

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7YZ8
Title	:	Triclinic crystal structure of YTHDF1 YTH domain (544AVV546 mutant)
Authors	:	Dalle Vedove, A.; Cazzanelli, G.; Lolli, G.
Deposited on	:	2022-02-19
Resolution	:	2.50 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
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
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)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.50 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.



Motric	Whole archive	Similar resolution
Wiethic	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	А	200	82%	12%	6%
1	В	200	86%	1	2% •
1	С	200	% • 84%	7%	8%
1	D	200	83%	9%	8%
1	Е	200	80%	13%	7%



Mol	Chain	Length	Quality of chain		
1	F	200	74%	17%	• 8%
1	G	200	77%	14%	• 8%
1	Н	200	78%	14%	7%
1	Ι	200	78%	14%	7%
1	J	200	76%	15%	8%
1	K	200	% 82%	10%	• 8%
1	L	200	% • 79%	11%	• 9%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18773 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	189	Total 1564	C 991	N 281	0 287	${f S}{5}$	0	1	0
1	В	195	Total 1609	C 1020	N 289	0 295	${ m S}{ m 5}$	0	1	0
1	С	183	Total 1512	C 959	N 272	0 276	${f S}{5}$	0	1	0
1	D	184	Total 1526	C 970	N 274	О 277	${f S}{5}$	0	1	0
1	Е	186	Total 1541	C 979	N 277	O 280	${f S}{5}$	0	1	0
1	F	185	Total 1535	C 976	N 276	0 278	${f S}{5}$	0	1	0
1	G	184	Total 1515	C 961	N 274	0 275	S 5	0	0	0
1	Н	186	Total 1534	C 972	N 278	0 279	S 5	0	0	0
1	Ι	186	Total 1539	C 978	N 277	0 279	S 5	0	1	0
1	J	184	Total 1530	C 972	N 275	0 278	${f S}{5}$	0	1	0
1	K	185	Total 1528	C 969	N 276	0 278	S 5	0	0	0
1	L	182	Total 1501	Ċ 953	N 270	0 273	$\begin{array}{c} \mathbf{S} \\ 5 \end{array}$	0	0	0

• Molecule 1 is a protein called YTH domain-containing family protein 1.

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	360	GLY	-	expression tag	UNP Q9BYJ9
А	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
А	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
А	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
В	360	GLY	-	expression tag	UNP Q9BYJ9



Chain	Residue	Modelled	Actual	Comment	Reference
В	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
В	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
В	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
С	360	GLY	-	expression tag	UNP Q9BYJ9
С	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
С	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
С	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
D	360	GLY	-	expression tag	UNP Q9BYJ9
D	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
D	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
D	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
Е	360	GLY	-	expression tag	UNP Q9BYJ9
Е	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
Е	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
Е	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
F	360	GLY	-	expression tag	UNP Q9BYJ9
F	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
F	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
F	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
G	360	GLY	-	expression tag	UNP Q9BYJ9
G	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
G	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
G	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
Н	360	GLY	-	expression tag	UNP Q9BYJ9
Н	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
Н	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
Н	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
Ι	360	GLY	-	expression tag	UNP Q9BYJ9
Ι	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
I	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
I	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
J	360	GLY	-	expression tag	UNP Q9BYJ9
J	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
J	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
J	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
K	360	GLY	-	expression tag	UNP Q9BYJ9
K	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
K	545	VAL	GLU	engineered mutation	UNP Q9BYJ9
K	546	VAL	GLU	engineered mutation	UNP Q9BYJ9
L	360	GLY	-	expression tag	UNP Q9BYJ9
L	544	ALA	GLU	engineered mutation	UNP Q9BYJ9
L	545	VAL	GLU	engineered mutation	UNP Q9BYJ9



Chain	Residue	Modelled	Actual	Comment	Reference
L	546	VAL	GLU	engineered mutation	UNP Q9BYJ9

• Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atom	S	ZeroOcc	AltConf
2	А	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 3 & 1 \end{array}$	N S 1 1	0	0
2	В	1	Total C 3 1	N S 1 1	0	0
2	С	1	Total C 3 1	N S 1 1	0	0
2	D	1	Total C 3 1	N S 1 1	0	0
2	Е	1	Total C 3 1	N S 1 1	0	0
2	F	1	Total C 3 1	N S 1 1	0	0
2	G	1	Total C 3 1	N S 1 1	0	0
2	Н	1	Total C 3 1	N S 1 1	0	0
2	Ι	1	Total C 3 1	N S 1 1	0	0
2	J	1	Total C 3 1	N S 1 1	0	0
2	К	1	Total C 3 1	N S 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total 3	С 1	N 1	S 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	37	Total O 37 37	0	0
3	В	37	Total O 37 37	0	0
3	С	30	Total O 30 30	0	0
3	D	35	Total O 35 35	0	0
3	Е	22	Total O 22 22	0	0
3	F	28	Total O 28 28	0	0
3	G	20	Total O 20 20	0	0
3	Н	19	Total O 19 19	0	0
3	Ι	24	TotalO2424	0	0
3	J	28	Total O 28 28	0	0
3	K	16	Total O 16 16	0	0
3	L	7	Total O 7 7	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: YTH domain-containing family protein 1





H538 K541 K542 V545 V546 V546 K558 GLM

• Molecule 1: YTH domain-containing family protein 1



• Molecule 1: YTH domain-containing family protein 1



• Molecule 1: YTH domain-containing family protein 1





D535 H538 H538 R542 V549 V549 N557 N557 Q559

• Molecule 1: YTH domain-containing family protein 1



- K558 GLN
- Molecule 1: YTH domain-containing family protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	71.22Å 92.57Å 113.94Å	Depositor
a, b, c, α , β , γ	72.87° 79.05° 67.87°	Depositor
Bosolution(Å)	48.09 - 2.50	Depositor
Resolution (A)	49.06 - 2.50	EDS
% Data completeness	98.2 (48.09-2.50)	Depositor
(in resolution range)	98.3(49.06-2.50)	EDS
R_{merge}	0.05	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.91 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R R.	0.184 , 0.243	Depositor
II, II, <i>free</i>	0.184 , 0.242	DCC
R_{free} test set	4294 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	52.2	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 41.0	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18773	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: SCN

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).

Mal	Chain	Bond	lengths	Bond	angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.55	0/1605	0.73	0/2158
1	В	0.54	0/1653	0.71	0/2226
1	С	0.52	0/1551	0.71	0/2086
1	D	0.50	0/1567	0.68	0/2109
1	Ε	0.52	0/1582	0.65	0/2128
1	F	0.52	0/1576	0.66	0/2120
1	G	0.50	0/1552	0.65	0/2088
1	Н	0.49	0/1571	0.67	0/2111
1	Ι	0.49	0/1580	0.67	0/2125
1	J	0.52	0/1571	0.69	0/2113
1	Κ	0.49	0/1565	0.67	0/2105
1	L	0.48	0/1537	0.66	0/2067
All	All	0.51	0/18910	0.68	0/25436

There are no bond length outliers.

There are no bond angle outliers.

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	А	1564	0	1543	19	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	1609	0	1584	22	0
1	С	1512	0	1498	12	0
1	D	1526	0	1508	17	0
1	Е	1541	0	1523	19	0
1	F	1535	0	1521	23	0
1	G	1515	0	1497	25	0
1	Н	1534	0	1518	19	0
1	Ι	1539	0	1524	23	0
1	J	1530	0	1511	20	0
1	Κ	1528	0	1511	19	0
1	L	1501	0	1488	18	0
2	А	3	0	0	0	0
2	В	3	0	0	0	0
2	С	3	0	0	0	0
2	D	3	0	0	1	0
2	Ε	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	Н	3	0	0	0	0
2	Ι	3	0	0	1	0
2	J	3	0	0	0	0
2	Κ	3	0	0	0	0
2	L	3	0	0	1	0
3	А	37	0	0	1	0
3	В	37	0	0	2	0
3	С	30	0	0	0	0
3	D	35	0	0	0	0
3	Ε	22	0	0	0	0
3	F	28	0	0	1	0
3	G	20	0	0	1	0
3	Н	19	0	0	1	0
3	Ι	24	0	0	1	0
3	J	28	0	0	1	0
3	K	16	0	0	1	0
3	L	7	0	0	0	0
All	All	18773	0	18226	212	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 6.

