



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 AM UTC

PDB ID : 2CE8 / pdb_00002ce8
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

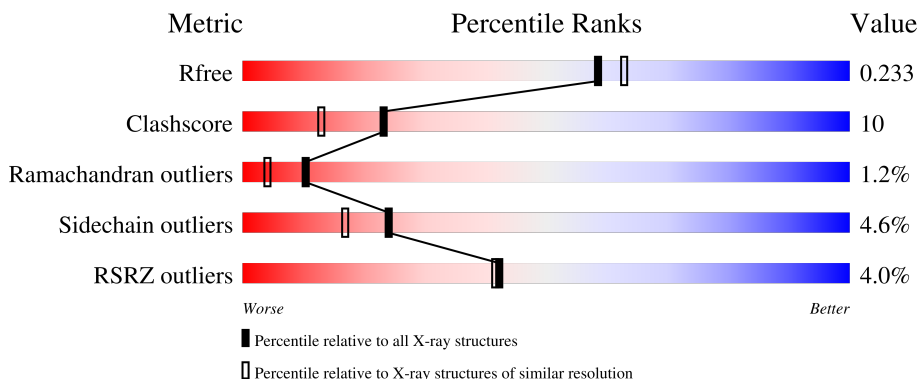
1 Overall quality at a glance

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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 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 $\leq 5\%$. 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	 2% 82% 15%
1	B	337	 4% 79% 16%
1	C	337	 2% 78% 20%
1	D	337	 5% 76% 19%
2	X	9	 56% 56% 22%

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Mol	Chain	Length	Quality of chain
2	Y	9	 <p>A horizontal bar chart representing the quality of chain Y. The bar is divided into four segments: a red segment (33%), a green segment (56%), a yellow segment (33%), and an orange segment (11%). The percentages are labeled above and below the segments.</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	337	2587	1628	445	497	17	0	0	0
1	B	337	2587	1628	445	497	17	0	0	0
1	C	337	2587	1628	445	497	17	0	0	0
1	D	337	2587	1628	445	497	17	0	0	0

- Molecule 2 is a protein called EH1 PEPTIDE.

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

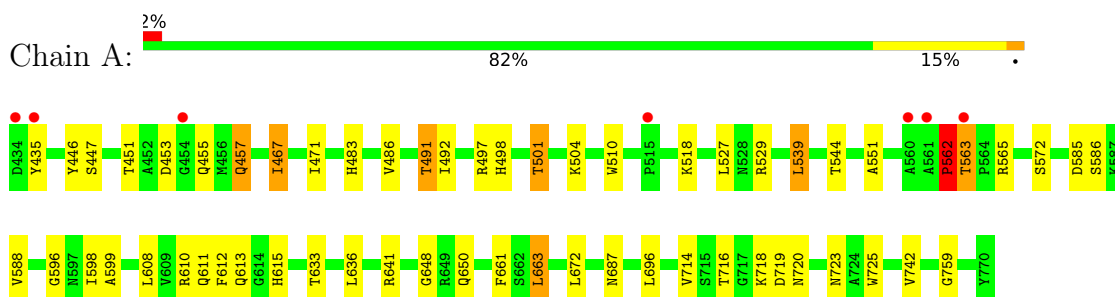
- Molecule 3 is water.

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

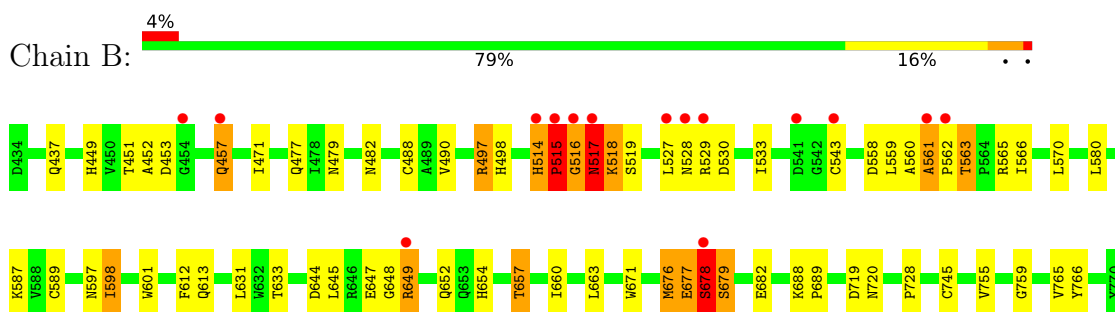
3 Residue-property plots i

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.

