Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:28 PM EDT

PDB ID	:	3HM7
Title	:	Crystal structure of allantoinase from Bacillus halodurans C-125
Authors	:	Patskovsky, Y.; Romero, R.; Rutter, M.; Miller, S.; Wasserman, S.R.; Sauder, J.M.; Raushel, F.M.; Burley, S.K.; Almo, S.C.; New York Structural GenomiX Research Consortium (NYSGXRC); New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-05-28
Resolution	:	2.60 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 (i) 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 (1)) were used in the production of this report:

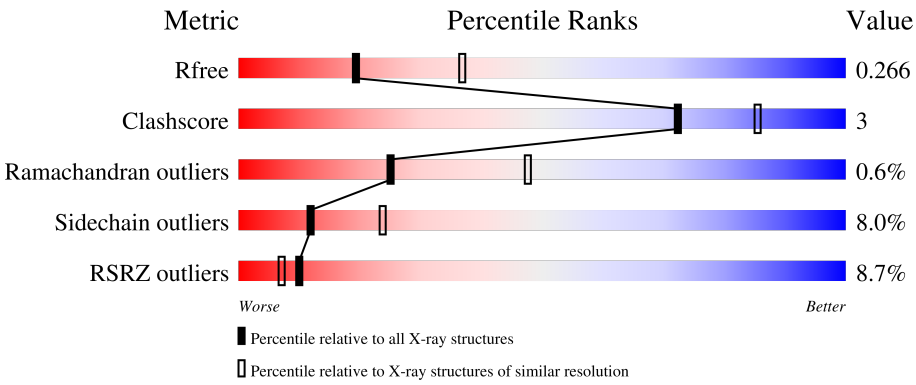
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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.



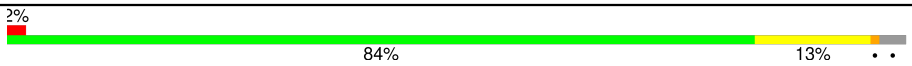
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	448	7%, 82%, 14%
1	B	448	5%, 82%, 15%
1	C	448	27%, 78%, 18%
1	D	448	7%, 81%, 15%
1	E	448	3%, 87%, 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	448	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20901 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 Allantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3425	2166	593	649	17	0	4	0
1	B	437	3437	2173	594	653	17	0	5	0
1	C	435	3410	2154	588	651	17	0	3	0
1	D	436	3415	2157	591	650	17	0	2	0
1	E	436	3412	2156	590	649	17	0	2	0
1	F	436	3425	2165	592	651	17	0	4	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q9KAH8
A	0	SER	-	expression tag	UNP Q9KAH8
A	1	LEU	-	expression tag	UNP Q9KAH8
A	439	GLU	-	expression tag	UNP Q9KAH8
A	440	GLY	-	expression tag	UNP Q9KAH8
A	441	HIS	-	expression tag	UNP Q9KAH8
A	442	HIS	-	expression tag	UNP Q9KAH8
A	443	HIS	-	expression tag	UNP Q9KAH8
A	444	HIS	-	expression tag	UNP Q9KAH8
A	445	HIS	-	expression tag	UNP Q9KAH8
A	446	HIS	-	expression tag	UNP Q9KAH8
B	-1	MET	-	expression tag	UNP Q9KAH8
B	0	SER	-	expression tag	UNP Q9KAH8
B	1	LEU	-	expression tag	UNP Q9KAH8
B	439	GLU	-	expression tag	UNP Q9KAH8
B	440	GLY	-	expression tag	UNP Q9KAH8
B	441	HIS	-	expression tag	UNP Q9KAH8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	442	HIS	-	expression tag	UNP Q9KAH8
B	443	HIS	-	expression tag	UNP Q9KAH8
B	444	HIS	-	expression tag	UNP Q9KAH8
B	445	HIS	-	expression tag	UNP Q9KAH8
B	446	HIS	-	expression tag	UNP Q9KAH8
C	-1	MET	-	expression tag	UNP Q9KAH8
C	0	SER	-	expression tag	UNP Q9KAH8
C	1	LEU	-	expression tag	UNP Q9KAH8
C	439	GLU	-	expression tag	UNP Q9KAH8
C	440	GLY	-	expression tag	UNP Q9KAH8
C	441	HIS	-	expression tag	UNP Q9KAH8
C	442	HIS	-	expression tag	UNP Q9KAH8
C	443	HIS	-	expression tag	UNP Q9KAH8
C	444	HIS	-	expression tag	UNP Q9KAH8
C	445	HIS	-	expression tag	UNP Q9KAH8
C	446	HIS	-	expression tag	UNP Q9KAH8
D	-1	MET	-	expression tag	UNP Q9KAH8
D	0	SER	-	expression tag	UNP Q9KAH8
D	1	LEU	-	expression tag	UNP Q9KAH8
D	439	GLU	-	expression tag	UNP Q9KAH8
D	440	GLY	-	expression tag	UNP Q9KAH8
D	441	HIS	-	expression tag	UNP Q9KAH8
D	442	HIS	-	expression tag	UNP Q9KAH8
D	443	HIS	-	expression tag	UNP Q9KAH8
D	444	HIS	-	expression tag	UNP Q9KAH8
D	445	HIS	-	expression tag	UNP Q9KAH8
D	446	HIS	-	expression tag	UNP Q9KAH8
E	-1	MET	-	expression tag	UNP Q9KAH8
E	0	SER	-	expression tag	UNP Q9KAH8
E	1	LEU	-	expression tag	UNP Q9KAH8
E	439	GLU	-	expression tag	UNP Q9KAH8
E	440	GLY	-	expression tag	UNP Q9KAH8
E	441	HIS	-	expression tag	UNP Q9KAH8
E	442	HIS	-	expression tag	UNP Q9KAH8
E	443	HIS	-	expression tag	UNP Q9KAH8
E	444	HIS	-	expression tag	UNP Q9KAH8
E	445	HIS	-	expression tag	UNP Q9KAH8
E	446	HIS	-	expression tag	UNP Q9KAH8
F	-1	MET	-	expression tag	UNP Q9KAH8
F	0	SER	-	expression tag	UNP Q9KAH8
F	1	LEU	-	expression tag	UNP Q9KAH8
F	439	GLU	-	expression tag	UNP Q9KAH8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	440	GLY	-	expression tag	UNP Q9KAH8
F	441	HIS	-	expression tag	UNP Q9KAH8
F	442	HIS	-	expression tag	UNP Q9KAH8
F	443	HIS	-	expression tag	UNP Q9KAH8
F	444	HIS	-	expression tag	UNP Q9KAH8
F	445	HIS	-	expression tag	UNP Q9KAH8
F	446	HIS	-	expression tag	UNP Q9KAH8