All (212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:553:ARG:HH21	1:G:553:ARG:HG3	1.26	0.97
1:K:550:ARG:HH11	1:K:550:ARG:HG2	1.34	0.92
1:I:378:ASN:HD21	1:I:481:VAL:H	1.18	0.91
1:A:380:LYS:HD2	1:H:381:GLU:HG2	1.60	0.83
1:G:485:PRO:HB2	1:G:487:ASN:OD1	1.77	0.83
1:A:521:LYS:NZ	1:G:373:ALA:HB1	1.98	0.79
1:L:367:VAL:HG23	1:L:536:PHE:HE1	1.47	0.79
1:I:390:ARG:HE	1:I:428:MET:HE2	1.51	0.76
1:L:380:LYS:HE2	1:L:381:GLU:OE2	1.85	0.75
1:I:552:GLU:HB3	1:I:556:ARG:NH1	2.04	0.73
1:A:551:LYS:O	1:A:551:LYS:HD3	1.88	0.72
1:E:389:GLY:HA2	1:E:428:MET:HE1	1.70	0.71
1:I:552:GLU:HB3	1:I:556:ARG:HH12	1.57	0.70
1:A:521:LYS:HZ2	1:G:373:ALA:HB1	1.57	0.69
1:G:407:LYS:HE3	1:G:540:GLU:OE2	1.92	0.69
1:G:553:ARG:HG3	1:G:553:ARG:NH2	1.97	0.67
1:E:380:LYS:HA	1:E:380:LYS:HE2	1.77	0.67
1:G:367:VAL:HG11	1:G:407:LYS:NZ	2.10	0.66
1:K:384:TRP:CE2	1:K:521:LYS:HD3	2.31	0.66
1:A:396:SER:HB3	1:A:440:VAL:HG22	1.78	0.65
1:K:550:ARG:HG2	1:K:550:ARG:NH1	2.09	0.65
1:K:483:ASP:OD2	1:K:530:THR:HG23	1.97	0.64
1:K:468:ASP:N	3:K:701:HOH:O	2.30	0.63
1:L:552:GLU:HB3	1:L:556:ARG:NH2	2.14	0.63
1:B:404:ARG:HH11	1:B:404:ARG:HG3	1.64	0.62
1:L:552:GLU:HB3	1:L:556:ARG:HH22	1.64	0.62
1:F:542:ARG:O	1:F:546:VAL:HG23	1.99	0.62
1:B:530:THR:CG2	1:D:556:ARG:HH11	2.13	0.61
1:A:551:LYS:HD3	1:A:551:LYS:C	2.19	0.61
1:D:415:GLU:HG2	1:D:471:LYS:HE2	1.83	0.61
1:F:364:SER:HB2	1:F:365:HIS:CD2	2.36	0.61
1:I:541:LYS:HE3	1:I:545:VAL:HG21	1.83	0.60
1:H:370:LYS:HE3	1:J:549:VAL:HG22	1.84	0.59
1:G:485:PRO:CB	1:G:487:ASN:OD1	2.51	0.59
1:D:375:HIS:HD2	1:D:477:GLN:HE22	1.51	0.59
1:H:542:ARG:O	1:H:546:VAL:HG23	2.04	0.58
1:I:364:SER:N	3:I:703:HOH:O	2.35	0.58
1:J:384:TRP:CZ2	1:J:521:LYS:HD2	2.39	0.58
1:I:511:VAL:HG23	1:I:516:ALA:HB2	1.85	0.58
1:A:431:LYS:HE3	1:E:513:LEU:HB3	1.86	0.57
1:E:541:LYS:HE3	1:E:545:VAL:HG21	1.87	0.57
1:G:367:VAL:HG11	1:G:407:LYS:HZ1	1.71	0.56



