:THR:HG22	1:C:78:VAL:HG13	1.92	0.51
1:E:329:ASN:ND2	1:E:352:ALA:O	2.43	0.51
1:E:460:ARG:NH1	1:E:614:GLN:O	2.44	0.51
1:E:63:ASN:HB3	1:E:89:TYR:CZ	2.47	0.51
1:C:512:ILE:HG22	1:C:577:LEU:HD21	1.94	0.50
1:F:372:HIS:NE2	1:F:412:GLU:OE1	2.43	0.50
1:E:329:ASN:OD1	1:E:355:ARG:NH2	2.42	0.50
1:D:142:GLY:O	1:D:190:GLN:NE2	2.41	0.50
1:F:257:GLY:O	1:F:304:LEU:HD12	2.12	0.50
1:B:150:ILE:HD12	1:B:164:LYS:HB3	1.94	0.49
1:D:156:ASP:O	1:D:222:ARG:NH1	2.42	0.49
1:C:63:ASN:HB3	1:C:89:TYR:CZ	2.47	0.49
1:D:150:ILE:HD13	1:D:165:LEU:HD21	1.95	0.49
1:A:9:HIS:CE1	1:A:42:TYR:CB	2.96	0.48
1:A:378:TYR:OH	1:B:366:GLU:HG3	2.14	0.48
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.94	0.48
1:B:128:THR:O	1:B:150:ILE:HG22	2.14	0.47
1:B:3:THR:HG22	1:B:78:VAL:HG13	1.96	0.47
1:C:397:GLU:OE2	1:C:400:ARG:NH1	2.48	0.47
1:F:63:ASN:HB3	1:F:89:TYR:CZ	2.49	0.47
1:A:381:LYS:HD2	1:A:423:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:GLY:O	1:F:190:GLN:NE2	2.46	0.47
1:D:315:ARG:CZ	1:D:339:ASP:O	2.62	0.47
1:B:107:LEU:HD13	1:B:129:GLY:HA3	1.96	0.47
1:F:114:ARG:HD2	1:F:200:ARG:CB	2.45	0.47
1:A:173:LEU:O	1:A:177:LEU:HB2	2.15	0.47
1:A:512:ILE:HD11	1:A:577:LEU:HD11	1.96	0.47
1:D:330:HIS:HB3	1:D:544:ILE:HG13	1.96	0.46
1:D:495:GLY:O	1:D:498:LEU:CD1	2.63	0.46
1:D:382:LYS:NZ	1:F:366:GLU:OE1	2.42	0.46
1:B:150:ILE:CD1	1:B:164:LYS:HB3	2.45	0.46
1:C:541:ARG:NH2	1:C:644:GLU:OE2	2.48	0.46
1:F:83:TYR:OH	3:F:701:ACT:H3	2.15	0.46
1:C:114:ARG:HD2	1:C:200:ARG:HA	1.98	0.46
1:D:120:VAL:HG21	1:D:128:THR:HG21	1.98	0.46
1:D:133:HIS:NE2	1:D:140:ASP:HA	2.30	0.46
1:B:63:ASN:HB3	1:B:89:TYR:CZ	2.50	0.46
1:C:64:HIS:HD2	1:C:65:PRO:HD2	1.81	0.46
1:F:330:HIS:HB3	1:F:544:ILE:HG13	1.98	0.46
1:B:193:ASN:N	1:B:193:ASN:OD1	2.48	0.45
1:D:601:ARG:NH2	1:E:294:GLN:HB3	2.30	0.45
1:E:528:ILE:HD13	1:E:609:TYR:CE2	2.51	0.45
1:F:9:HIS:CD2	1:F:42:TYR:CB	2.99	0.45
1:A:334:ARG:NH1	1:A:338:GLU:OE2	2.49	0.45
1:E:107:LEU:HD21	1:E:149:ARG:HG2	1.97	0.45
1:A:315:ARG:CZ	1:A:361:HIS:CE1	3.00	0.45
1:F:334:ARG:NH1	1:F:338:GLU:OE2	2.49	0.45
1:E:141:ALA:HA	1:E:190:GLN:HE22	1.82	0.45
1:B:64:HIS:NE2	1:E:529:ASP:OD1	2.50	0.45
1:C:114:ARG:HD2	1:C:200:ARG:CA	2.46	0.45
1:E:173:LEU:O	1:E:177:LEU:HB2	2.17	0.45
1:D:144:ILE:HG13	1:D:190:GLN:HG3	1.99	0.45