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

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

- Molecule 3 is water.

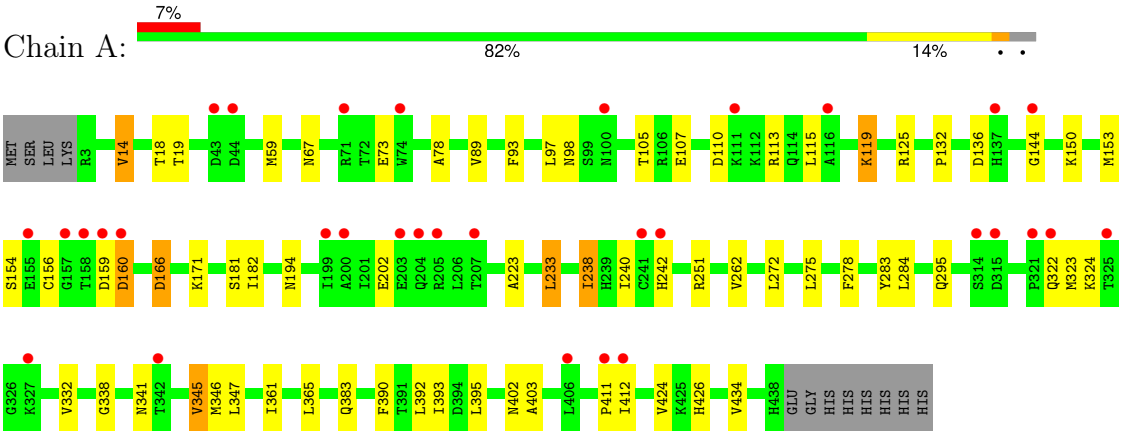
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	53	53	53	0	0
3	B	69	69	69	0	0
3	C	39	39	39	0	0
3	D	47	47	47	0	0
3	E	74	74	74	0	0
3	F	89	89	89	0	0

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.

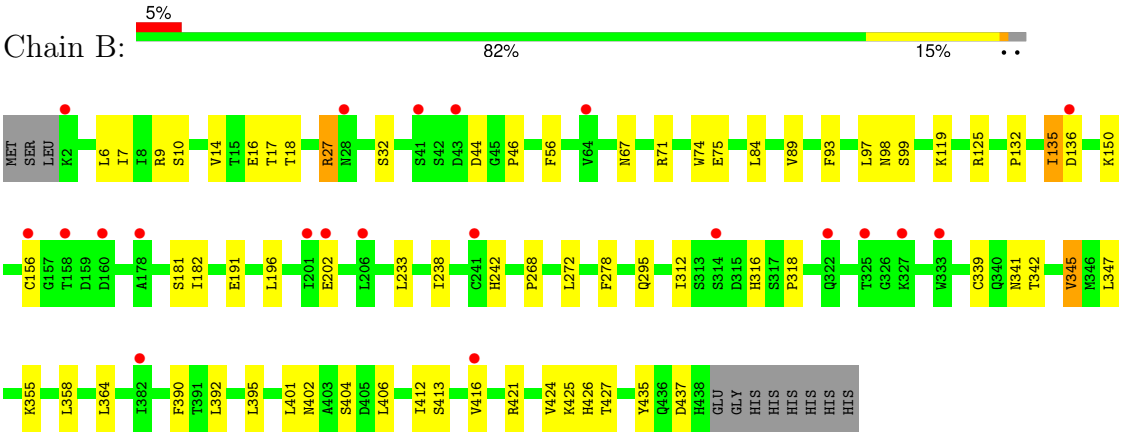
- Molecule 1: Allantoinase

Chain A:



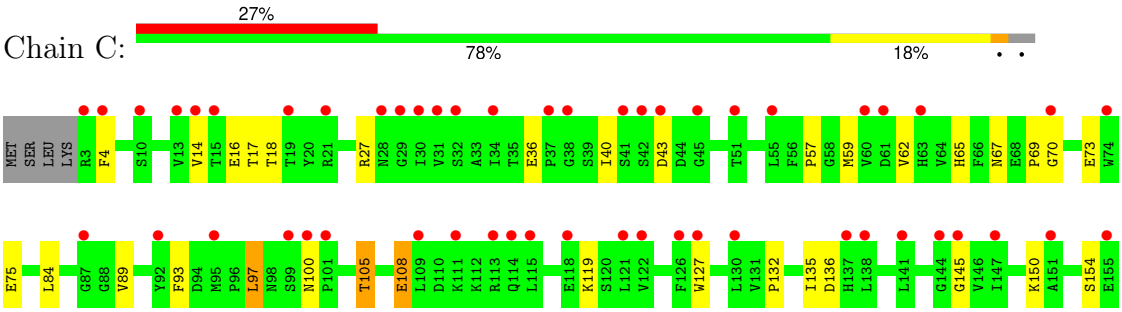
- Molecule 1: Allantoinase

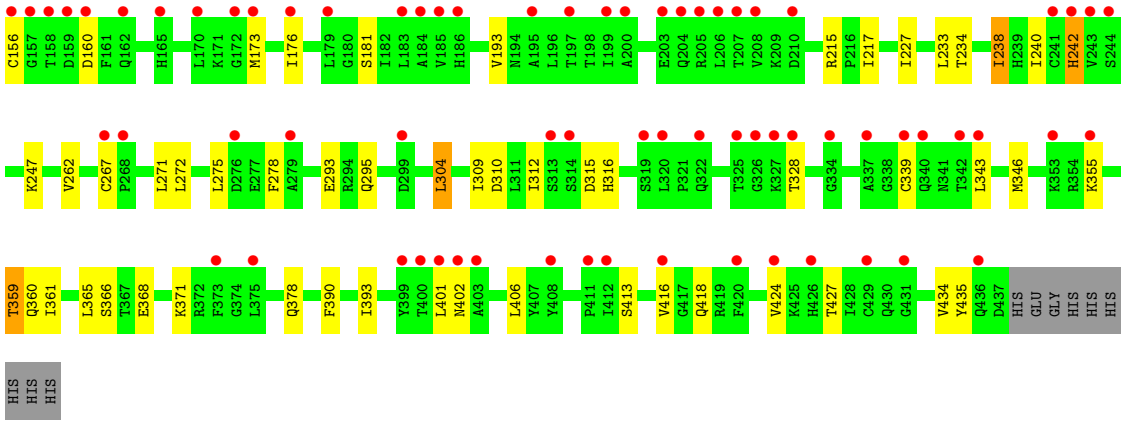
Chain B:



- Molecule 1: Allantoinase

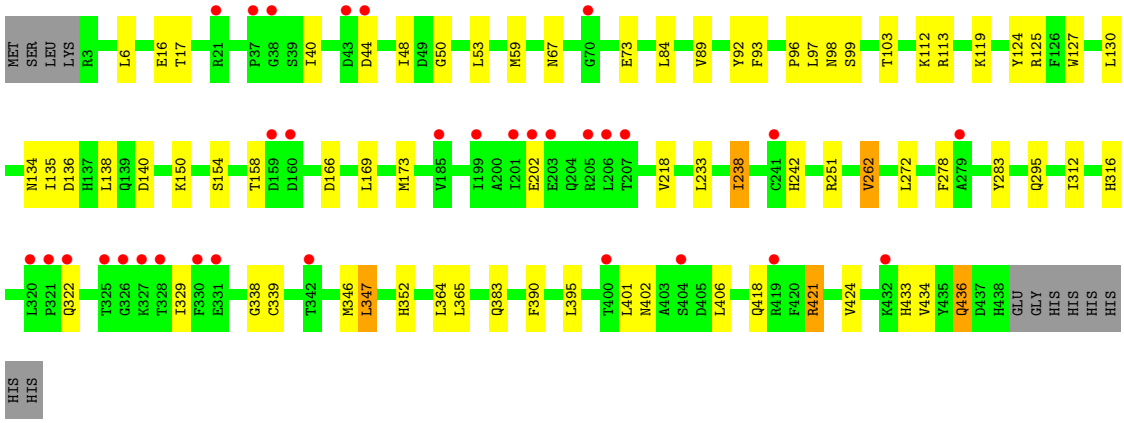
Chain C:





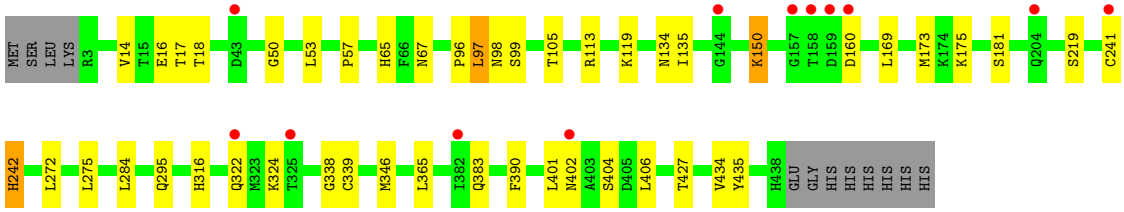
• Molecule 1: Allantoinase

Chain D:



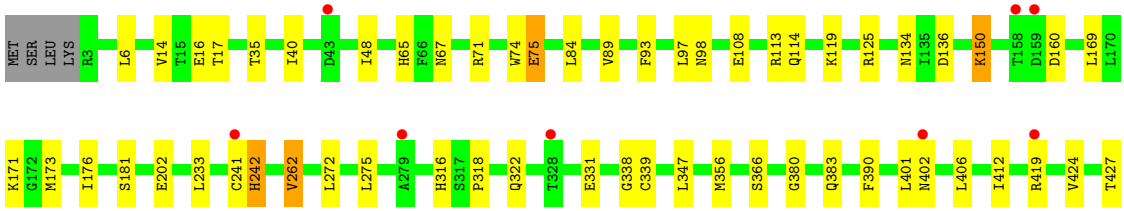
• Molecule 1: Allantoinase

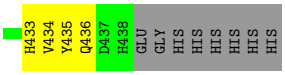
Chain E:



• Molecule 1: Allantoinase

Chain F:




H433
V434
Y435
Q436
D437
H438
GLU
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	157.66Å 157.66Å 418.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 27.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (27.39-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.240 , 0.267 0.240 , 0.266	Depositor DCC
R_{free} test set	2853 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20901	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4571e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.41	0/3507	0.60	0/4749
1	B	0.44	0/3523	0.61	1/4770 (0.0%)
1	C	0.43	0/3485	0.62	0/4720
1	D	0.42	0/3488	0.59	0/4724
1	E	0.43	0/3488	0.59	0/4724
1	F	0.41	0/3508	0.61	1/4752 (0.0%)
All	All	0.42	0/20999	0.60	2/28439 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	395	LEU	CA-CB-CG	6.19	129.54	115.30
1	F	262	VAL	CB-CA-C	-5.13	101.65	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ASP	Peptide
1	A	160	ASP	Peptide

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	3425	0	3404	27	0
1	B	3437	0	3411	25	0
1	C	3410	0	3376	32	0
1	D	3415	0	3379	29	0
1	E	3412	0	3380	16	0
1	F	3425	0	3393	19	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	53	0	0	0	0
3	B	69	0	0	0	0
3	C	39	0	0	0	0
3	D	47	0	0	0	0
3	E	74	0	0	0	0
3	F	89	0	0	0	0
All	All	20901	0	20343	138	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 3.