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:J:493:ARG:NH1	1:J:499:ASN:O	2.35	0.56	
1:K:380:LYS:H	1:K:380:LYS:HD2	1.70	0.56	
1:A:531:SER:HB3	1:A:533:PHE:H	1.71	0.56	
1:E:530:THR:CG2	1:I:556:ARG:HE	2.19	0.55	
1:I:437:LEU:HD13	1:I:519:VAL:HG11	1.88	0.55	
1:I:542:ARG:O	1:I:546:VAL:HG23	2.07	0.55	
1:B:370:LYS:NZ	3:B:702:HOH:O	2.39	0.55	
1:I:407:LYS:NZ	1:I:540:GLU:OE1	2.40	0.55	
1:D:538:HIS:CE1	1:D:542:ARG:HD2	2.42	0.55	
1:J:518:GLN:O	1:J:522:ILE:HD12	2.06	0.54	
1:B:551:LYS:NZ	3:B:704:HOH:O	2.39	0.54	
1:E:530:THR:HG22	1:I:556:ARG:HE	1.71	0.54	
1:E:396:SER:HB3	1:E:440:VAL:HG22	1.88	0.54	
1:I:378:ASN:ND2	1:I:480:PHE:HA	2.23	0.54	
1:K:550:ARG:HH11	1:K:550:ARG:CG	2.12	0.54	
1:G:469:LYS:N	3:G:701:HOH:O	2.41	0.53	
1:F:530:THR:HG23	1:F:534:ASP:OD2	2.08	0.53	
1:G:396:SER:HB3	1:G:440:VAL:HG22	1.90	0.53	
1:F:530:THR:CG2	1:J:556:ARG:HE	2.22	0.53	
1:F:385:ASN:HD21	1:F:387:LYS:HE2	1.74	0.53	
1:L:380:LYS:HG3	1:L:381:GLU:OE1	2.08	0.53	
1:F:530:THR:HG21	1:J:556:ARG:HE	1.73	0.52	
1:C:514:GLU:OE1	1:I:431:LYS:NZ	2.42	0.52	
1:A:551:LYS:NZ	3:A:702:HOH:O	2.42	0.52	
1:B:551:LYS:O	1:B:551:LYS:HD3	2.10	0.52	
1:B:535:ASP:O	1:B:538:HIS:HB3	2.10	0.52	
1:F:551:LYS:O	1:F:555:SER:N	2.40	0.51	
1:G:367:VAL:HB	1:G:536:PHE:HE1	1.75	0.51	
1:D:415:GLU:OE1	1:D:471:LYS:HE2	2.10	0.51	
1:H:396:SER:HB3	1:H:440:VAL:HG22	1.91	0.51	
1:B:530:THR:HG21	1:D:556:ARG:HH11	1.75	0.50	
1:G:542:ARG:O	1:G:546:VAL:HG23	2.11	0.50	
1:A:521:LYS:HZ1	1:G:373:ALA:HB1	1.72	0.50	
1:D:415:GLU:CG	1:D:471:LYS:HE2	2.42	0.50	
1:K:550:ARG:NH1	1:K:550:ARG:CG	2.73	0.50	
1:A:538:HIS:CE1	1:A:542:ARG:HD2	2.47	0.50	
1:E:420:ARG:NH2	1:E:508:THR:O	2.37	0.50	
1:C:365:HIS:N	1:C:366:PRO:HD3	2.26	0.49	
1:F:389:GLY:HA2	1:F:428:MET:HE2	1.94	0.49	
1:H:395:LYS:HB3	1:H:441:ASN:HD21	1.77	0.49	
1:J:538:HIS:CE1	1:J:542:ARG:HD2	2.48	0.49	