1:D:148:LEU:HB2	1:D:172:LEU:HD12	1.97	0.45
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.99	0.45
1:A:135:MET:O	1:A:136:VAL:HG13	2.17	0.44
1:B:175:GLN:HG3	1:B:176:THR:HG23	1.99	0.44
1:B:421:VAL:O	1:B:424:ARG:NH1	2.49	0.44
1:A:134:ARG:NH2	1:A:187:GLU:OE2	2.40	0.44
1:C:113:GLY:HA3	1:C:198:PHE:H	1.83	0.44
1:B:655:LEU:O	1:B:656:THR:CB	2.66	0.44
1:F:512:ILE:HG13	1:F:513:THR:N	2.33	0.44
1:C:228:TRP:HB3	1:C:229:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:SD	1:D:181:LYS:HA	2.57	0.44
1:D:314:ARG:NH2	1:D:317:ARG:CZ	2.81	0.43
1:A:412:GLU:OE1	1:A:415:ARG:NH1	2.44	0.43
1:C:175:GLN:HG2	1:C:176:THR:HG23	2.00	0.43
1:D:114:ARG:HD2	1:D:200:ARG:CB	2.49	0.43
1:C:112:ARG:NH2	1:C:190:GLN:OE1	2.51	0.43
1:E:394:THR:HG22	1:E:396:ILE:HG22	1.99	0.43
1:C:134:ARG:O	1:C:142:GLY:HA3	2.18	0.43
1:A:391:ALA:HB3	1:A:506:ILE:HD11	2.01	0.43
1:C:330:HIS:HB3	1:C:544:ILE:HG13	2.00	0.43
1:E:196:THR:CG2	1:E:198:PHE:CE1	3.02	0.43
1:C:314:ARG:NH2	1:C:317:ARG:CZ	2.81	0.42
1:D:19:LEU:HD13	1:D:177:LEU:HD21	2.01	0.42
1:E:127:GLU:OE2	1:E:149:ARG:NH1	2.52	0.42
1:C:64:HIS:CD2	1:C:65:PRO:HD2	2.54	0.42
1:D:438:MET:SD	1:D:614:GLN:NE2	2.93	0.42
1:E:330:HIS:HB3	1:E:544:ILE:HG13	2.01	0.42
1:F:315:ARG:NH2	1:F:339:ASP:O	2.53	0.42
1:A:134:ARG:O	1:A:142:GLY:HA3	2.20	0.42
1:C:104:HIS:CD2	1:C:108:LEU:HD21	2.55	0.42
1:D:387:LEU:HD12	1:D:428:ILE:HB	2.01	0.42
1:D:14:LEU:HD21	1:D:166:CYS:HA	2.01	0.42
1:C:173:LEU:O	1:C:177:LEU:HB2	2.19	0.42
1:B:93:LEU:HD12	1:B:100:ALA:HB3	2.02	0.41
1:E:434:GLU:OE1	1:E:460:ARG:NH2	2.53	0.41
1:E:138:ARG:HB2	1:E:141:ALA:HB3	2.01	0.41
1:F:90:ASP:HA	1:F:93:LEU:HB2	2.02	0.41
1:B:434:GLU:HG2	1:B:619:ARG:NH2	2.26	0.41
1:E:300:GLN:HA	1:E:301:GLY:HA2	1.90	0.41
1:E:8:TYR:CE2	1:E:9:HIS:CE1	3.09	0.41
1:F:549:ARG:NH1	1:F:631:ASP:O	2.50	0.41
1:A:381:LYS:HD2	1:A:423:TYR:CD1	2.54	0.41
1:A:6:PHE:CZ	1:A:92:ILE:HD11	2.56	0.41
1:D:246:ARG:HB3	1:D:275:GLU:HB3	2.02	0.41
1:B:146:ALA:CB	1:B:176:THR:HG21	2.50	0.41
1:E:512:ILE:HG13	1:E:513:THR:N	2.36	0.41
1:F:491:PHE:CZ	1:F:621:PRO:HB3	2.55	0.41
1:D:315:ARG:NH2	1:D:339:ASP:O	2.54	0.41
1:F:59:PRO:HG2	1:F:62:VAL:HG22	2.03	0.41
1:D:173:LEU:CD2	1:D:177:LEU:HD22	2.50	0.41