All (138) 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:67:ASN:ND2	1:D:98:ASN:HB2	1.96	0.80
1:F:75:GLU:HG2	1:F:318:PRO:HG3	1.69	0.73
1:B:75:GLU:HG2	1:B:318:PRO:HG3	1.76	0.68
1:E:67:ASN:ND2	1:E:98:ASN:HB2	2.09	0.67
1:F:67:ASN:ND2	1:F:98:ASN:HB2	2.09	0.67
1:B:67:ASN:ND2	1:B:98:ASN:HB2	2.10	0.67
1:D:96:PRO:HD3	1:D:127:TRP:HB2	1.76	0.67
1:D:97:LEU:O	1:D:98:ASN:HB2	1.94	0.66
1:A:393:ILE:HG22	1:A:395:LEU:HD23	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:TYR:HE1	1:D:329:ILE:HA	1.63	0.62
1:C:70:GLY:HA3	1:C:100:ASN:H	1.64	0.62
1:F:16[B]:GLU:HG3	1:F:17:THR:HG23	1.83	0.61
1:C:359:THR:HG22	1:C:360:GLN:N	2.16	0.60
1:A:18:THR:HG21	1:E:383:GLN:HE22	1.67	0.60
1:B:18:THR:HG21	1:F:383:GLN:HE22	1.67	0.60
1:D:67:ASN:ND2	1:D:98:ASN:CB	2.64	0.59
1:B:316:HIS:HB2	1:B:339:CYS:HB3	1.85	0.58
1:A:14:VAL:HG12	1:A:19:THR:HG22	1.86	0.58
1:E:16[B]:GLU:HG3	1:E:17:THR:HG23	1.86	0.57
1:C:359:THR:CG2	1:C:360:GLN:N	2.67	0.57
1:E:65:HIS:HB3	1:E:67:ASN:HD21	1.69	0.57
1:C:18:THR:HG21	1:D:383:GLN:HE22	1.68	0.57
1:D:346:MET:HG3	1:D:365:LEU:HD11	1.88	0.55
1:D:283:TYR:CE1	1:D:329:ILE:HA	2.40	0.55
1:B:84:LEU:HB3	1:B:89:VAL:HB	1.87	0.55
1:B:9:ARG:O	1:B:10:SER:HB2	2.07	0.55
1:C:62:VAL:HA	1:C:93:PHE:HB2	1.89	0.54
1:B:392:LEU:HB2	1:B:426:HIS:HB2	1.90	0.54
1:D:97:LEU:C	1:D:99:SER:H	2.12	0.53
1:F:427:THR:HB	1:F:435:TYR:HB3	1.91	0.53
1:A:18:THR:HG21	1:E:383:GLN:NE2	2.23	0.53
1:B:56:PHE:HZ	1:B:358:LEU:HD22	1.73	0.53
1:B:268:PRO:HG3	1:B:342:THR:HG23	1.91	0.53
1:C:238:ILE:HD11	1:C:240:ILE:HD11	1.91	0.53
1:D:316:HIS:HB2	1:D:339:CYS:HB3	1.91	0.52
1:F:433:HIS:HE1	1:F:436:GLN:HB2	1.73	0.52
1:C:4:PHE:HE2	1:C:40:ILE:HG12	1.75	0.52
1:D:84:LEU:HB3	1:D:89:VAL:HB	1.90	0.52
1:C:346:MET:HG3	1:C:365:LEU:HD11	1.91	0.52
1:F:65:HIS:HB3	1:F:67:ASN:HD21	1.75	0.52
1:C:368:GLU:HA	1:C:371:LYS:HB2	1.92	0.51
1:D:50:GLY:HA2	1:D:53:LEU:HD12	1.91	0.51
1:A:166:ASP:HB2	1:B:191:GLU:HG3	1.93	0.51
1:D:59:MET:HB2	1:D:89:VAL:HG22	1.93	0.51
1:A:403:ALA:HB1	1:A:411:PRO:HB2	1.93	0.51
1:D:96:PRO:HD3	1:D:127:TRP:CB	2.41	0.50
1:C:65:HIS:HB3	1:C:67:ASN:HD21	1.77	0.50
1:C:401:LEU:HD21	1:C:406:LEU:HD21	1.94	0.50
1:D:401:LEU:HD21	1:D:406:LEU:HD21	1.92	0.50
1:C:16[A]:GLU:HG2	1:C:17:THR:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:PHE:CD1	1:F:125:ARG:HB2	2.47	0.49
1:D:16[B]:GLU:HG3	1:D:17:THR:HG23	1.94	0.49
1:A:383:GLN:NE2	1:E:18:THR:HG21	2.28	0.49
1:A:78:ALA:HB2	1:A:119:LYS:HG3	1.95	0.48
1:A:341:ASN:O	1:A:345:VAL:HG12	2.13	0.48
1:E:346:MET:HG3	1:E:365:LEU:HD11	1.96	0.48
1:B:16[B]:GLU:HG3	1:B:17:THR:HG23	1.95	0.47
1:C:173:MET:HB3	1:C:234:THR:HG21	1.96	0.47
1:C:271:LEU:HD11	1:C:304:LEU:HD13	1.97	0.47
1:F:176:ILE:HG23	1:F:181:SER:HB3	1.97	0.47
1:C:217:ILE:HG21	1:C:247:LYS:HD2	1.96	0.47
1:A:110:ASP:HA	1:A:113:ARG:HB3	1.97	0.47
1:A:153:MET:CE	1:A:223:ALA:HB1	2.45	0.47
1:C:267:CYS:SG	1:C:315:ASP:HB2	2.54	0.47
1:E:316:HIS:HB2	1:E:339:CYS:HB3	1.97	0.46
1:A:233:LEU:HD21	1:B:196:LEU:HD11	1.96	0.46
1:C:427:THR:HB	1:C:435:TYR:HB3	1.98	0.46
1:F:316:HIS:HB2	1:F:339:CYS:HB3	1.97	0.46
1:A:93:PHE:CD1	1:A:125:ARG:HB2	2.51	0.46
1:A:383:GLN:HE22	1:E:18:THR:HG21	1.81	0.46
1:C:59:MET:HA	1:C:366:SER:HB2	1.98	0.46
1:F:401:LEU:HD21	1:F:406:LEU:HD21	1.96	0.46
1:A:181:SER:OG	1:A:182:ILE:N	2.49	0.46
1:D:130:LEU:HD13	1:D:138:LEU:HD11	1.98	0.46
1:F:169:LEU:HB3	1:F:173:MET:HE3	1.98	0.46
1:E:169:LEU:HB3	1:E:173:MET:HE2	1.98	0.45
1:F:150:LYS:NZ	1:F:241:CYS:SG	2.89	0.45
1:C:304:LEU:HD12	1:C:309:ILE:HD12	1.99	0.45
1:D:6:LEU:HD11	1:D:48:ILE:HG12	1.99	0.45
1:E:401:LEU:HD21	1:E:406:LEU:HD21	1.98	0.45