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:F:378:ASN:O	1:F:380:LYS:HE2	2.13	0.49
1:B:556:ARG:HE	1:D:530:THR:HG21	1.78	0.49
1:B:391:VAL:HG21	1:B:516:ALA:HB1	1.94	0.48
1:A:530:THR:HG22	1:A:531:SER:N	2.28	0.48
1:D:532:ILE:HD12	2:D:601:SCN:S	2.53	0.48
1:D:530:THR:HG23	1:D:534:ASP:OD2	2.13	0.48
1:H:535:ASP:O	1:H:538:HIS:HB3	2.14	0.48
1:K:368:LEU:HB2	1:K:536:PHE:CD1	2.49	0.48
1:E:399:GLU:H	1:E:399:GLU:CD	2.17	0.48
1:B:404:ARG:HG3	1:B:404:ARG:NH1	2.27	0.48
1:H:430:SER:HB2	1:H:431:LYS:NZ	2.29	0.48
1:J:530:THR:HG23	1:J:534:ASP:OD2	2.13	0.48
1:F:557:ASN:ND2	3:F:704:HOH:O	2.45	0.48
1:H:365:HIS:CD2	1:H:366:PRO:HD2	2.49	0.48
1:I:378:ASN:HD22	1:I:480:PHE:HA	1.79	0.48
1:F:397[A]:TYR:OH	1:J:401:ASP:OD2	2.24	0.47
1:H:513:LEU:HB2	3:H:707:HOH:O	2.14	0.47
1:K:538:HIS:CE1	1:K:542:ARG:HD2	2.49	0.47
1:F:541:LYS:NZ	1:H:369:GLU:OE1	2.42	0.47
1:C:494:LEU:HD21	1:C:502:VAL:HG23	1.96	0.47
1:F:413:SER:OG	1:F:414:THR:N	2.47	0.47
1:J:390:ARG:HE	1:J:428:MET:CE	2.27	0.47
1:L:458:TYR:CE1	1:L:471:LYS:NZ	2.83	0.47
1:G:538:HIS:CE1	1:G:542:ARG:HD2	2.50	0.47
1:G:553:ARG:HH21	1:G:553:ARG:CG	2.07	0.47
1:I:532:ILE:HD12	2:I:601:SCN:S	2.54	0.46
1:H:394:ILE:HG21	1:H:438:PHE:CE2	2.51	0.46
1:B:413:SER:OG	1:B:414:THR:N	2.49	0.46
1:G:399:GLU:HG2	1:G:539:TYR:OH	2.16	0.46
1:G:425:PHE:CE2	1:G:455:PRO:HD3	2.51	0.46
1:G:367:VAL:HB	1:G:536:PHE:CE1	2.50	0.46
1:A:525:SER:O	1:A:527:LYS:HD2	2.16	0.46
1:K:551:LYS:HA	1:K:551:LYS:HD2	1.56	0.46
1:L:532:ILE:HD12	2:L:601:SCN:S	2.55	0.46
1:H:551:LYS:NZ	1:H:555:SER:OG	2.49	0.45
1:A:365:HIS:HA	1:A:366:PRO:HD3	1.73	0.45
1:C:514:GLU:HG2	1:K:430:SER:CB	2.46	0.45
1:H:395:LYS:HE2	1:H:441:ASN:HD22	1.80	0.45
1:J:384:TRP:CH2	1:J:521:LYS:HD2	2.52	0.45
1:J:416:HIS:CE1	1:J:419:LYS:HZ3	2.35	0.45
1:J:416:HIS:CE1	1:J:419:LYS:NZ	2.85	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:495:GLU:OE1	1:B:515:LYS:NZ	2.49	0.45
1:L:395:LYS:HA	1:L:395:LYS:HD2	1.72	0.45
1:D:415:GLU:HG2	1:D:471:LYS:CE	2.46	0.45
1:J:535:ASP:O	1:J:538:HIS:HB3	2.16	0.45
1:E:367:VAL:HG23	1:E:536:PHE:HE1	1.80	0.45
1:I:395:LYS:HA	1:I:395:LYS:HD2	1.74	0.45
1:B:556:ARG:HE	1:D:530:THR:CG2	2.30	0.44
1:C:506:ARG:HH12	1:I:419:LYS:HZ3	1.66	0.44
1:D:407:LYS:HE3	1:D:408:TYR:CZ	2.52	0.44
1:J:396:SER:HB3	1:J:440:VAL:HG22	1.99	0.44
1:B:437:LEU:HD13	1:B:519:VAL:HG11	1.99	0.44
1:D:530:THR:HG22	1:D:531:SER:N	2.32	0.44
1:K:538:HIS:O	1:K:541:LYS:HB3	2.16	0.44
1:B:375:HIS:CD2	1:B:477:GLN:HE22	2.36	0.44
1:F:535:ASP:O	1:F:538:HIS:HB3	2.18	0.44
1:L:410:ILE:HG13	1:L:470:TRP:HZ3	1.82	0.44
1:L:388:SER:O	1:L:433:PRO:HD2	2.18	0.43
1:L:543:GLN:O	1:L:546:VAL:HG22	2.18	0.43
1:C:538:HIS:CE1	1:C:542:ARG:HD2	2.53	0.43
1:G:483:ASP:OD2	1:G:530:THR:HG23	2.19	0.43
1:K:368:LEU:HB2	1:K:536:PHE:CE1	2.54	0.43
1:C:405:SER:HB2	1:C:411:TRP:HE3	1.84	0.43
1:C:413:SER:OG	1:C:414:THR:N	2.52	0.43
1:L:390:ARG:O	1:L:434:VAL:HA	2.18	0.43
1:E:428:MET:HE3	1:E:428:MET:HB3	1.89	0.43
1:G:495:GLU:OE2	1:G:515:LYS:NZ	2.44	0.43
1:B:530:THR:HG22	1:B:531:SER:N	2.34	0.43
1:B:553:ARG:HH21	1:D:483:ASP:CG	2.23	0.43
1:G:542:ARG:O	1:G:545:VAL:HG12	2.19	0.43
1:F:513:LEU:HD12	1:F:513:LEU:HA	1.81	0.42
1:H:482:LYS:HE3	1:H:528:HIS:ND1	2.34	0.42
1:L:425:PHE:HE2	1:L:455:PRO:HD3	1.84	0.42
1:J:412:CYS:HB3	1:J:470:TRP:CD2	2.54	0.42
1:A:513:LEU:HD23	1:E:431:LYS:HE3	2.01	0.42
1:F:395:LYS:HZ3	1:F:395:LYS:HB3	1.84	0.42
1:A:530:THR:CG2	1:C:556:ARG:HH11	2.32	0.42
1:H:394:ILE:HG13	1:H:436:LEU:HB3	2.01	0.42
1:G:513:LEU:HD12	1:G:513:LEU:HA	1.87	0.42
1:L:471:LYS:HB3	1:L:471:LYS:HE3	1.68	0.42