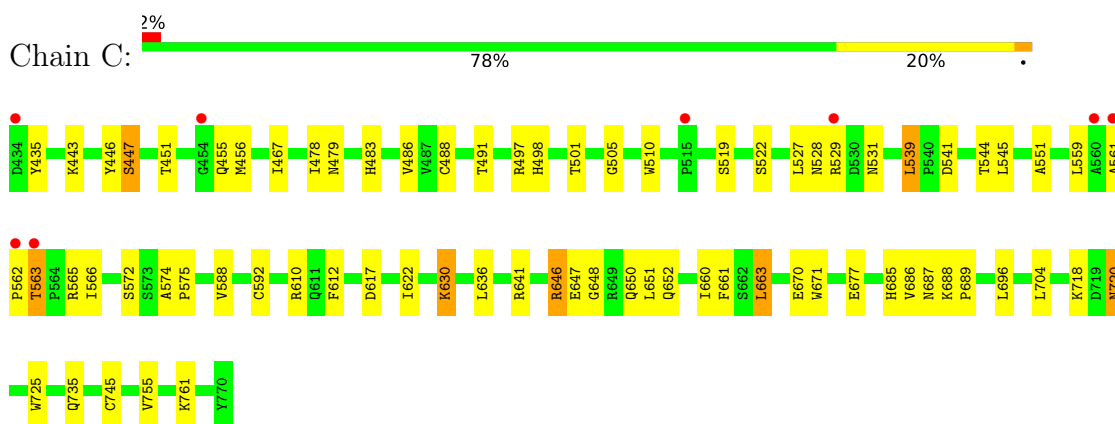
- Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1



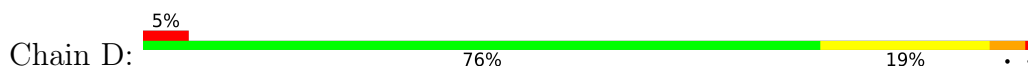
- Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

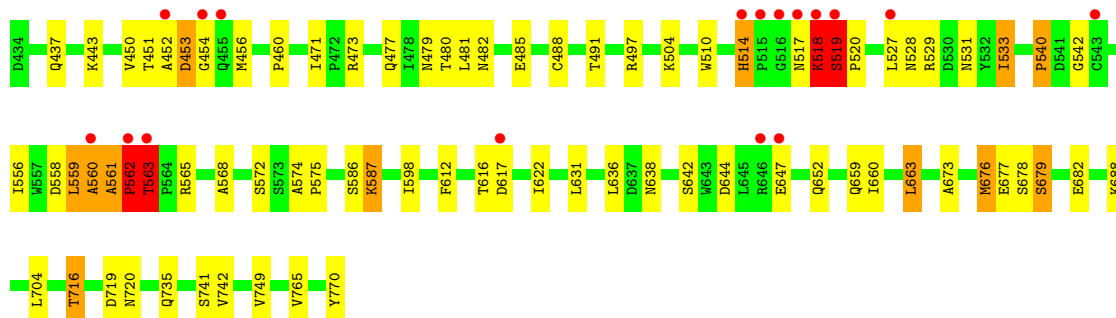


- Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

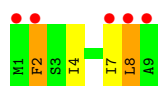


- Molecule 1: TRANSDUCIN-LIKE ENHANCER PROTEIN 1

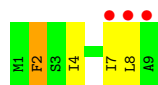




- Molecule 2: EH1 PEPTIDE



- Molecule 2: EH1 PEPTIDE



4 Data and refinement statistics

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 – 2.03 115.86 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.4 (116.25-2.03) 97.0 (115.86-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.179 , 0.238 0.178 , 0.233	Depositor DCC
R_{free} test set	4380 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.298	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

