



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2017 – 08:27 AM EDT

PDB ID : 2CE8  
Title : An EH1 peptide bound to the Groucho-TLE WD40 domain.  
Authors : Pickles, L.M.; Roe, S.M.; Pearl, L.H.  
Deposited on : 2006-02-03  
Resolution : 2.03 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029077

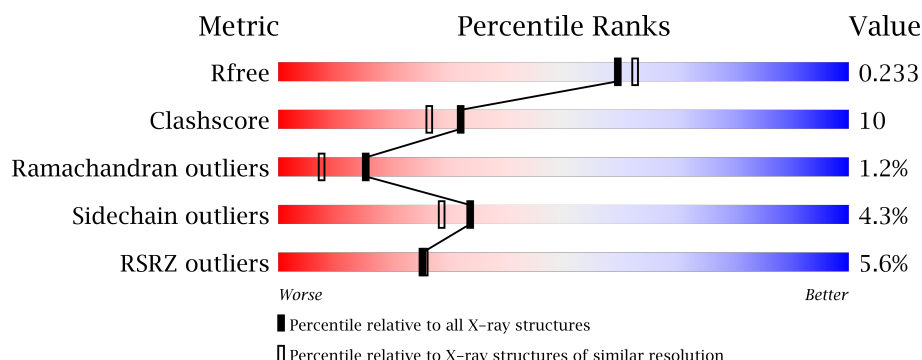
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	337	<div> <div>4%</div> <div>83%</div> <div>16%</div> <div>..</div> </div>
1	B	337	<div> <div>5%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
1	C	337	<div> <div>4%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	D	337	<div> <div>7%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	X	9	<div> <div>44%</div> <div>56%</div> <div>22%</div> <div>22%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Y	9	 A horizontal bar chart showing the quality of chain Y. The bar is divided into four segments: red (44%), green (56%), yellow (33%), and orange (11%). The percentages are labeled above or below the segments. The red segment is the largest, followed by green, then yellow, and finally orange.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 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 TRANSDUCIN-LIKE ENHANCER PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	B	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	C	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			
1	D	337	Total	C	N	O	S	0	0	0
			2587	1628	445	497	17			

- Molecule 2 is a protein called EH1 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	9	Total	C	N	O	S	0	0	0
			70	46	10	13	1			
2	Y	9	Total	C	N	O	S	0	0	0
			70	46	10	13	1			

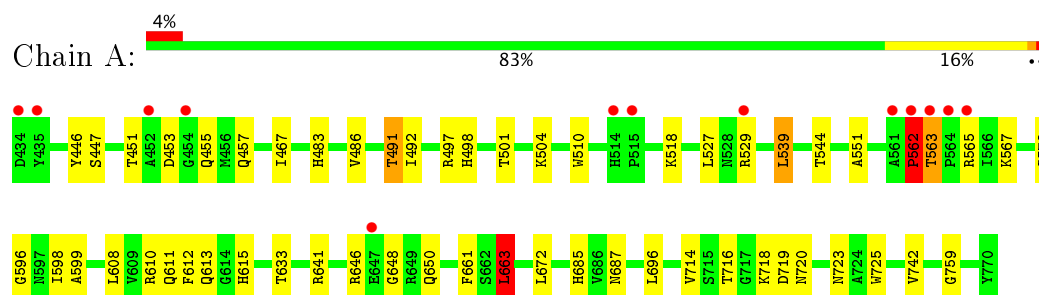
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total	O	0	0
			291	291		
3	B	279	Total	O	0	0
			279	279		
3	C	265	Total	O	0	0
			265	265		
3	D	235	Total	O	0	0
			235	235		
3	X	4	Total	O	0	0
			4	4		
3	Y	3	Total	O	0	0
			3	3		

