



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:37 PM GMT

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 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/ValidationPDFNotes.html>

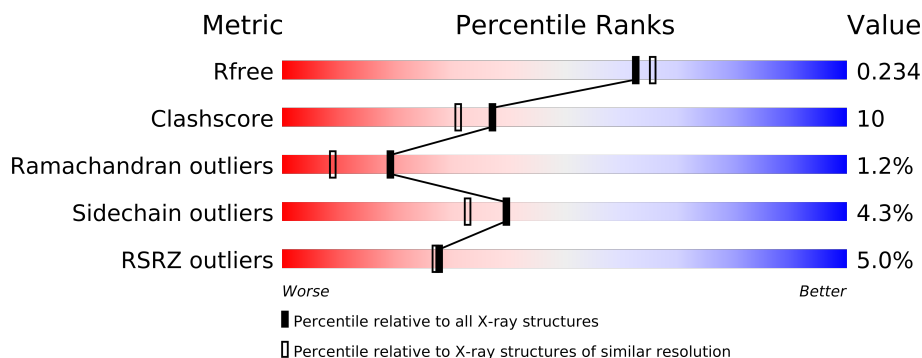
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	
2	X	9	
2	Y	9	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11565 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

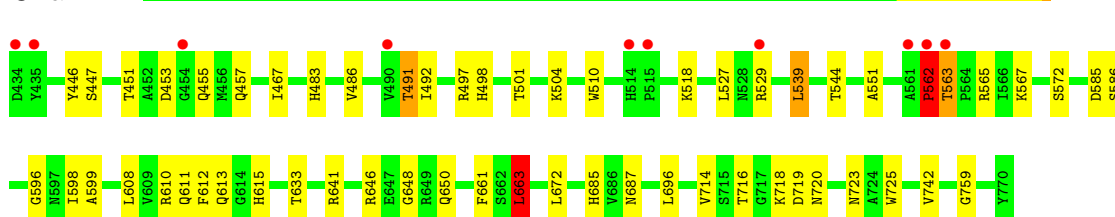
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	291	Total	O	0	0
			291	291		
3	B	279	Total	O	0	0
			279	279		
3	C	265	Total	O	0	0
			265	265		
3	D	235	Total	O	0	0
			235	235		
3	X	4	Total	O	0	0
			4	4		
3	Y	3	Total	O	0	0
			3	3		

3 Residue-property plots

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.

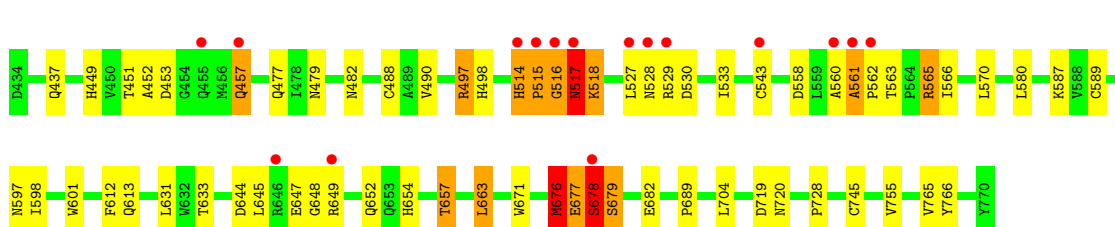
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain A:



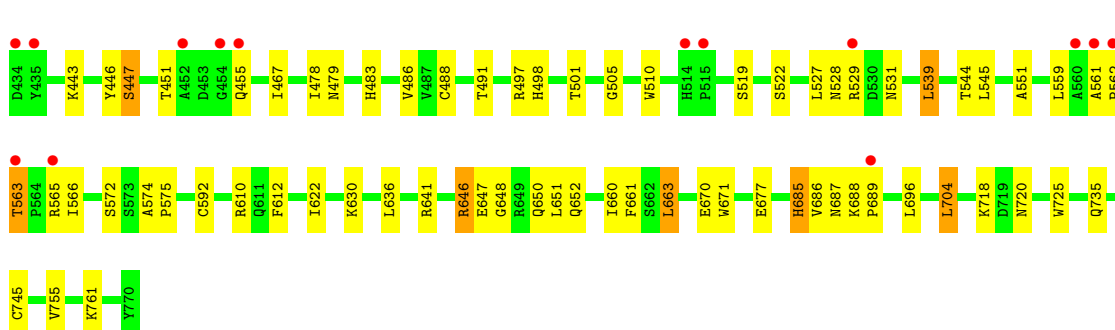
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain B:



• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

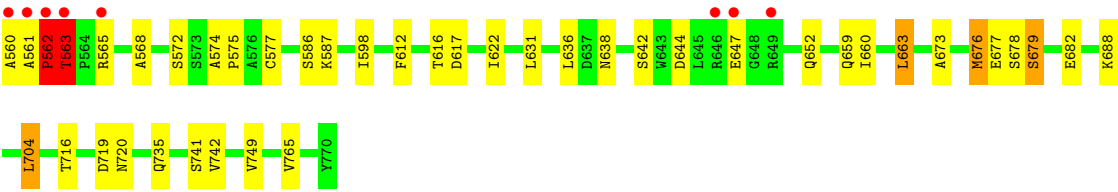
Chain C:



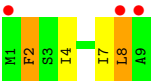
• Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

Chain D:

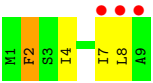




• Molecule 2: EH1 PEPTIDE



• Molecule 2: EH1 PEPTIDE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 96.4 (31.84-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.179 , 0.238 0.179 , 0.234	Depositor DCC
R_{free} test set	4380 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	7 of 87638 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11565	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Y	3	0	0	0	0
All	All	11565	0	10158	208	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (208) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:D:562:PRO:HB2	1:D:563:THR:HB	1.80	0.63
1:A:539:LEU:HG	1:A:544:THR:HB	1.79	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:D:510:TRP:HE3	1:D:518:LYS:CB	2.15	0.58
1:B:652:GLN:NE2	1:B:654:HIS:CE1	2.66	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:D:617:ASP:HB2	3:D:2126:HOH:O	2.04	0.58
1:A:491:THR:HG21	3:A:2096:HOH:O	2.03	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:648:GLY:O	1:B:649:ARG:HG2	2.07	0.55
1:B:515:PRO:CB	1:B:516:GLY:HA3	2.36	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:C:539:LEU:HG	1:C:544:THR:HB	1.91	0.53
1:A:585:ASP:O	1:A:586:SER:HB2	2.08	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:D:481:LEU:CD2	1:D:518:LYS:HG3	2.43	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:504:LYS:HE3	1:A:529:ARG:O	2.13	0.48
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:D:518:LYS:CA	1:D:519:SER:CB	2.83	0.47
1:B:676:MET:CE	1:B:682:GLU:HG3	2.43	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:D:540:PRO:HD2	1:D:586:SER:OG	2.14	0.47
1:A:716:THR:HB	1:A:742:VAL:HB	1.97	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:C:630:LYS:HE3	1:C:651:LEU:CD1	2.45	0.46
1:A:567:LYS:NZ	3:A:2111:HOH:O	2.44	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:C:562:PRO:HA	1:C:563:THR:O	2.16	0.45
1:B:560:ALA:HB3	1:B:561:ALA:HA	1.97	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:D:481:LEU:HD22	1:D:518:LYS:HG3	1.99	0.44
1:B:527:LEU:HD22	3:B:2154:HOH:O	2.17	0.44
1:C:545:LEU:HB2	1:C:559:LEU:HD11	1.98	0.44
1:B:719:ASP:O	1:B:720:ASN:HB2	2.17	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:661:PHE:CD2	2:Y:2:PHE:CE2	3.05	0.44
1:C:630:LYS:HE3	1:C:651:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:636:LEU:HD22	1:D:659:GLN:HE21	1.83	0.44
1:C:498:HIS:HA	1:C:510:TRP:O	2.18	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:D:644:ASP:HB3	1:D:647:GLU:HB2	2.00	0.43
1:B:671:TRP:CD2	1:B:728:PRO:HB3	2.54	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:645:LEU:HA	1:B:645:LEU:HD23	1.72	0.41
1:B:570:LEU:HB3	1:B:601:TRP:CZ3	2.55	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:D:540:PRO:CD	1:D:586:SER:OG	2.69	0.41
1:C:720:ASN:N	1:C:720:ASN:HD22	2.19	0.41
1:C:592:CYS:SG	1:C:622:ILE:HB	2.60	0.41
1:D:488:CYS:HB2	1:D:533:ILE:O	2.21	0.41
1:B:529:ARG:HH11	1:B:529:ARG:HG2	1.84	0.41
1:A:641:ARG:HH11	1:A:650:GLN:NE2	2.19	0.41
1:A:599:ALA:HB1	1:A:608:LEU:CD1	2.50	0.41
1:D:443:LYS:NZ	1:D:735:GLN:HE22	2.17	0.41
1:A:598:ILE:CD1	1:A:633:THR:HG21	2.50	0.41
1:C:565:ARG:HG2	3:C:2098:HOH:O	2.21	0.41
1:C:636:LEU:HD11	2:Y:2:PHE:CD1	2.56	0.41
1:D:716:THR:HB	1:D:742:VAL:HB	2.03	0.41
1:C:670:GLU:HB3	1:C:671:TRP:CD1	2.56	0.40
1:B:745:CYS:HA	1:B:755:VAL:O	2.20	0.40
1:C:745:CYS:HA	1:C:755:VAL:O	2.21	0.40
1:A:598:ILE:HD12	1:A:633:THR:HG21	2.04	0.40
1:A:451:THR:O	1:A:453:ASP:O	2.39	0.40
1:A:596:GLY:O	1:A:615:HIS:HB2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:488:CYS:SG	2:Y:4:ILE:HG13	2.61	0.40
1:D:528:ASN:HB3	1:D:531:ASN:ND2	2.35	0.40
1:C:574:ALA:HA	1:C:575:PRO:HD3	1.92	0.40
1:D:574:ALA:HA	1:D:575:PRO:HD3	1.93	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