1:B:551:LYS:HD3	1:B:551:LYS:C	2.40	0.42
1:E:386:LEU:O	1:E:517:LYS:HE2	2.20	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:I:535:ASP:O	1:I:538:HIS:HB3	2.19	0.42
1:L:499:ASN:HD22	1:L:499:ASN:HA	1.66	0.42
1:C:506:ARG:NH1	1:I:419:LYS:NZ	2.68	0.42
1:F:412:CYS:HB3	1:F:470:TRP:CD2	2.55	0.42
1:I:378:ASN:ND2	1:I:481:VAL:H	2.01	0.42
1:A:395:LYS:HA	1:A:439:SER:O	2.20	0.42
1:I:368:LEU:HB2	1:I:536:PHE:CD1	2.54	0.42
1:A:425:PHE:CE2	1:A:455:PRO:HD3	2.55	0.41
1:F:530:THR:HG22	1:F:531:SER:N	2.35	0.41
1:B:375:HIS:HD2	1:B:477:GLN:HE22	1.67	0.41
1:F:437:LEU:HD13	1:F:519:VAL:HG11	2.02	0.41
1:H:365:HIS:HD2	1:H:367:VAL:H	1.68	0.41
1:E:542:ARG:O	1:E:546:VAL:HG23	2.20	0.41
1:H:431:LYS:N	1:H:431:LYS:HD2	2.35	0.41
1:L:383:GLU:HG3	1:L:383:GLU:O	2.21	0.41
1:K:494:LEU:HD21	1:K:502:VAL:HG23	2.02	0.41
1:B:431:LYS:HD2	1:B:431:LYS:H	1.84	0.41
1:D:374:ALA:O	1:F:548:VAL:HG21	2.21	0.41
1:F:368:LEU:HB2	1:F:536:PHE:CD1	2.56	0.41
1:C:405:SER:HB2	1:C:411:TRP:CE3	2.55	0.41
1:C:495:GLU:CD	1:C:495:GLU:H	2.22	0.41
1:E:415:GLU:OE2	1:E:471:LYS:HE2	2.20	0.41
1:J:365:HIS:N	3:J:705:HOH:O	2.54	0.41
1:F:452:MET:HG3	1:F:474:PHE:CD1	2.55	0.41
1:H:391:VAL:HG21	1:H:516:ALA:HB1	2.03	0.41
1:A:482:LYS:HE3	1:A:528:HIS:ND1	2.36	0.41
1:B:365:HIS:HD2	1:B:367:VAL:H	1.67	0.41
1:G:437:LEU:HD13	1:G:519:VAL:HG11	2.02	0.41
1:I:410:ILE:HG13	1:I:470:TRP:HZ3	1.86	0.41
1:K:391:VAL:HG22	1:K:511:VAL:HB	2.02	0.41
1:K:538:HIS:NE2	1:K:542:ARG:HD2	2.36	0.41
1:D:413:SER:OG	1:D:414:THR:N	2.54	0.41
1:B:404:ARG:NH1	1:B:465:TRP:O	2.54	0.40
1:F:378:ASN:O	1:F:380:LYS:CE	2.69	0.40
1:H:431:LYS:HD2	1:H:431:LYS:H	1.86	0.40
1:J:368:LEU:HD11	1:J:372:LYS:HE3	2.03	0.40
1:E:453:LYS:HA	1:E:453:LYS:HD2	1.83	0.40
1:K:542:ARG:O	1:K:546:VAL:HG23	2.22	0.40
1:L:368:LEU:HB2	1:L:536:PHE:CE1	2.57	0.40
1:G:488:GLN:O	1:G:491:HIS:HE1	2.05	0.40
1:E:482:LYS:HB2	1:E:528:HIS:CG	2.57	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:535:ASP:O	1:E:538:HIS:HB3	2.22	0.40
1:K:537:ALA:O	1:K:541:LYS:N	2.49	0.40
1:E:367:VAL:HG23	1:E:536:PHE:CE1	2.56	0.40
1:L:552:GLU:O	1:L:556:ARG:HG3	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	Perce	entiles
1	А	186/200~(93%)	178 (96%)	8 (4%)	0	100	100
1	В	194/200~(97%)	188 (97%)	6 (3%)	0	100	100
1	С	180/200~(90%)	175 (97%)	5(3%)	0	100	100
1	D	181/200 (90%)	175 (97%)	6 (3%)	0	100	100
1	Е	183/200~(92%)	177 (97%)	6 (3%)	0	100	100
1	F	182/200~(91%)	176 (97%)	5 (3%)	1 (0%)	29	48
1	G	180/200~(90%)	175 (97%)	5(3%)	0	100	100
1	Н	182/200~(91%)	179 (98%)	3 (2%)	0	100	100
1	Ι	183/200~(92%)	176 (96%)	7 (4%)	0	100	100
1	J	181/200 (90%)	176 (97%)	5(3%)	0	100	100
1	Κ	181/200~(90%)	176 (97%)	5(3%)	0	100	100
1	L	178/200~(89%)	174 (98%)	4 (2%)	0	100	100
All	All	2191/2400 (91%)	2125 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	F	366	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Rotameric Outliers		Percentiles		
1	А	175/182~(96%)	172~(98%)	3~(2%)	60	82		
1	В	179/182~(98%)	178~(99%)	1 (1%)	86	95		
1	С	170/182~(93%)	168~(99%)	2(1%)	71	88		
1	D	171/182~(94%)	170~(99%)	1 (1%)	86	95		
1	Ε	172/182~(94%)	172 (100%)	0	100	100		
1	F	172/182~(94%)	168~(98%)	4 (2%)	50	76		
1	G	169/182~(93%)	165~(98%)	4 (2%)	49	74		
1	Н	171/182~(94%)	167~(98%)	4 (2%)	50	76		
1	Ι	172/182~(94%)	170~(99%)	2(1%)	71	88		
1	J	171/182~(94%)	164~(96%)	7 (4%)	30	55		
1	Κ	171/182~(94%)	166~(97%)	5(3%)	42	69		
1	L	$16\overline{8/182} \ (92\overline{\%})$	$1\overline{65}\ (98\%)$	$\overline{3(2\%)}$	59	81		
All	All	2061/2184~(94%)	2025 (98%)	36(2%)	60	82		