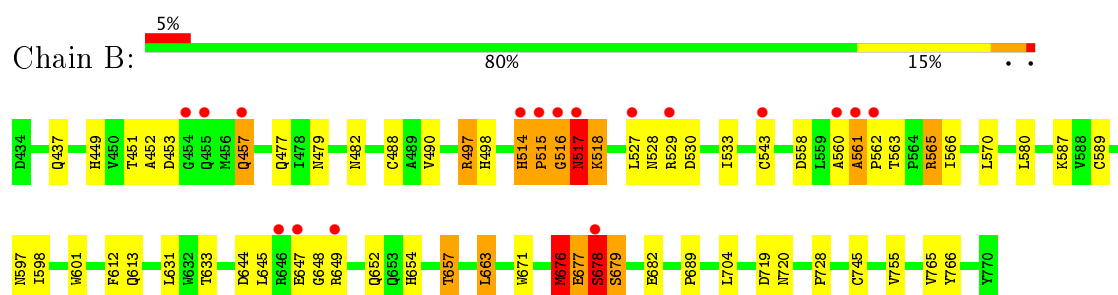
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

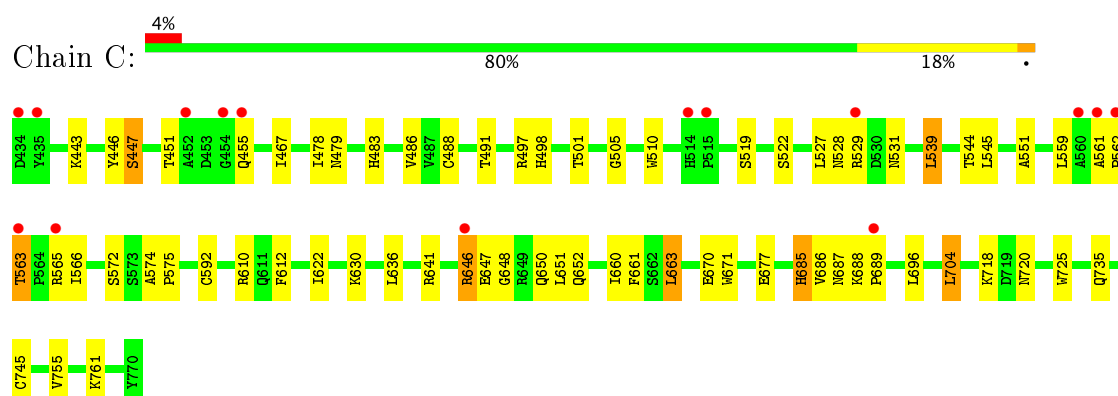
#### • Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1



#### • Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

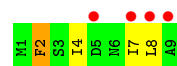


#### • Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1



#### • Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.58Å 56.35Å 125.25Å 90.00° 112.32° 90.00°	Depositor
Resolution (Å)	116.25 – 2.03 31.84 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.4 (116.25-2.03) 96.5 (31.84-2.03)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.238 0.178 , 0.233	Depositor DCC
$R_{free}$ test set	4378 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 82.34 % 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 2.8585e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.88	0/2653	0.84	1/3612 (0.0%)
1	B	0.90	1/2653 (0.0%)	0.90	6/3612 (0.2%)
1	C	0.83	0/2653	0.80	1/3612 (0.0%)
1	D	0.83	0/2653	0.90	6/3612 (0.2%)
2	X	0.75	0/70	0.93	0/93
2	Y	0.69	0/70	0.83	0/93
All	All	0.86	1/10752 (0.0%)	0.86	14/14634 (0.1%)

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	1
1	B	0	2
1	D	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	677	GLU	CG-CD	5.46	1.60	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	663	LEU	CA-CB-CG	9.15	136.35	115.30
1	D	704	LEU	CA-CB-CG	7.56	132.70	115.30
1	B	663	LEU	CA-CB-CG	7.38	132.27	115.30
1	C	704	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	663	LEU	CA-CB-CG	6.69	130.69	115.30
1	D	519	SER	C-N-CD	-6.48	106.35	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	562	PRO	C-N-CA	6.12	137.00	121.70
1	B	704	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	678	SER	CA-CB-OG	-6.01	94.98	111.20
1	B	678	SER	N-CA-CB	5.68	119.03	110.50
1	B	678	SER	CB-CA-C	-5.58	99.50	110.10
1	B	676	MET	CG-SD-CE	-5.54	91.33	100.20
1	D	704	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	D	616	THR	C-N-CA	-5.10	108.95	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	PRO	Peptide
1	B	514	HIS	Peptide
1	B	516	GLY	Peptide
1	D	518	LYS	Peptide
1	D	559	LEU	Peptide
1	D	562	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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	2587	0	2503	42	0
1	B	2587	0	2503	51	0
1	C	2587	0	2503	49	0
1	D	2587	0	2503	65	0
2	X	70	0	73	5	0
2	Y	70	0	73	6	0
3	A	291	0	0	13	0
3	B	279	0	0	11	0
3	C	265	0	0	10	0
3	D	235	0	0	12	1
3	X	4	0	0	0	0
3	Y	3	0	0	0	0
All	All	11565	0	10158	208	1

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 10.