1:D:9:HIS:CE1	1:D:42:TYR:CB	3.05	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:GLY:O	1:E:304:LEU:HD12	2.21	0.41
1:B:616:VAL:HG21	1:B:619:ARG:HH21	1.86	0.40
1:F:373:SER:HB2	1:F:375:TRP:CD2	2.56	0.40
1:F:373:SER:HB3	1:F:375:TRP:CH2	2.56	0.40
1:B:114:ARG:HH11	1:B:200:ARG:HH11	1.70	0.40
1:A:110:LYS:NZ	1:A:194:GLU:O	2.54	0.40
1:D:648:PHE:O	1:D:652:THR:HG23	2.21	0.40
2:D:701[B]:DTT:H41	1:F:375:TRP:HB3	2.04	0.40
1:C:292:LEU:HD13	1:C:296:LEU:HD12	2.04	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	628/660 (95%)	613 (98%)	14 (2%)	1 (0%)	52	80
1	B	637/660 (96%)	623 (98%)	13 (2%)	1 (0%)	52	80
1	C	629/660 (95%)	617 (98%)	12 (2%)	0	100	100
1	D	633/660 (96%)	619 (98%)	14 (2%)	0	100	100
1	E	637/660 (96%)	619 (97%)	17 (3%)	1 (0%)	52	80
1	F	629/660 (95%)	618 (98%)	11 (2%)	0	100	100
All	All	3793/3960 (96%)	3709 (98%)	81 (2%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	E	136	VAL
1	B	136	VAL

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	528/559 (94%)	515 (98%)	13 (2%)	55	84
1	B	532/559 (95%)	517 (97%)	15 (3%)	51	81
1	C	529/559 (95%)	513 (97%)	16 (3%)	48	79
1	D	528/559 (94%)	514 (97%)	14 (3%)	52	82
1	E	531/559 (95%)	513 (97%)	18 (3%)	44	75
1	F	528/559 (94%)	507 (96%)	21 (4%)	38	69
All	All	3176/3354 (95%)	3079 (97%)	97 (3%)	47	78

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	47	ARG
1	A	91	GLU
1	A	92	ILE
1	A	93	LEU
1	A	107	LEU
1	A	121	LEU
1	A	196	THR
1	A	292	LEU
1	A	365	VAL
1	A	387	LEU
1	A	501	LEU
1	A	637	ASP
1	B	9	HIS
1	B	35	ASN
1	B	91	GLU
1	B	103	LEU
1	B	107	LEU
1	B	193	ASN
1	B	247	VAL
1	B	298	LEU
1	B	366	GLU

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Mol	Chain	Res	Type
1	B	396	ILE
1	B	435	VAL
1	B	512	ILE
1	B	517	LEU
1	B	618	HIS
1	B	634	PRO
1	C	91	GLU
1	C	92	ILE
1	C	93	LEU
1	C	103	LEU
1	C	107	LEU
1	C	121	LEU
1	C	164	LYS
1	C	175	GLN
1	C	271	ASP
1	C	292	LEU
1	C	298	LEU
1	C	365	VAL
1	C	373	SER
1	C	387	LEU
1	C	634	PRO
1	C	656	THR
1	D	3	THR
1	D	4	VAL
1	D	9	HIS
1	D	91	GLU
1	D	128	THR
1	D	173	LEU
1	D	220	MET
1	D	247	VAL
1	D	266	LEU
1	D	292	LEU
1	D	365	VAL
1	D	401	ASN
1	D	604	GLU
1	D	634	PRO
1	E	3	THR
1	E	91	GLU
1	E	103	LEU
1	E	107	LEU
1	E	112	ARG
1	E	186	LEU

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Mol	Chain	Res	Type
1	E	205	ASP
1	E	209	GLU