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

5 Model quality

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	1.07	4/2653 (0.2%)	1.00	3/3612 (0.1%)
1	B	1.07	2/2653 (0.1%)	1.08	14/3612 (0.4%)
1	C	1.00	0/2653	0.96	2/3612 (0.1%)
1	D	0.99	1/2653 (0.0%)	1.12	20/3612 (0.6%)
2	X	0.97	0/70	1.11	0/93
2	Y	0.87	0/70	1.00	0/93
All	All	1.03	7/10752 (0.1%)	1.04	39/14634 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	ILE	CA-CB	6.78	1.62	1.54
1	A	467	ILE	CA-CB	5.85	1.61	1.55
1	B	660	ILE	CA-CB	5.38	1.60	1.54
1	B	471	ILE	CA-CB	5.35	1.60	1.54
1	A	435	TYR	N-CA	5.35	1.53	1.46
1	A	471	ILE	CA-CB	5.28	1.60	1.54
1	A	501	THR	CA-CB	5.20	1.60	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	559	LEU	N-CA-C	10.20	124.24	111.69
1	D	562	PRO	CA-C-N	8.50	137.00	121.70
1	D	562	PRO	C-N-CA	8.50	137.00	121.70
1	B	678	SER	CA-CB-OG	-8.06	94.98	111.10
1	B	688	LYS	CA-C-N	-7.21	112.72	120.94
1	B	688	LYS	C-N-CA	-7.21	112.72	120.94
1	C	435	TYR	N-CA-C	6.62	118.15	111.07
1	D	616	THR	CA-C-N	-6.54	108.95	122.82
1	D	616	THR	C-N-CA	-6.54	108.95	122.82
1	D	519	SER	C-N-CD	-6.48	106.35	120.60
1	D	519	SER	CA-C-N	6.31	142.15	127.00
1	D	519	SER	C-N-CA	6.31	142.15	127.00
1	D	563	THR	CA-C-N	5.95	125.96	119.89
1	D	563	THR	C-N-CA	5.95	125.96	119.89
1	D	561	ALA	CA-C-N	5.94	127.27	119.84
1	D	561	ALA	C-N-CA	5.94	127.27	119.84
1	B	677	GLU	CA-C-N	-5.89	110.28	121.54
1	B	677	GLU	C-N-CA	-5.89	110.28	121.54
1	C	617	ASP	N-CA-C	-5.88	100.63	108.74
1	D	663	LEU	CA-CB-CG	5.73	136.35	116.30
1	D	560	ALA	CA-C-N	5.67	131.91	121.70
1	D	560	ALA	C-N-CA	5.67	131.91	121.70
1	B	678	SER	CB-CA-C	-5.49	99.50	110.42
1	D	616	THR	N-CA-C	5.42	119.90	113.12
1	B	563	THR	CA-C-N	5.29	125.21	119.76
1	B	563	THR	C-N-CA	5.29	125.21	119.76
1	B	649	ARG	N-CA-C	5.29	122.07	110.80
1	D	562	PRO	N-CA-C	5.28	123.36	112.47
1	D	716	THR	CA-C-N	-5.25	118.56	122.18
1	D	716	THR	C-N-CA	-5.25	118.56	122.18
1	B	515	PRO	CB-CA-C	5.23	120.18	111.56
1	A	562	PRO	CA-C-N	5.14	130.95	121.70
1	A	562	PRO	C-N-CA	5.14	130.95	121.70
1	D	454	GLY	N-CA-C	-5.14	108.53	115.21
1	B	678	SER	N-CA-CB	5.05	119.03	110.49
1	B	759	GLY	N-CA-C	-5.05	109.12	114.67
1	A	636	LEU	N-CA-C	-5.03	107.11	113.20
1	B	519	SER	CA-C-N	-5.01	114.79	119.85
1	B	519	SER	C-N-CA	-5.01	114.79	119.85