All (208) 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:518:LYS:CB	1:D:519:SER:HB2	1.51	1.39
1:D:518:LYS:HB3	1:D:519:SER:CB	1.78	1.11
1:B:649:ARG:HD3	3:B:2140:HOH:O	1.54	1.06
1:A:562:PRO:HB2	1:A:563:THR:CB	1.91	1.01
1:A:562:PRO:CB	1:A:563:THR:HB	1.90	1.00
1:A:562:PRO:HB2	1:A:563:THR:HB	0.98	0.97
1:D:518:LYS:HB3	1:D:519:SER:HB2	0.97	0.96
1:D:485:GLU:HG2	1:D:504:LYS:HB3	1.45	0.94
1:D:560:ALA:HB3	1:D:561:ALA:HB3	1.47	0.94
1:B:515:PRO:O	1:B:517:ASN:ND2	2.00	0.94
1:D:518:LYS:CA	1:D:519:SER:HB2	1.98	0.94
1:C:447:SER:H	1:D:437:GLN:HE22	1.18	0.92
1:D:749:VAL:HG22	3:D:2045:HOH:O	1.71	0.91
1:B:649:ARG:HB3	3:B:2167:HOH:O	1.72	0.89
1:B:543:CYS:SG	3:B:2092:HOH:O	2.29	0.88
1:D:519:SER:HB3	1:D:520:PRO:HA	1.56	0.86
1:B:652:GLN:HE21	1:B:654:HIS:HE1	1.23	0.85
1:D:560:ALA:HB3	1:D:561:ALA:CB	2.08	0.83
1:A:611:GLN:HE21	1:A:613:GLN:HE21	1.26	0.82
1:D:518:LYS:CB	1:D:519:SER:CB	2.46	0.81
1:D:519:SER:HB3	1:D:520:PRO:CA	2.10	0.80
1:B:515:PRO:HB2	1:B:516:GLY:HA3	1.64	0.80
1:A:447:SER:H	1:B:437:GLN:HE22	1.31	0.79
1:D:510:TRP:CE3	1:D:518:LYS:HB2	2.17	0.79
1:B:490:VAL:HB	3:B:2052:HOH:O	1.83	0.78
1:D:676:MET:HE3	1:D:682:GLU:HG3	1.65	0.77
1:B:652:GLN:NE2	1:B:654:HIS:HE1	1.83	0.77
1:B:652:GLN:HE21	1:B:654:HIS:CE1	2.03	0.76
1:D:558:ASP:OD1	1:D:560:ALA:HB2	1.86	0.76
1:B:517:ASN:O	1:B:518:LYS:HB2	1.88	0.74
1:C:562:PRO:HA	1:C:563:THR:C	2.10	0.72
1:B:482:ASN:ND2	3:B:2046:HOH:O	2.22	0.71
1:D:560:ALA:CB	1:D:561:ALA:HB3	2.22	0.69
1:C:446:TYR:H	1:D:437:GLN:NE2	1.90	0.69
1:B:449:HIS:O	1:B:457:GLN:NE2	2.25	0.69
1:C:641:ARG:HH11	1:C:650:GLN:HE22	1.41	0.68
1:B:560:ALA:N	1:B:561:ALA:HB2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ILE:HG21	3:A:2269:HOH:O	1.91	0.68
1:A:611:GLN:HE21	1:A:613:GLN:NE2	1.90	0.68
1:B:517:ASN:OD1	1:B:518:LYS:N	2.28	0.67
1:A:687:ASN:HB3	3:A:2222:HOH:O	1.94	0.67
1:B:631:LEU:HB2	1:B:645:LEU:HD21	1.76	0.66
1:A:446:TYR:H	1:B:437:GLN:NE2	1.93	0.66
1:C:491:THR:HG21	3:C:2085:HOH:O	1.96	0.66
1:D:460:PRO:HB2	3:D:2016:HOH:O	1.95	0.66
1:D:485:GLU:HG2	1:D:504:LYS:CB	2.23	0.65
2:X:2:PHE:O	2:X:2:PHE:HD1	1.79	0.65
1:B:649:ARG:HD2	3:B:2167:HOH:O	1.97	0.65
1:D:676:MET:CE	1:D:682:GLU:HG3	2.27	0.65
2:X:2:PHE:O	2:X:2:PHE:CD1	2.50	0.64
1:D:451:THR:HG22	1:D:452:ALA:H	1.62	0.64
1:A:529:ARG:HG3	3:A:2088:HOH:O	1.97	0.64