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	381	GLU
1	А	529	THR
1	А	531	SER
1	В	460	THR
1	С	495	GLU
1	С	525	SER
1	D	380	LYS
1	F	364	SER
1	F	395	LYS
1	F	469	LYS



Mol	Chain	Res	Type
1	F	504	ASN
1	G	430	SER
1	G	545	VAL
1	G	553	ARG
1	G	557	ASN
1	Н	386	LEU
1	Н	493	ARG
1	Н	551	LYS
1	Н	558	LYS
1	Ι	364	SER
1	Ι	493	ARG
1	J	376	SER
1	J	397[A]	TYR
1	J	397[B]	TYR
1	J	404	ARG
1	J	557	ASN
1	J	558	LYS
1	J	559	GLN
1	K	380	LYS
1	Κ	391	VAL
1	K	419	LYS
1	К	473	LYS
1	К	550	ARG
1	L	499	ASN
1	L	552	GLU
1	L	554	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	365	HIS
1	А	375	HIS
1	А	554	GLN
1	А	559	GLN
1	В	365	HIS
1	В	375	HIS
1	В	538	HIS
1	D	477	GLN
1	Е	375	HIS
1	Е	441	ASN
1	Е	477	GLN
1	Е	538	HIS



Mol	Chain	Res	Type
1	F	365	HIS
1	F	385	ASN
1	F	403	HIS
1	F	499	ASN
1	G	365	HIS
1	Н	365	HIS
1	Н	375	HIS
1	Н	441	ASN
1	Ι	378	ASN
1	J	365	HIS
1	J	416	HIS
1	J	487	ASN
1	J	538	HIS
1	J	557	ASN
1	K	365	HIS
1	К	375	HIS
1	L	488	GLN
1	L	499	ASN
1	L	509	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)