1:D:352:HIS:CD2	1:D:421:ARG:HB3	2.52	0.45
1:C:84:LEU:HB3	1:C:89:VAL:HB	1.99	0.45
1:A:238:ILE:HD11	1:A:240:ILE:HD11	1.99	0.45
1:B:135:ILE:H	1:B:135:ILE:HG13	1.56	0.45
1:B:312:ILE:HG12	1:B:364:LEU:HB3	1.99	0.44
1:A:392:LEU:HB2	1:A:426:HIS:HB2	2.00	0.44
1:B:427:THR:HB	1:B:435:TYR:HB3	2.00	0.44
1:D:84:LEU:HD22	1:D:89:VAL:HG11	1.99	0.44
1:E:284:LEU:HD23	1:E:324:LYS:HG2	2.00	0.44
1:B:27:ARG:HB2	1:B:32:SER:HB2	1.99	0.44
1:F:84:LEU:HB3	1:F:89:VAL:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:THR:HG23	1:C:108:GLU:HB2	2.00	0.43
1:E:150:LYS:NZ	1:E:241:CYS:SG	2.89	0.43
1:B:18:THR:HG21	1:F:383:GLN:NE2	2.32	0.43
1:D:312:ILE:HG12	1:D:364:LEU:HB3	1.99	0.43
1:A:346:MET:HG3	1:A:365:LEU:HD11	1.99	0.43
1:B:401:LEU:HD21	1:B:406:LEU:HD21	1.99	0.43
1:C:93:PHE:HB3	1:C:127:TRP:NE1	2.34	0.43
1:C:14:VAL:O	1:C:57:PRO:HD3	2.19	0.43
1:A:284:LEU:HD23	1:A:324:LYS:HE3	2.01	0.43
1:C:275:LEU:HB2	1:C:293:GLU:HA	2.01	0.43
1:A:275:LEU:HD12	1:A:275:LEU:HA	1.94	0.42
1:A:283:TYR:CD1	1:A:332:VAL:HG21	2.53	0.42
1:F:35:THR:HG21	1:F:40:ILE:HD13	2.01	0.42
1:D:92:TYR:CZ	1:D:124:TYR:HB3	2.54	0.42
1:D:251:ARG:HA	1:D:251:ARG:HD2	1.85	0.42
1:E:96:PRO:HD2	1:E:97:LEU:HD23	2.02	0.42
1:B:413:SER:HB3	1:B:416:VAL:HG23	2.02	0.42
1:E:427:THR:HB	1:E:435:TYR:HB3	2.00	0.42
1:B:71:ARG:HD3	1:B:74:TRP:CZ2	2.54	0.42
1:F:6:LEU:HD11	1:F:48:ILE:HG12	2.01	0.42
1:B:425:LYS:HA	1:B:437:ASP:HB2	2.02	0.42
1:D:93:PHE:CD1	1:D:125:ARG:HB2	2.55	0.42
1:B:181:SER:OG	1:B:182:ILE:N	2.50	0.41
1:A:59:MET:HB2	1:A:89:VAL:HG22	2.01	0.41
1:A:113:ARG:NH1	1:A:144:GLY:O	2.53	0.41
1:D:169:LEU:HB3	1:D:173:MET:HE3	2.02	0.41
1:D:433:HIS:HE1	1:D:436:GLN:HG3	1.85	0.41
1:C:18:THR:HG21	1:D:383:GLN:NE2	2.35	0.41
1:F:71:ARG:HD3	1:F:74:TRP:CZ2	2.55	0.41
1:B:6:LEU:HD12	1:B:46:PRO:HB2	2.01	0.41
1:C:193:VAL:HG22	1:C:215:ARG:HA	2.01	0.41
1:C:316:HIS:HB2	1:C:339:CYS:HB3	2.01	0.41
1:A:67:ASN:ND2	1:A:98:ASN:HB3	2.35	0.41
1:C:176:ILE:HG23	1:C:181:SER:HB3	2.01	0.41
1:D:238:ILE:HG23	1:D:262:VAL:HG13	2.02	0.41
1:E:50:GLY:HA2	1:E:53:LEU:HD12	2.03	0.41
1:A:153:MET:HE2	1:A:223:ALA:HB1	2.02	0.41
1:A:251:ARG:HA	1:A:251:ARG:HD2	1.94	0.41
1:C:413:SER:HB3	1:C:416:VAL:HG23	2.02	0.41
1:D:347:LEU:HD12	1:D:347:LEU:HA	1.86	0.41
1:C:65:HIS:HE1	1:C:97:LEU:HD21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CD1	1:B:125:ARG:HB2	2.56	0.40
1:B:341:ASN:O	1:B:345:VAL:HG12	2.21	0.40
1:C:16[B]:GLU:HG3	1:C:17:THR:HG23	2.02	0.40
1:C:73:GLU:H	1:C:73:GLU:HG2	1.66	0.40
1:A:283:TYR:CE1	1:A:332:VAL:HG21	2.57	0.40
1:F:366:SER:OG	1:F:380:GLY:HA2	2.21	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	438/448 (98%)	410 (94%)	25 (6%)	3 (1%)	22	43
1	B	440/448 (98%)	425 (97%)	13 (3%)	2 (0%)	29	52
1	C	436/448 (97%)	397 (91%)	35 (8%)	4 (1%)	17	35
1	D	436/448 (97%)	416 (95%)	18 (4%)	2 (0%)	29	52
1	E	436/448 (97%)	419 (96%)	15 (3%)	2 (0%)	29	52
1	F	438/448 (98%)	424 (97%)	12 (3%)	2 (0%)	29	52
All	All	2624/2688 (98%)	2491 (95%)	118 (4%)	15 (1%)	25	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PRO
1	A	242	HIS
1	B	242	HIS
1	C	242	HIS
1	D	242	HIS
1	E	242	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	242	HIS
1	D	338	GLY
1	F	338	GLY
1	C	145	GLY
1	E	338	GLY
1	B	132	PRO
1	C	132	PRO
1	A	338	GLY
1	C	69	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	375/382 (98%)	343 (92%)	32 (8%)	10	21
1	B	377/382 (99%)	351 (93%)	26 (7%)	15	31
1	C	373/382 (98%)	336 (90%)	37 (10%)	8	15
1	D	373/382 (98%)	340 (91%)	33 (9%)	10	19
1	E	373/382 (98%)	350 (94%)	23 (6%)	18	37
1	F	375/382 (98%)	347 (92%)	28 (8%)	13	27
All	All	2246/2292 (98%)	2067 (92%)	179 (8%)	12	24