1:C:455:GLN:N	3:C:2016:HOH:O	2.31	0.63
1:A:539:LEU:HG	1:A:544:THR:HB	1.79	0.63
1:D:562:PRO:HB2	1:D:563:THR:HB	1.80	0.63
1:A:612:PHE:HE2	1:A:648:GLY:HA2	1.65	0.62
1:D:562:PRO:HB2	1:D:563:THR:CG2	2.30	0.62
1:B:644:ASP:HB3	1:B:647:GLU:HB2	1.81	0.61
1:A:483:HIS:HD2	1:A:501:THR:OG1	1.83	0.61
1:D:510:TRP:CZ3	1:D:518:LYS:HB2	2.36	0.60
1:D:510:TRP:HE3	1:D:518:LYS:HB2	1.61	0.60
1:C:612:PHE:HE2	1:C:648:GLY:HA2	1.66	0.60
1:C:528:ASN:HB3	1:C:531:ASN:ND2	2.16	0.60
1:B:518:LYS:HE3	3:B:2042:HOH:O	2.00	0.60
1:B:558:ASP:HB3	1:B:565:ARG:HG3	1.83	0.60
1:D:451:THR:HG22	1:D:452:ALA:N	2.16	0.59
1:D:562:PRO:HB2	1:D:563:THR:HG22	1.84	0.59
1:D:497:ARG:NH1	3:D:2047:HOH:O	2.35	0.59
1:B:652:GLN:NE2	1:B:654:HIS:CE1	2.66	0.58
1:D:510:TRP:HE3	1:D:518:LYS:CB	2.15	0.58
1:D:514:HIS:HD2	3:D:2053:HOH:O	1.85	0.58
1:C:483:HIS:HD2	1:C:501:THR:OG1	1.86	0.58
1:A:491:THR:HG21	3:A:2096:HOH:O	2.03	0.58
1:D:617:ASP:HB2	3:D:2126:HOH:O	2.04	0.58
1:C:527:LEU:HD22	1:C:551:ALA:HB3	1.86	0.57
1:D:562:PRO:HB2	1:D:563:THR:CB	2.34	0.57
1:A:457:GLN:NE2	3:A:2020:HOH:O	2.38	0.57
1:B:452:ALA:HB2	1:B:689:PRO:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ARG:HH11	1:A:650:GLN:HE22	1.53	0.56
1:D:482:ASN:ND2	3:D:2035:HOH:O	2.38	0.55
1:C:761:LYS:HD3	3:C:2255:HOH:O	2.06	0.55
1:B:515:PRO:CB	1:B:516:GLY:HA3	2.36	0.55
1:B:648:GLY:O	1:B:649:ARG:HG2	2.07	0.55
1:C:528:ASN:HB3	1:C:531:ASN:HD22	1.69	0.55
1:B:561:ALA:H	1:B:562:PRO:HA	1.73	0.54
1:C:497:ARG:HB3	3:C:2054:HOH:O	2.06	0.54
2:Y:2:PHE:CD2	2:Y:7:ILE:HD11	2.42	0.54
1:A:687:ASN:CG	3:A:2222:HOH:O	2.45	0.54
1:A:572:SER:HB2	3:A:2177:HOH:O	2.07	0.53
1:D:622:ILE:HD11	1:D:631:LEU:HD11	1.89	0.53
1:A:585:ASP:O	1:A:586:SER:HB2	2.08	0.53
1:C:539:LEU:HG	1:C:544:THR:HB	1.91	0.53
1:C:661:PHE:CE1	1:C:677:GLU:HB2	2.43	0.53
1:C:451:THR:OG1	1:C:455:GLN:HB3	2.09	0.52
2:Y:2:PHE:CD1	2:Y:2:PHE:O	2.63	0.52
1:C:479:ASN:HB3	3:C:2038:HOH:O	2.09	0.52
1:D:480:THR:H	1:D:517:ASN:ND2	2.08	0.52
1:C:486:VAL:HG21	2:Y:8:LEU:HD21	1.91	0.52
1:C:572:SER:HB2	3:C:2155:HOH:O	2.09	0.52
1:A:687:ASN:CB	3:A:2222:HOH:O	2.57	0.52
1:B:580:LEU:HD22	1:B:589:CYS:SG	2.50	0.51
1:D:572:SER:HB2	3:D:2093:HOH:O	2.10	0.51
1:B:517:ASN:OD1	1:B:518:LYS:CA	2.59	0.51
1:D:479:ASN:HB2	1:D:765:VAL:HB	1.93	0.51
1:D:563:THR:HG23	1:D:563:THR:O	2.11	0.51