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 [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	2587	0	2503	41	0
1	B	2587	0	2503	54	0
1	C	2587	0	2503	50	0
1	D	2587	0	2503	67	0
2	X	70	0	73	5	0
2	Y	70	0	73	6	0
3	A	291	0	0	12	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	213	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 (213) 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:D:676:MET:HE1	1:D:682:GLU:HG3	1.36	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:676:MET:HE1	1:B:682:GLU:HG3	1.50	0.92
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:C:562:PRO:HA	1:C:563:THR:C	2.10	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:676:MET:HE1	1:D:682:GLU:CG	2.14	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: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:B:676:MET:HE1	1:B:682:GLU:CG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:687:ASN:CG	3:A:2222:HOH:O	2.45	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:A:641:ARG:HH11	1:A:650:GLN:HE22	1.53	0.56
1:B:452:ALA:HB2	1:B:689:PRO:HG2	1.86	0.56
1:D:482:ASN:ND2	3:D:2035:HOH:O	2.38	0.55
1:B:677:GLU:O	1:B:678:SER:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:663:LEU:HD12	1:C:663:LEU:C	2.35	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:LYS:HE2	2:X:7:ILE:O	2.15	0.47
1:D:450:VAL:HG22	1:D:456:MET:HG2	1.96	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:630:LYS:HE3	1:C:651:LEU:CD1	2.45	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:A:661:PHE:CD2	2:X:2:PHE:HE2	2.34	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:D:676:MET:CE	1:D:682:GLU:HG3	2.27	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:559:LEU:C	1:B:561:ALA:HB2	2.41	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
1:C:661:PHE:CD2	2:Y:2:PHE:CE2	3.05	0.44
1:D:636:LEU:HD22	1:D:659:GLN:HE21	1.83	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:C:456:MET:HE3	1:C:456:MET:HB2	1.93	0.43
1:D:644:ASP:HB3	1:D:647:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:MET:HB2	1:B:676:MET:HE2	1.54	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: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:D:676:MET:HB2	1:D:676:MET:HE2	1.32	0.42
1:B:570:LEU:HB3	1:B:601:TRP:CZ3	2.55	0.41
1:B:645:LEU:HD23	1:B:645:LEU:HA	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:C:541:ASP:OD1	1:C:541:ASP:C	2.64	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:C:565:ARG:HG2	3:C:2098:HOH:O	2.21	0.41
1:D:443:LYS:NZ	1:D:735:GLN:HE22	2.17	0.41
1:D:473:ARG:HE	1:D:770:TYR:C	2.29	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	335/337 (99%)	322 (96%)	12 (4%)	1 (0%)	36 31
1	B	335/337 (99%)	311 (93%)	16 (5%)	8 (2%)	4 1
1	C	335/337 (99%)	318 (95%)	16 (5%)	1 (0%)	36 31
1	D	335/337 (99%)	313 (93%)	16 (5%)	6 (2%)	6 2
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%)	10 4

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
1	B	679	SER

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Mol	Chain	Res	Type
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 [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	288/288 (100%)	279 (97%)	9 (3%)	35	31
1	B	288/288 (100%)	277 (96%)	11 (4%)	29	23
1	C	288/288 (100%)	273 (95%)	15 (5%)	21	13
1	D	288/288 (100%)	272 (94%)	16 (6%)	19	12
2	X	8/8 (100%)	6 (75%)	2 (25%)	0	0
2	Y	8/8 (100%)	7 (88%)	1 (12%)	4	1
All	All	1168/1168 (100%)	1114 (95%)	54 (5%)	24	17

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	A	457	GLN
1	A	467	ILE
1	A	491	THR
1	A	539	LEU
1	A	563	THR
1	A	565	ARG
1	A	588	VAL