1	E	266	LEU
1	E	292	LEU
1	E	298	LEU
1	E	314	ARG
1	E	315	ARG
1	E	415	ARG
1	E	434	GLU
1	E	517	LEU
1	E	634	PRO
1	E	656	THR
1	F	9	HIS
1	F	33	THR
1	F	91	GLU
1	F	103	LEU
1	F	107	LEU
1	F	112	ARG
1	F	126	THR
1	F	149	ARG
1	F	176	THR
1	F	247	VAL
1	F	292	LEU
1	F	298	LEU
1	F	366	GLU
1	F	373	SER
1	F	396	ILE
1	F	401	ASN
1	F	604	GLU
1	F	618	HIS
1	F	619	ARG
1	F	644	GLU
1	F	656	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	B	9	HIS
1	B	588	HIS
1	C	64	HIS
1	D	104	HIS

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Mol	Chain	Res	Type
1	D	118	ASN
1	E	190	GLN
1	E	372	HIS
1	F	9	HIS
1	F	64	HIS
1	F	248	HIS
1	F	363	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTT	A	701[A]	-	7,7,7	0.67	0	4,8,8	1.13	0
2	DTT	A	701[B]	-	7,7,7	0.56	0	4,8,8	0.35	0
3	ACT	A	702	-	0,3,3	0.00	-	0,3,3	0.00	-
2	DTT	D	701[A]	-	7,7,7	0.55	0	4,8,8	0.27	0
2	DTT	D	701[B]	-	7,7,7	0.52	0	4,8,8	0.25	0
3	ACT	F	701	-	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	A	701[A]	-	-	0/8/8/8	0/0/0/0
2	DTT	A	701[B]	-	-	0/8/8/8	0/0/0/0
3	ACT	A	702	-	-	0/0/0/0	0/0/0/0
2	DTT	D	701[A]	-	-	0/8/8/8	0/0/0/0
2	DTT	D	701[B]	-	-	0/8/8/8	0/0/0/0
3	ACT	F	701	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701[B]	DTT	1	0
3	F	701	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	636/660 (96%)	0.43	26 (4%) 41 41	19, 51, 96, 152	0
1	B	643/660 (97%)	0.50	41 (6%) 23 21	20, 56, 105, 170	0
1	C	637/660 (96%)	0.43	23 (3%) 46 46	27, 55, 103, 158	0
1	D	641/660 (97%)	0.98	113 (17%) 2 1	20, 71, 157, 204	0
1	E	643/660 (97%)	0.41	30 (4%) 35 34	16, 49, 98, 147	0
1	F	637/660 (96%)	0.47	33 (5%) 31 30	30, 60, 100, 146	0
All	All	3837/3960 (96%)	0.54	266 (6%) 20 18	16, 55, 121, 204	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	79	ILE	13.2
1	D	100	ALA	12.1
1	D	101	PHE	8.7
1	E	608	TYR	7.5
1	D	136	VAL	7.4
1	D	180	ILE	7.4
1	B	609	TYR	6.7
1	D	24	TYR	6.5
1	D	254	ALA	6.2
1	D	92	ILE	6.2
1	D	99	GLY	6.1
1	D	135	MET	6.0
1	D	189	ALA	5.7
1	D	209	GLU	5.7
1	B	608	TYR	5.7
1	A	655	LEU	5.4
1	D	193	ASN	5.3
1	D	95	LEU	5.0
1	D	161	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	148	LEU	4.9
1	D	191	ARG	4.8
1	D	97	PRO	4.8
1	D	108	LEU	4.8
1	E	611	LYS	4.7
1	D	195	ALA	4.7
1	D	80	PHE	4.7
1	E	612	GLY	4.7
1	D	251	ALA	4.7