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	Distance(Å)	Clash(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%)	50	43
1	B	335/337 (99%)	311 (93%)	16 (5%)	8 (2%)	9	2
1	C	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	50	43
1	D	335/337 (99%)	313 (93%)	16 (5%)	6 (2%)	13	4
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%)	19	9

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	PRO
1	B	514	HIS
1	B	515	PRO
1	B	517	ASN
1	B	518	LYS

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Mol	Chain	Res	Type
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%)	52	48
1	B	288/288 (100%)	277 (96%)	11 (4%)	44	38
1	C	288/288 (100%)	275 (96%)	13 (4%)	38	31
1	D	288/288 (100%)	274 (95%)	14 (5%)	35	27
2	X	8/8 (100%)	6 (75%)	2 (25%)	1	0
2	Y	8/8 (100%)	7 (88%)	1 (12%)	7	3
All	All	1168/1168 (100%)	1118 (96%)	50 (4%)	40	33

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
1	A	539	LEU
1	A	563	THR
1	A	565	ARG
1	A	646	ARG
1	A	663	LEU

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Mol	Chain	Res	Type
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
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
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 ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	337/337 (100%)	-0.25	10 (2%) 48 48	7, 14, 36, 52	0
1	B	337/337 (100%)	-0.07	16 (4%) 30 29	8, 16, 39, 52	0
1	C	337/337 (100%)	-0.16	14 (4%) 35 34	9, 16, 38, 56	0
1	D	337/337 (100%)	0.03	22 (6%) 18 17	9, 18, 44, 54	0
2	X	9/9 (100%)	1.75	3 (33%) 1 1	37, 42, 51, 54	0
2	Y	9/9 (100%)	1.92	3 (33%) 1 1	39, 41, 57, 59	0
All	All	1366/1366 (100%)	-0.09	68 (4%) 28 27	7, 16, 41, 59	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	GLY	7.7
1	C	561	ALA	7.7
2	Y	9	ALA	7.4
1	C	562	PRO	7.3
1	A	561	ALA	7.0
1	D	562	PRO	6.3
2	X	9	ALA	5.3
1	B	515	PRO	5.2
1	B	562	PRO	5.2
1	D	516	GLY	5.1
1	D	452	ALA	5.0
1	A	562	PRO	4.9
1	B	517	ASN	4.8
1	B	527	LEU	4.5
1	C	434	ASP	4.2
1	D	454	GLY	4.1
1	D	560	ALA	4.1
1	D	527	LEU	4.1
1	D	455	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	515	PRO	4.0
1	B	561	ALA	3.9
1	D	514	HIS	3.8
1	B	514	HIS	3.8
1	C	563	THR	3.7
1	D	647	GLU	3.4
1	D	543	CYS	3.4
1	B	560	ALA	3.4
1	A	563	THR	3.4
1	D	563	THR	3.3
2	X	8	LEU	3.2
1	A	454	GLY	3.2
2	X	1	MET	3.1
2	Y	8	LEU	3.1
1	B	646	ARG	3.1
1	C	435	TYR	3.1
1	A	435	TYR	3.1
1	B	529	ARG	3.1
1	A	434	ASP	3.0
1	D	517	ASN	3.0
1	D	561	ALA	3.0
1	D	559	LEU	2.9
1	D	519	SER	2.9
1	C	560	ALA	2.9
1	B	649	ARG	2.7
1	D	649	ARG	2.7
1	D	456	MET	2.7
1	C	529	ARG	2.7
1	C	455	GLN	2.6
1	D	646	ARG	2.6
1	C	452	ALA	2.6
1	B	543	CYS	2.6
1	A	515	PRO	2.5
1	B	516	GLY	2.5
1	C	515	PRO	2.4
1	B	678	SER	2.4
1	C	514	HIS	2.4
2	Y	7	ILE	2.3
1	A	514	HIS	2.3
1	A	529	ARG	2.3
1	B	457	GLN	2.3
1	D	453	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	490	VAL	2.1
1	B	455	GLN	2.1
1	D	565	ARG	2.1
1	B	528	ASN	2.1
1	C	565	ARG	2.1
1	C	689	PRO	2.1
1	D	451	THR	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.