1:B:677:GLU:O	1:B:678:SER:C	2.46	0.50
1:D:453:ASP:N	1:D:453:ASP:OD1	2.42	0.50
1:D:529:ARG:HD3	3:D:2070:HOH:O	2.10	0.50
1:C:652:GLN:NE2	1:C:687:ASN:OD1	2.43	0.50
1:B:497:ARG:HD3	1:B:498:HIS:CE1	2.46	0.49
1:B:678:SER:OG	1:B:679:SER:N	2.34	0.49
1:C:646:ARG:HG2	1:C:647:GLU:HG3	1.94	0.49
1:A:497:ARG:HB3	3:A:2061:HOH:O	2.12	0.49
1:A:696:LEU:HB2	1:A:725:TRP:CH2	2.48	0.49
1:D:481:LEU:CD2	1:D:518:LYS:HG3	2.43	0.49
1:D:556:ILE:HD12	1:D:568:ALA:HB3	1.93	0.49
1:B:597:ASN:OD1	1:B:613:GLN:HG2	2.13	0.49
1:D:477:GLN:HB3	3:D:2032:HOH:O	2.13	0.48
1:A:504:LYS:HE3	1:A:529:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ILE:HB	1:B:612:PHE:HB2	1.95	0.48
1:D:678:SER:O	1:D:679:SER:CB	2.61	0.48
1:B:479:ASN:HB2	1:B:765:VAL:HB	1.96	0.48
1:B:676:MET:CE	1:B:682:GLU:HG3	2.43	0.47
1:D:518:LYS:CA	1:D:519:SER:CB	2.83	0.47
1:A:486:VAL:HG13	1:A:759:GLY:HA2	1.95	0.47
1:C:483:HIS:HE1	3:C:2058:HOH:O	1.98	0.47
1:B:517:ASN:OD1	1:B:518:LYS:HA	2.14	0.47
1:D:450:VAL:HG22	1:D:456:MET:HG2	1.96	0.47
1:A:718:LYS:HE2	2:X:7:ILE:O	2.15	0.47
1:A:716:THR:HB	1:A:742:VAL:HB	1.97	0.47
1:D:540:PRO:HD2	1:D:586:SER:OG	2.14	0.47
1:C:670:GLU:HG2	1:C:685:HIS:CE1	2.50	0.47
1:D:719:ASP:O	1:D:720:ASN:HB2	2.15	0.47
1:C:641:ARG:HH11	1:C:650:GLN:NE2	2.11	0.46
1:B:649:ARG:CD	3:B:2140:HOH:O	2.35	0.46
1:C:663:LEU:C	1:C:663:LEU:HD12	2.35	0.46
1:A:567:LYS:NZ	3:A:2111:HOH:O	2.44	0.46
1:C:630:LYS:HE3	1:C:651:LEU:CD1	2.45	0.46
1:D:676:MET:HE3	1:D:682:GLU:CG	2.43	0.46
1:C:641:ARG:NH1	1:C:650:GLN:HE22	2.10	0.46
1:D:642:SER:HB3	1:D:652:GLN:H	1.81	0.46
1:D:519:SER:CB	1:D:520:PRO:CA	2.88	0.46
1:C:610:ARG:HD2	3:C:2134:HOH:O	2.16	0.46
1:D:673:ALA:HB3	1:D:704:LEU:HD21	1.98	0.45
1:A:663:LEU:HD13	1:A:672:LEU:HD11	1.98	0.45
1:C:696:LEU:HB2	1:C:725:TRP:CH2	2.52	0.45
1:B:560:ALA:HB3	1:B:561:ALA:HA	1.97	0.45
1:C:562:PRO:HA	1:C:563:THR:O	2.16	0.45
1:A:661:PHE:CD2	2:X:2:PHE:HE2	2.34	0.45
1:D:519:SER:N	3:D:2055:HOH:O	2.08	0.45
1:D:587:LYS:HG3	3:D:2114:HOH:O	2.17	0.45
1:C:478:ILE:HG13	1:C:479:ASN:HD22	1.82	0.45
1:B:527:LEU:HD22	3:B:2154:HOH:O	2.17	0.44
1:D:481:LEU:HD22	1:D:518:LYS:HG3	1.99	0.44
1:B:719:ASP:O	1:B:720:ASN:HB2	2.17	0.44
1:C:545:LEU:HB2	1:C:559:LEU:HD11	1.98	0.44
1:B:457:GLN:HG2	3:B:2024:HOH:O	2.17	0.44
2:X:4:ILE:HG22	2:X:8:LEU:HD22	1.98	0.44