1	D	74	LEU	4.5
1	D	145	VAL	4.5
1	E	613	TYR	4.4
1	C	655	LEU	4.4
1	D	94	GLN	4.4
1	D	247	VAL	4.4
1	D	111	TYR	4.4
1	F	574	ILE	4.3
1	B	249	PRO	4.3
1	D	109	PRO	4.3
1	D	16	ILE	4.3
1	D	173	LEU	4.2
1	D	220	MET	4.2
1	D	131	THR	4.2
1	D	274	LEU	4.2
1	D	190	GLN	4.2
1	C	656	THR	4.2
1	D	88	ILE	4.1
1	F	630	LEU	4.1
1	C	36	PRO	4.1
1	E	609	TYR	4.0
1	D	112	ARG	4.0
1	D	267	ILE	4.0
1	D	143	ALA	4.0
1	A	208	LEU	4.0
1	D	144	ILE	3.9
1	D	207	PHE	3.9
1	B	211	HIS	3.9
1	D	117	LEU	3.9
1	D	19	LEU	3.9
1	D	149	ARG	3.8
1	D	177	LEU	3.8
1	D	301	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	216	VAL	3.8
1	A	656	THR	3.8
1	D	172	LEU	3.8
1	E	607	SER	3.8
1	E	614	GLN	3.8
1	D	139	ALA	3.7
1	D	296	LEU	3.7
1	D	165	LEU	3.6
1	D	78	VAL	3.6
1	D	134	ARG	3.6
1	B	617	GLU	3.6
1	F	97	PRO	3.5
1	B	612	GLY	3.5
1	D	87	LEU	3.5
1	D	170	ARG	3.5
1	D	228	TRP	3.5
1	D	141	ALA	3.5
1	A	217	LEU	3.5
1	C	608	TYR	3.5
1	F	656	THR	3.5
1	B	184	ASN	3.4
1	C	71	ILE	3.4
1	D	266	LEU	3.4
1	D	4	VAL	3.4
1	D	6	PHE	3.4
1	D	261	SER	3.3
1	D	62	VAL	3.3
1	D	176	THR	3.3
1	B	512	ILE	3.3
1	C	285	ILE	3.3
1	B	424	ARG	3.3
1	D	260	ILE	3.3
1	B	138	ARG	3.3
1	B	79	ILE	3.3
1	F	66	LEU	3.3
1	D	292	LEU	3.2
1	A	299	VAL	3.2
1	C	250	HIS	3.2
1	B	88	ILE	3.2
1	E	601	ARG	3.2
1	D	276	ILE	3.2
1	C	203	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	64	HIS	3.2
1	D	123	ASN	3.2
1	D	250	HIS	3.2
1	D	196	THR	3.2
1	F	303	ARG	3.1
1	D	252	SER	3.1
1	D	259	VAL	3.1
1	D	107	LEU	3.1
1	D	248	HIS	3.1
1	F	340	HIS	3.1
1	D	90	ASP	3.1
1	D	118	ASN	3.0
1	A	92	ILE	3.0
1	C	89	TYR	3.0
1	D	133	HIS	3.0
1	A	654	ASP	3.0
1	A	220	MET	3.0
1	D	223	ALA	2.9
1	A	95	LEU	2.9
1	B	132	LEU	2.9
1	B	614	GLN	2.9
1	C	92	ILE	2.9
1	D	132	LEU	2.9
1	D	146	ALA	2.9
1	D	130	VAL	2.9
1	E	95	LEU	2.9
1	F	387	LEU	2.9
1	A	1	MET	2.9
1	E	247	VAL	2.9
1	D	91	GLU	2.8
1	F	655	LEU	2.8
1	A	607	SER	2.8
1	F	537	PHE	2.8
1	D	227	PRO	2.8
1	D	147	GLN	2.7
1	B	94	GLN	2.7
1	C	299	VAL	2.7
1	D	221	VAL	2.7
1	E	57	TYR	2.7
1	F	203	PRO	2.7
1	D	505	ARG	2.7
1	A	534	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	203	PRO	2.7
1	F	301	GLY	2.7
1	B	619	ARG	2.7
1	C	88	ILE	2.7
1	E	512	ILE	2.7
1	B	656	THR	2.7
1	E	606	SER	2.7
1	D	249	PRO	2.6
1	D	337	ARG	2.6
1	F	343	VAL	2.6
1	E	208	LEU	2.6
1	A	528	ILE	2.6
1	C	619	ARG	2.6