12 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



Mal	Trune	Chain	Dec	Tinle	B	ond leng	gths	E	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SCN	D	601	-	1,2,2	0.89	0	$0,\!1,\!1$	-	-
2	SCN	Н	601	-	1,2,2	1.03	0	0,1,1	-	-
2	SCN	F	601	-	1,2,2	0.88	0	$0,\!1,\!1$	-	-
2	SCN	G	601	-	1,2,2	0.96	0	$0,\!1,\!1$	-	-
2	SCN	Ι	601	-	1,2,2	0.77	0	0,1,1	-	-
2	SCN	K	601	-	1,2,2	0.93	0	$0,\!1,\!1$	-	-
2	SCN	J	601	-	1,2,2	0.79	0	$0,\!1,\!1$	-	-
2	SCN	L	601	-	1,2,2	0.72	0	$0,\!1,\!1$	-	-
2	SCN	В	601	-	1,2,2	0.88	0	0,1,1	-	-
2	SCN	С	601	-	1,2,2	0.85	0	0,1,1	-	-
2	SCN	А	601	-	1,2,2	0.88	0	0,1,1	-	-
2	SCN	E	601	-	1,2,2	0.75	0	0,1,1	-	-

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).

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	SCN	1	0
2	Ι	601	SCN	1	0
2	L	601	SCN	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 (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RS	RZ>	>2	$OWAB(Å^2)$	Q<0.9
1	А	189/200~(94%)	-0.23	0 100	1	00	29, 46, 80, 111	0
1	В	195/200~(97%)	-0.20	1 (0%)	91	91	30, 52, 83, 95	0
1	С	183/200~(91%)	-0.09	2 (1%)	80	82	35, 49, 86, 107	0
1	D	184/200~(92%)	-0.29	1 (0%)	91	91	35, 55, 91, 102	0
1	Е	186/200~(93%)	-0.14	2 (1%)	80	82	36, 59, 95, 119	0
1	F	185/200~(92%)	-0.26	2 (1%)	80	82	42, 56, 92, 110	0
1	G	184/200~(92%)	-0.13	1 (0%)	91	91	40, 60, 96, 119	0
1	Н	186/200~(93%)	-0.06	3 (1%)	72	74	41, 71, 98, 122	0
1	Ι	186/200~(93%)	-0.04	3 (1%)	72	74	40, 64, 96, 107	0
1	J	184/200~(92%)	-0.18	1 (0%)	91	91	45, 59, 90, 105	0
1	Κ	185/200~(92%)	-0.00	2(1%)	80	82	44, 68, 94, 103	0
1	L	$18\overline{2}/200~(91\%)$	0.08	2 (1%)	80	82	50, 73, 114, 128	0
All	All	2229/2400~(92%)	-0.13	20 (0%)	84	86	29, 59, 95, 128	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	471	LYS	4.3
1	D	470	TRP	3.6
1	Κ	397	TYR	3.6
1	F	470	TRP	3.3
1	С	471	LYS	3.2
1	J	470	TRP	3.2
1	Е	367	VAL	2.8
1	Ι	397[A]	TYR	2.8
1	В	397[A]	TYR	2.8
1	Н	397	TYR	2.8
1	L	470	TRP	2.6



Mol	Chain	Res	Type	RSRZ
1	Е	397[A]	TYR	2.5
1	Ι	471	LYS	2.4
1	Κ	533	PHE	2.4
1	Н	381	GLU	2.4
1	Н	380	LYS	2.3
1	G	548	VAL	2.3
1	С	397[A]	TYR	2.1
1	Ι	365	HIS	2.0
1	F	397[A]	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	SCN	Н	601	3/3	0.87	0.30	$95,\!95,\!97,\!98$	0
2	SCN	K	601	3/3	0.91	0.24	110,110,120,135	0
2	SCN	Е	601	3/3	0.92	0.36	126,126,132,144	0
2	SCN	J	601	3/3	0.95	0.23	97,97,101,104	0
2	SCN	L	601	3/3	0.95	0.31	77,77,82,96	0
2	SCN	F	601	3/3	0.96	0.14	55,55,69,84	0
2	SCN	G	601	3/3	0.97	0.23	63,63,78,84	0
2	SCN	А	601	3/3	0.97	0.17	67,67,77,82	0
2	SCN	Ι	601	3/3	0.97	0.25	71,71,77,86	0
2	SCN	В	601	3/3	0.98	0.25	72,72,83,92	0
2	SCN	D	601	3/3	0.98	0.16	47,47,57,67	0
2	SCN	С	601	3/3	0.99	0.18	64,64,70,75	0



6.5 Other polymers (i)

There are no such residues in this entry.