1:C:498:HIS:HA	1:C:510:TRP:O	2.18	0.44
1:C:630:LYS:HE3	1:C:651:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:LEU:HD22	1:D:659:GLN:HE21	1.83	0.44
1:C:661:PHE:CD2	2:Y:2:PHE:CE2	3.05	0.44
1:A:518:LYS:HD2	3:A:2074:HOH:O	2.17	0.44
1:A:498:HIS:HA	1:A:510:TRP:O	2.19	0.43
1:C:689:PRO:HD2	3:C:2205:HOH:O	2.18	0.43
1:B:477:GLN:HG2	1:B:766:TYR:CE2	2.54	0.43
1:B:671:TRP:CD2	1:B:728:PRO:HB3	2.54	0.43
1:D:644:ASP:HB3	1:D:647:GLU:HB2	2.00	0.43
1:B:657:THR:HG21	3:B:2176:HOH:O	2.18	0.43
1:C:660:ILE:HD12	1:C:660:ILE:N	2.33	0.43
1:A:610:ARG:NE	3:A:2144:HOH:O	2.51	0.43
1:B:488:CYS:HB2	1:B:533:ILE:O	2.18	0.43
1:A:719:ASP:O	1:A:720:ASN:HB2	2.19	0.42
1:C:443:LYS:NZ	1:C:735:GLN:HE22	2.18	0.42
1:C:505:GLY:HA3	1:C:529:ARG:HA	2.01	0.42
1:C:443:LYS:HZ1	1:C:735:GLN:HE22	1.66	0.42
1:B:598:ILE:HG13	1:B:633:THR:HG21	2.01	0.42
1:D:598:ILE:HB	1:D:612:PHE:HB2	2.02	0.42
1:B:570:LEU:HB3	1:B:601:TRP:CZ3	2.55	0.41
1:B:645:LEU:HA	1:B:645:LEU:HD23	1.72	0.41
1:A:650:GLN:NE2	3:A:2179:HOH:O	2.46	0.41
1:D:638:ASN:ND2	3:D:2144:HOH:O	2.53	0.41
1:C:686:VAL:O	1:C:687:ASN:HB2	2.21	0.41
1:A:714:VAL:HA	1:A:723:ASN:O	2.20	0.41
1:C:592:CYS:SG	1:C:622:ILE:HB	2.60	0.41
1:C:720:ASN:N	1:C:720:ASN:HD22	2.19	0.41
1:D:540:PRO:CD	1:D:586:SER:OG	2.69	0.41
1:B:529:ARG:HH11	1:B:529:ARG:HG2	1.84	0.41
1:D:488:CYS:HB2	1:D:533:ILE:O	2.21	0.41
1:A:599:ALA:HB1	1:A:608:LEU:CD1	2.50	0.41
1:A:641:ARG:HH11	1:A:650:GLN:NE2	2.19	0.41
1:A:598:ILE:CD1	1:A:633:THR:HG21	2.50	0.41
1:D:443:LYS:NZ	1:D:735:GLN:HE22	2.17	0.41
1:C:565:ARG:HG2	3:C:2098:HOH:O	2.21	0.41
1:D:716:THR:HB	1:D:742:VAL:HB	2.03	0.41
1:C:636:LEU:HD11	2:Y:2:PHE:CD1	2.56	0.41
1:B:745:CYS:HA	1:B:755:VAL:O	2.20	0.40
1:C:670:GLU:HB3	1:C:671:TRP:CD1	2.56	0.40
1:C:745:CYS:HA	1:C:755:VAL:O	2.21	0.40
1:A:451:THR:O	1:A:453:ASP:O	2.39	0.40
1:A:598:ILE:HD12	1:A:633:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:GLY:O	1:A:615:HIS:HB2	2.21	0.40
1:C:488:CYS:SG	2:Y:4:ILE:HG13	2.61	0.40
1:A:527:LEU:HD22	1:A:551:ALA:HB3	2.02	0.40
1:B:451:THR:O	1:B:453:ASP:O	2.39	0.40
1:C:574:ALA:HA	1:C:575:PRO:HD3	1.92	0.40
1:D:528:ASN:HB3	1:D:531:ASN:ND2	2.35	0.40
1:D:574:ALA:HA	1:D:575:PRO:HD3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2052:HOH:O	3:D:2220:HOH:O[2_645]	1.84	0.36