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Mol	Chain	Res	Type
1	A	663	LEU
1	B	457	GLN
1	B	517	ASN
1	B	528	ASN
1	B	530	ASP
1	B	563	THR
1	B	566	ILE
1	B	587	LYS
1	B	598	ILE
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	588	VAL
1	C	630	LYS
1	C	646	ARG
1	C	663	LEU
1	C	688	LYS
1	C	704	LEU
1	C	718	LYS
1	C	720	ASN
1	D	453	ASP
1	D	491	THR
1	D	518	LYS
1	D	519	SER
1	D	527	LEU
1	D	533	ILE
1	D	540	PRO
1	D	563	THR
1	D	565	ARG
1	D	587	LYS
1	D	660	ILE
1	D	663	LEU
1	D	676	MET
1	D	677	GLU
1	D	688	LYS

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	685	HIS
1	A	720	ASN
1	A	735	GLN
1	B	437	GLN
1	B	457	GLN
1	B	482	ASN
1	B	531	ASN
1	B	652	GLN
1	B	654	HIS
1	B	723	ASN
1	B	735	GLN
1	C	482	ASN
1	C	483	HIS
1	C	531	ASN
1	C	611	GLN
1	C	650	GLN
1	C	659	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	605	ASN
1	D	652	GLN
1	D	654	HIS
1	D	659	GLN

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Mol	Chain	Res	Type
1	D	680	ASN
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 oligosaccharides 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 [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	337/337 (100%)	-0.47	7 (2%) 63 63	7, 14, 36, 52	0
1	B	337/337 (100%)	-0.16	15 (4%) 38 37	8, 16, 39, 52	0
1	C	337/337 (100%)	-0.34	8 (2%) 59 60	9, 16, 38, 56	0
1	D	337/337 (100%)	-0.08	17 (5%) 34 33	9, 18, 44, 54	0
2	X	9/9 (100%)	1.84	5 (55%) 0 0	37, 42, 51, 54	0
2	Y	9/9 (100%)	2.17	3 (33%) 1 1	39, 41, 57, 59	0
All	All	1366/1366 (100%)	-0.23	55 (4%) 42 41	7, 16, 41, 59	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	519	SER	6.2
2	Y	9	ALA	5.3
1	A	561	ALA	5.0
1	C	454	GLY	4.8
1	B	515	PRO	4.7
1	C	562	PRO	4.6
1	B	517	ASN	4.3
2	X	9	ALA	4.3
1	B	561	ALA	4.2
1	C	434	ASP	4.1
1	D	527	LEU	4.0
1	D	452	ALA	3.9
1	B	516	GLY	3.8
1	B	678	SER	3.8
1	C	561	ALA	3.8
1	D	560	ALA	3.8
1	D	517	ASN	3.8
1	B	562	PRO	3.5
1	D	454	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	563	THR	3.5
1	D	562	PRO	3.5
1	D	515	PRO	3.4
1	A	434	ASP	3.3
1	D	516	GLY	3.3
2	Y	8	LEU	3.2
1	B	649	ARG	3.1
1	B	527	LEU	3.1
1	D	518	LYS	3.1
2	Y	7	ILE	3.0
1	D	543	CYS	2.8
1	B	528	ASN	2.7
1	D	455	GLN	2.7
1	C	563	THR	2.7
1	D	647	GLU	2.6
2	X	7	ILE	2.6
1	D	617	ASP	2.6
1	B	514	HIS	2.6
1	C	515	PRO	2.6
2	X	8	LEU	2.5
2	X	1	MET	2.4
1	D	514	HIS	2.4
2	X	2	PHE	2.3
1	A	563	THR	2.3
1	A	560	ALA	2.3
1	B	454	GLY	2.3
1	B	529	ARG	2.3
1	D	646	ARG	2.2
1	A	454	GLY	2.2
1	B	543	CYS	2.2
1	B	457	GLN	2.2
1	C	529	ARG	2.2
1	C	560	ALA	2.2
1	A	435	TYR	2.1
1	B	541	ASP	2.0
1	A	515	PRO	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 oligosaccharides 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.