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	73	GLU
1	A	97	LEU
1	A	105	THR
1	A	107	GLU
1	A	115	LEU
1	A	119	LYS
1	A	136	ASP
1	A	150	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	SER
1	A	156	CYS
1	A	160	ASP
1	A	166	ASP
1	A	171	LYS
1	A	194	ASN
1	A	202	GLU
1	A	233	LEU
1	A	238	ILE
1	A	262	VAL
1	A	272	LEU
1	A	278	PHE
1	A	295	GLN
1	A	322	GLN
1	A	323	MET
1	A	345	VAL
1	A	347	LEU
1	A	361	ILE
1	A	390	PHE
1	A	402	ASN
1	A	412	ILE
1	A	424	VAL
1	A	434	VAL
1	B	7	ILE
1	B	14	VAL
1	B	27	ARG
1	B	44	ASP
1	B	97	LEU
1	B	99	SER
1	B	119	LYS
1	B	135	ILE
1	B	136	ASP
1	B	150	LYS
1	B	156	CYS
1	B	202	GLU
1	B	233	LEU
1	B	238	ILE
1	B	272	LEU
1	B	278	PHE
1	B	295	GLN
1	B	345	VAL
1	B	347	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	LYS
1	B	390	PHE
1	B	402	ASN
1	B	404	SER
1	B	412	ILE
1	B	421	ARG
1	B	424	VAL
1	C	27	ARG
1	C	36	GLU
1	C	43	ASP
1	C	75	GLU
1	C	97	LEU
1	C	105	THR
1	C	108	GLU
1	C	119	LYS
1	C	135	ILE
1	C	136	ASP
1	C	150	LYS
1	C	154	SER
1	C	156	CYS
1	C	160	ASP
1	C	227	ILE
1	C	233	LEU
1	C	238	ILE
1	C	242	HIS
1	C	262	VAL
1	C	272	LEU
1	C	278	PHE
1	C	295	GLN
1	C	304	LEU
1	C	310	ASP
1	C	312	ILE
1	C	328	THR
1	C	343	LEU
1	C	355	LYS
1	C	359	THR
1	C	361	ILE
1	C	378	GLN
1	C	390	PHE
1	C	393	ILE
1	C	402	ASN
1	C	418	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	424	VAL
1	C	434	VAL
1	D	40	ILE
1	D	44	ASP
1	D	73	GLU
1	D	103	THR
1	D	112	LYS
1	D	113	ARG
1	D	119	LYS
1	D	134	ASN
1	D	135	ILE
1	D	136	ASP
1	D	140	ASP
1	D	150	LYS
1	D	154	SER
1	D	158	THR
1	D	166	ASP
1	D	202	GLU
1	D	218	VAL
1	D	233	LEU
1	D	238	ILE
1	D	262	VAL
1	D	272	LEU
1	D	278	PHE
1	D	295	GLN
1	D	322	GLN
1	D	347	LEU
1	D	390	PHE
1	D	395	LEU
1	D	402	ASN
1	D	418	GLN
1	D	421	ARG
1	D	424	VAL
1	D	434	VAL
1	D	436	GLN
1	E	14	VAL
1	E	57	PRO
1	E	97	LEU
1	E	99	SER
1	E	105	THR
1	E	113	ARG
1	E	119	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	134	ASN
1	E	135	ILE
1	E	150	LYS
1	E	160	ASP
1	E	175	LYS
1	E	181	SER
1	E	219	SER
1	E	242	HIS
1	E	272	LEU
1	E	275	LEU
1	E	295	GLN
1	E	322	GLN
1	E	390	PHE
1	E	402	ASN
1	E	404	SER
1	E	434	VAL
1	F	14	VAL
1	F	75	GLU
1	F	97	LEU
1	F	108	GLU
1	F	113	ARG
1	F	114	GLN
1	F	119	LYS
1	F	134	ASN
1	F	136	ASP
1	F	150	LYS
1	F	160	ASP
1	F	171	LYS
1	F	202	GLU
1	F	233	LEU
1	F	242	HIS
1	F	262	VAL
1	F	272	LEU
1	F	275	LEU
1	F	322	GLN
1	F	331	GLU
1	F	347	LEU
1	F	356	MET
1	F	390	PHE
1	F	402	ASN
1	F	412	ILE
1	F	419	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	424	VAL
1	F	434	VAL