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	335/337 (99%)	322 (96%)	12 (4%)	1 (0%)	44	39
1	B	335/337 (99%)	311 (93%)	16 (5%)	8 (2%)	7	2
1	C	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	44	39
1	D	335/337 (99%)	313 (93%)	16 (5%)	6 (2%)	10	3
2	X	7/9 (78%)	7 (100%)	0	0	100	100
2	Y	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1354/1366 (99%)	1277 (94%)	61 (4%)	16 (1%)	15	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	PRO

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Mol	Chain	Res	Type
1	B	514	HIS
1	B	515	PRO
1	B	517	ASN
1	B	518	LYS
1	B	679	SER
1	D	514	HIS
1	D	519	SER
1	D	562	PRO
1	B	561	ALA
1	D	542	GLY
1	D	679	SER
1	B	497	ARG
1	D	563	THR
1	B	678	SER
1	C	561	ALA

### 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	288/288 (100%)	279 (97%)	9 (3%)	45	43
1	B	288/288 (100%)	277 (96%)	11 (4%)	38	34
1	C	288/288 (100%)	275 (96%)	13 (4%)	32	27
1	D	288/288 (100%)	274 (95%)	14 (5%)	29	23
2	X	8/8 (100%)	6 (75%)	2 (25%)	1	0
2	Y	8/8 (100%)	7 (88%)	1 (12%)	5	2
All	All	1168/1168 (100%)	1118 (96%)	50 (4%)	33	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	A	467	ILE
1	A	491	THR