1	B	642	ILE	2.6
1	B	527	LEU	2.6
1	A	512	ILE	2.6
1	B	528	ILE	2.6
1	B	150	ILE	2.5
1	B	100	ALA	2.5
1	D	72	ALA	2.5
1	B	511	ALA	2.5
1	E	656	THR	2.5
1	C	581	LEU	2.5
1	D	120	VAL	2.5
1	E	6	PHE	2.5
1	A	237	ASN	2.5
1	D	211	HIS	2.5
1	E	180	ILE	2.5
1	D	121	LEU	2.5
1	A	64	HIS	2.5
1	B	602	VAL	2.5
1	F	616	VAL	2.5
1	E	74	LEU	2.5
1	A	89	TYR	2.5
1	B	246	ARG	2.5
1	F	90	ASP	2.5
1	F	182	HIS	2.4
1	A	159	ILE	2.4
1	D	581	LEU	2.4
1	E	516	ILE	2.4
1	B	601	ARG	2.4
1	B	60	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	246	ARG	2.4
1	A	262	VAL	2.4
1	B	62	VAL	2.4
1	B	255	GLN	2.4
1	A	519	LEU	2.4
1	D	208	LEU	2.4
1	F	607	SER	2.4
1	E	565	ILE	2.4
1	B	616	VAL	2.4
1	D	298	LEU	2.3
1	E	66	LEU	2.3
1	E	266	LEU	2.3
1	E	210	TRP	2.3
1	E	89	TYR	2.3
1	C	304	LEU	2.3
1	D	96	ALA	2.3
1	F	89	TYR	2.3
1	F	577	LEU	2.3
1	D	89	TYR	2.3
1	D	224	VAL	2.3
1	F	36	PRO	2.3
1	C	35	ASN	2.3
1	C	96	ALA	2.3
1	C	256	PRO	2.3
1	B	89	TYR	2.2
1	F	385	VAL	2.2
1	D	93	LEU	2.2
1	D	577	LEU	2.2
1	B	611	LYS	2.2
1	F	506	ILE	2.2
1	F	654	ASP	2.2
1	D	119	TRP	2.2
1	E	335	LEU	2.2
1	F	590	LEU	2.2
1	C	85	ARG	2.2
1	D	257	GLY	2.2
1	D	232	PHE	2.2
1	E	619	ARG	2.2
1	F	460	ARG	2.2
1	B	607	SER	2.2
1	F	642	ILE	2.2
1	A	255	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	650	LEU	2.2
1	B	90	ASP	2.2
1	D	169	ALA	2.2
1	E	88	ILE	2.1
1	C	95	LEU	2.1
1	E	590	LEU	2.1
1	B	603	VAL	2.1
1	B	613	TYR	2.1
1	A	507	GLY	2.1
1	D	610	GLY	2.1
1	D	49	ALA	2.1
1	D	192	GLU	2.1
1	A	371	ILE	2.1
1	A	574	ILE	2.1
1	D	11	MET	2.1
1	D	565	ILE	2.1
1	B	97	PRO	2.1
1	C	220	MET	2.1
1	C	114	ARG	2.1
1	A	186	LEU	2.1
1	B	16	ILE	2.1
1	E	600	PHE	2.1
1	C	380	VAL	2.1
1	D	517	LEU	2.1
1	D	185	ILE	2.1
1	F	615	ASP	2.1
1	F	653	VAL	2.1
1	B	67	TRP	2.1
1	E	396	ILE	2.0
1	F	191	ARG	2.0
1	F	598	ALA	2.0
1	B	136	VAL	2.0
1	A	506	ILE	2.0
1	D	20	LEU	2.0
1	D	187	GLU	2.0
1	B	141	ALA	2.0
1	F	578	GLY	2.0

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	A	702	4/4	0.95	0.41	5.53	20,20,44,44	0
2	DTT	A	701[B]	8/8	0.80	0.34	3.98	55,55,55,55	18
2	DTT	A	701[A]	8/8	0.80	0.34	3.77	32,55,55,55	18
2	DTT	D	701[B]	8/8	0.81	0.28	2.90	46,64,64,64	18
2	DTT	D	701[A]	8/8	0.81	0.28	2.51	35,64,64,64	18
3	ACT	F	701	4/4	0.87	0.28	2.49	20,20,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.