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	98	ASN
1	A	114	GLN
1	A	142	HIS
1	A	378	GLN
1	A	383	GLN
1	A	433	HIS
1	B	67	ASN
1	B	98	ASN
1	B	242	HIS
1	B	378	GLN
1	B	418	GLN
1	C	67	ASN
1	C	98	ASN
1	C	114	GLN
1	C	142	HIS
1	C	418	GLN
1	D	67	ASN
1	D	162	GLN
1	D	242	HIS
1	D	352	HIS
1	D	378	GLN
1	D	418	GLN
1	D	433	HIS
1	E	67	ASN
1	E	142	HIS
1	E	352	HIS
1	E	378	GLN
1	F	67	ASN
1	F	98	ASN
1	F	142	HIS
1	F	322	GLN
1	F	383	GLN
1	F	418	GLN
1	F	436	GLN

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 (i)

Of 6 ligands modelled in this entry, 6 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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	436/448 (97%)	0.30	32 (7%)	15	11	22, 38, 54, 77	0
1	B	437/448 (97%)	0.09	21 (4%)	30	24	28, 37, 52, 66	0
1	C	435/448 (97%)	1.48	122 (28%)	0	0	22, 39, 51, 74	0
1	D	436/448 (97%)	0.22	32 (7%)	15	11	26, 38, 53, 70	0
1	E	436/448 (97%)	-0.02	12 (2%)	53	46	25, 37, 47, 68	0
1	F	436/448 (97%)	-0.06	8 (1%)	68	64	26, 37, 48, 64	0
All	All	2616/2688 (97%)	0.33	227 (8%)	10	7	22, 37, 52, 77	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	THR	9.2
1	C	402	ASN	7.6
1	A	157	GLY	7.3
1	C	156	CYS	6.9
1	C	113	ARG	5.8
1	A	322	GLN	5.7
1	C	144	GLY	5.5
1	C	322	GLN	5.4
1	C	400	THR	5.3
1	C	159	ASP	5.2
1	A	111	LYS	5.1
1	C	111	LYS	5.0
1	C	109	LEU	4.8
1	C	31	VAL	4.8
1	C	141	LEU	4.7
1	C	157	GLY	4.7
1	C	205	ARG	4.6
1	C	241	CYS	4.6
1	A	204	GLN	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	201	ILE	4.6
1	C	210	ASP	4.5
1	C	21	ARG	4.5
1	C	122	VAL	4.5
1	C	121	LEU	4.5
1	C	4	PHE	4.5
1	D	43	ASP	4.4
1	C	334	GLY	4.3
1	D	202	GLU	4.3
1	A	325	THR	4.2
1	C	70	GLY	4.2
1	C	411	PRO	4.2
1	C	28	ASN	4.2
1	C	43	ASP	4.1
1	C	416	VAL	4.1
1	C	206	LEU	4.1
1	E	322	GLN	4.1
1	C	403	ALA	4.1
1	C	138	LEU	4.0
1	C	179	LEU	4.0
1	C	431	GLY	4.0
1	C	328	THR	4.0
1	C	412	ILE	4.0
1	C	327	LYS	4.0
1	B	201	ILE	4.0
1	C	339	CYS	4.0
1	D	199	ILE	3.9
1	D	38	GLY	3.9
1	C	319	SER	3.9
1	D	326	GLY	3.8
1	B	322	GLN	3.8
1	C	375	LEU	3.8
1	B	2	LYS	3.8
1	A	327	LYS	3.8
1	A	43	ASP	3.8
1	C	130	LEU	3.7
1	C	155	GLU	3.7
1	E	157	GLY	3.7
1	A	160	ASP	3.7
1	C	325	THR	3.7
1	B	158	THR	3.7
1	A	321	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	159	ASP	3.6
1	C	203	GLU	3.6
1	C	145	GLY	3.6
1	E	402	ASN	3.6
1	C	429	CYS	3.5
1	C	32	SER	3.5
1	A	158	THR	3.4
1	C	186	HIS	3.4
1	C	172	GLY	3.4
1	B	43	ASP	3.4
1	C	313	SER	3.4
1	E	159	ASP	3.4
1	C	199	ILE	3.4
1	B	178	ALA	3.4
1	C	115	LEU	3.3
1	C	195	ALA	3.3
1	C	137	HIS	3.3
1	D	327	LYS	3.3
1	D	328	THR	3.2
1	C	92	TYR	3.2
1	E	160	ASP	3.2
1	C	60	VAL	3.2
1	C	38	GLY	3.2
1	D	160	ASP	3.1
1	A	406	LEU	3.1
1	B	160	ASP	3.1
1	C	10	SER	3.0
1	D	205	ARG	3.0
1	F	43	ASP	3.0
1	A	241	CYS	3.0
1	C	126	PHE	3.0
1	C	299	ASP	3.0
1	C	267	CYS	3.0
1	B	41	SER	3.0
1	C	101	PRO	3.0
1	C	30	ILE	3.0
1	D	320	LEU	3.0
1	C	45	GLY	3.0
1	C	200	ALA	3.0
1	E	43	ASP	2.9
1	C	42	SER	2.9
1	C	399	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	156	CYS	2.9
1	C	184	ALA	2.9
1	C	100	ASN	2.9
1	D	203	GLU	2.9
1	C	355	LYS	2.9
1	C	41	SER	2.8
1	C	63	HIS	2.8
1	C	99	SER	2.8
1	D	404	SER	2.8
1	A	159	ASP	2.8
1	C	401	LEU	2.8
1	B	325	THR	2.8
1	E	325	THR	2.8
1	C	13	VAL	2.8
1	C	3	ARG	2.8
1	B	28	ASN	2.7
1	C	340	GLN	2.7
1	C	204	GLN	2.7
1	A	203	GLU	2.7
1	D	279	ALA	2.7
1	C	165	HIS	2.7
1	C	87	GLY	2.7
1	C	55	LEU	2.7
1	D	37	PRO	2.7
1	C	147	ILE	2.7
1	B	327	LYS	2.7
1	D	330	PHE	2.7
1	C	114	GLN	2.7
1	C	14	VAL	2.6
1	C	320	LEU	2.6
1	D	325	THR	2.6
1	D	400	THR	2.6
1	C	118	GLU	2.6
1	C	342	THR	2.6
1	C	408	TYR	2.6
1	D	206	LEU	2.6
1	C	242	HIS	2.5
1	D	21	ARG	2.5
1	C	176	ILE	2.5
1	B	416	VAL	2.5
1	F	419	ARG	2.5
1	D	321	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	242	HIS	2.5
1	C	160	ASP	2.5
1	F	279	ALA	2.5
1	B	333	TRP	2.5
1	D	70	GLY	2.4
1	B	202	GLU	2.4
1	C	197	THR	2.4
1	C	207	THR	2.4
1	A	74	TRP	2.4
1	A	314	SER	2.4
1	B	136	ASP	2.4
1	E	204	GLN	2.4
1	B	241	CYS	2.4
1	A	116	ALA	2.4
1	C	337	ALA	2.4
1	A	205	ARG	2.4
1	B	314	SER	2.4
1	D	419	ARG	2.4
1	D	322	GLN	2.4
1	A	199	ILE	2.4
1	E	241	CYS	2.4
1	A	207	THR	2.3
1	D	185	VAL	2.3
1	C	151	ALA	2.3
1	C	74	TRP	2.3
1	C	353	LYS	2.3
1	D	44	ASP	2.3
1	C	426	HIS	2.3
1	A	200	ALA	2.3
1	D	342	THR	2.3
1	F	402	ASN	2.3
1	C	162	GLN	2.3
1	D	241	CYS	2.3
1	D	207	THR	2.3
1	C	183	LEU	2.3
1	C	276	ASP	2.3
1	C	343	LEU	2.3
1	A	71	ARG	2.3
1	C	243	VAL	2.3
1	E	158	THR	2.2
1	F	158	THR	2.2
1	F	159	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	HIS	2.2
1	A	144	GLY	2.2
1	C	326	GLY	2.2
1	F	241	CYS	2.2
1	C	436	GLN	2.2
1	B	206	LEU	2.2
1	C	185	VAL	2.2
1	A	44	ASP	2.2
1	C	61	ASP	2.2
1	C	208	VAL	2.2
1	A	155	GLU	2.2
1	A	411	PRO	2.2
1	C	95	MET	2.2
1	C	15	THR	2.2
1	A	100	ASN	2.1
1	C	268	PRO	2.1
1	C	127	TRP	2.1
1	C	420	PHE	2.1
1	C	34	ILE	2.1
1	E	382	ILE	2.1
1	C	29	GLY	2.1
1	B	382	ILE	2.1
1	C	244	SER	2.1
1	A	315	ASP	2.1
1	C	279	ALA	2.1
1	C	173	MET	2.1
1	D	331	GLU	2.1
1	A	412	ILE	2.1
1	B	64	VAL	2.1
1	A	342	THR	2.0
1	C	19	THR	2.0
1	F	328	THR	2.0
1	C	373	PHE	2.0
1	C	170	LEU	2.0
1	C	37	PRO	2.0
1	D	432	LYS	2.0
1	C	314	SER	2.0
1	E	144	GLY	2.0
1	C	51	THR	2.0
1	C	424	VAL	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	447	1/1	0.84	0.20	40,40,40,40	1
2	ZN	C	447	1/1	0.93	0.20	50,50,50,50	1
2	ZN	F	447	1/1	0.94	0.22	39,39,39,39	1
2	ZN	E	447	1/1	0.96	0.08	39,39,39,39	1
2	ZN	B	447	1/1	0.96	0.08	39,39,39,39	1
2	ZN	A	447	1/1	0.97	0.06	43,43,43,43	1

6.5 Other polymers (i)

There are no such residues in this entry.