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Mol	Chain	Res	Type
1	A	539	LEU
1	A	563	THR
1	A	565	ARG
1	A	646	ARG
1	A	663	LEU
1	A	685	HIS
1	B	457	GLN
1	B	517	ASN
1	B	528	ASN
1	B	530	ASP
1	B	563	THR
1	B	565	ARG
1	B	566	ILE
1	B	587	LYS
1	B	657	THR
1	B	663	LEU
1	B	676	MET
1	C	447	SER
1	C	467	ILE
1	C	519	SER
1	C	522	SER
1	C	539	LEU
1	C	563	THR
1	C	566	ILE
1	C	646	ARG
1	C	663	LEU
1	C	685	HIS
1	C	688	LYS
1	C	704	LEU
1	C	718	LYS
1	D	453	ASP
1	D	491	THR
1	D	519	SER
1	D	527	LEU
1	D	540	PRO
1	D	563	THR
1	D	565	ARG
1	D	577	CYS
1	D	660	ILE
1	D	663	LEU
1	D	676	MET
1	D	677	GLU

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Mol	Chain	Res	Type
1	D	688	LYS
1	D	741	SER
2	X	2	PHE
2	X	8	LEU
2	Y	2	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	ASN
1	A	483	HIS
1	A	531	ASN
1	A	613	GLN
1	A	650	GLN
1	A	652	GLN
1	A	659	GLN
1	A	680	ASN
1	A	685	HIS
1	A	720	ASN
1	A	735	GLN
1	B	437	GLN
1	B	531	ASN
1	B	606	GLN
1	B	652	GLN
1	B	654	HIS
1	B	659	GLN
1	B	720	ASN
1	B	723	ASN
1	B	735	GLN
1	C	483	HIS
1	C	531	ASN
1	C	613	GLN
1	C	650	GLN
1	C	680	ASN
1	C	685	HIS
1	C	720	ASN
1	C	735	GLN
1	D	437	GLN
1	D	479	ASN
1	D	517	ASN
1	D	531	ASN
1	D	606	GLN

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Mol	Chain	Res	Type
1	D	613	GLN
1	D	638	ASN
1	D	652	GLN
1	D	654	HIS
1	D	659	GLN
1	D	720	ASN
1	D	723	ASN
1	D	735	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	337/337 (100%)	-0.28	13 (3%)	40 41	7, 14, 36, 52	0
1	B	337/337 (100%)	-0.08	17 (5%)	30 30	8, 16, 39, 52	0
1	C	337/337 (100%)	-0.21	15 (4%)	34 34	9, 16, 38, 56	0
1	D	337/337 (100%)	0.01	24 (7%)	17 17	9, 18, 44, 54	0
2	X	9/9 (100%)	1.95	4 (44%)	0 0	37, 42, 51, 54	0
2	Y	9/9 (100%)	2.35	4 (44%)	0 0	39, 41, 57, 59	0
All	All	1366/1366 (100%)	-0.11	77 (5%)	25 26	7, 16, 41, 59	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	9	ALA	9.5
1	C	454	GLY	7.9
1	C	561	ALA	7.3
1	C	562	PRO	7.2
1	D	562	PRO	6.5
1	A	561	ALA	6.3
2	X	9	ALA	6.2
1	B	515	PRO	6.1
1	D	452	ALA	5.8
1	D	516	GLY	5.8
1	B	562	PRO	5.5
1	D	515	PRO	5.4
1	A	562	PRO	5.3
1	B	527	LEU	5.3
1	D	527	LEU	5.2
1	C	434	ASP	4.9
1	B	517	ASN	4.7
1	B	646	ARG	4.5
1	B	514	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	514	HIS	4.3
1	D	454	GLY	4.3
1	D	455	GLN	4.1
1	B	561	ALA	3.9
1	D	560	ALA	3.9
1	B	560	ALA	3.6
1	C	563	THR	3.6
1	B	516	GLY	3.5
1	D	543	CYS	3.5
1	D	559	LEU	3.5
1	C	435	TYR	3.5
1	A	515	PRO	3.4
2	X	1	MET	3.4
1	D	647	GLU	3.4
1	A	563	THR	3.4
1	A	435	TYR	3.4
1	A	434	ASP	3.4
1	C	515	PRO	3.3
1	D	563	THR	3.3
1	A	454	GLY	3.3
1	D	646	ARG	3.2
2	Y	8	LEU	3.2
1	D	519	SER	3.2
1	B	529	ARG	3.1
1	C	514	HIS	3.0
1	B	649	ARG	3.0
1	A	514	HIS	3.0
1	C	560	ALA	3.0
1	C	529	ARG	2.9
1	D	517	ASN	2.9
1	B	543	CYS	2.9
1	A	529	ARG	2.8
1	D	451	THR	2.7
2	X	8	LEU	2.7
1	D	561	ALA	2.7
1	D	453	ASP	2.7
1	D	456	MET	2.7
1	D	565	ARG	2.6
1	C	452	ALA	2.6
1	D	649	ARG	2.6
2	Y	7	ILE	2.6
1	B	678	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	455	GLN	2.4
1	A	452	ALA	2.4
1	B	457	GLN	2.3
1	D	530	ASP	2.2
2	Y	5	ASP	2.2
1	B	647	GLU	2.2
1	A	647	GLU	2.2
1	A	565	ARG	2.1
1	C	455	GLN	2.1
1	C	689	PRO	2.1
1	B	454	GLY	2.1
1	C	565	ARG	2.0
1	A	564	PRO	2.0
1	D	518	LYS	2.0
2	X	2	PHE	2.0
1	C	646	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.