



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:52 AM GMT

PDB ID : 2C0M
Title : APO FORM OF THE TPR DOMAIN OF THE PEX5P RECEPTOR
Authors : Stanley, W.A.; Kursula, P.; Wilmanns, M.
Deposited on : 2005-09-05
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

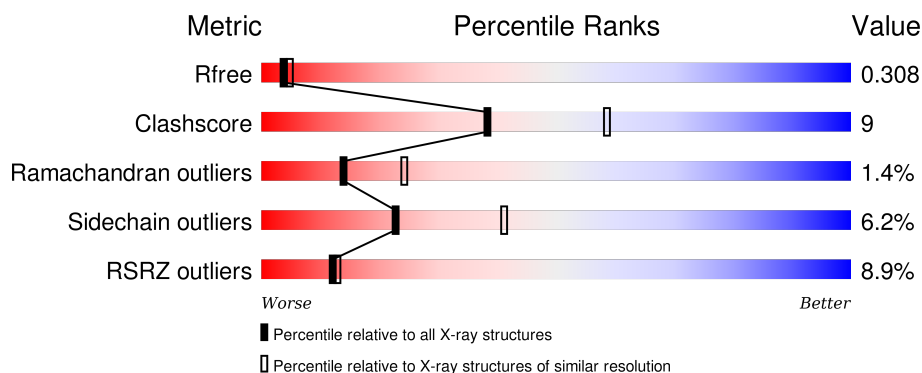
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	319	<div> <div> <div></div> <div>65%</div> <div>25%</div> <div>• • 7%</div> </div> </div>
1	B	319	<div> <div> <div>2%</div> <div>71%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	C	319	<div> <div> <div>16%</div> <div>76%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	F	319	<div> <div> <div>15%</div> <div>77%</div> <div>15%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9629 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 PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR.

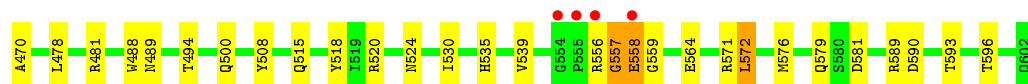
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	3	0
			2364	1482	418	453	11			
1	B	297	Total	C	N	O	S	0	4	0
			2374	1489	419	455	11			
1	C	302	Total	C	N	O	S	0	1	0
			2377	1493	417	456	11			
1	F	302	Total	C	N	O	S	0	0	0
			2368	1488	416	453	11			

There are 4 discrepancies between the modelled and reference sequences:

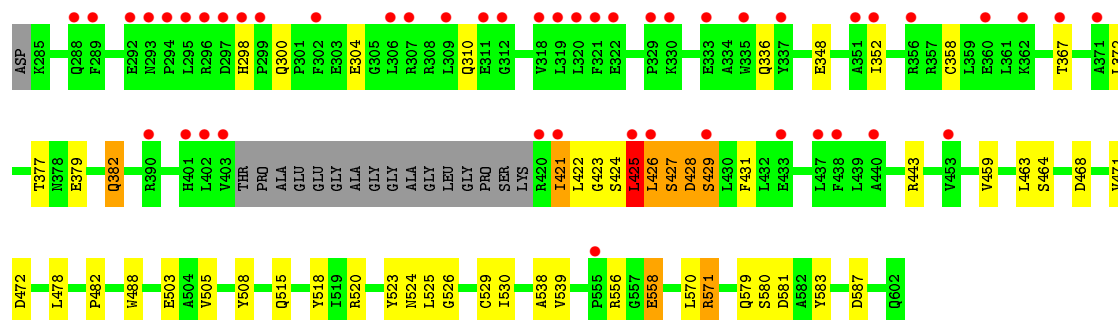
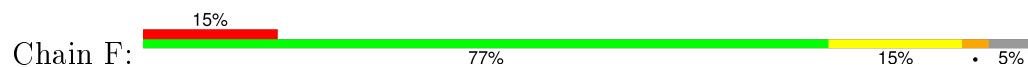
Chain	Residue	Modelled	Actual	Comment	Reference
A	388	ILE	THR	CONFLICT	UNP P50542
B	388	ILE	THR	CONFLICT	UNP P50542
C	388	ILE	THR	CONFLICT	UNP P50542
F	388	ILE	THR	CONFLICT	UNP P50542

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		
2	B	57	Total	O	0	0
			57	57		
2	C	14	Total	O	0	0
			14	14		
2	F	21	Total	O	0	0
			21	21		



● Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.47Å 85.55Å 88.89Å 71.17° 89.99° 73.43°	Depositor
Resolution (Å)	19.54 – 2.50 19.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.54-2.50) 79.1 (19.53-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.263 , 0.309 0.296 , 0.308	Depositor DCC
R_{free} test set	2363 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , -4.0	EDS
Estimated twinning fraction	0.229 for h,h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 47256 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9629	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.86	3/2409 (0.1%)	0.85	6/3265 (0.2%)
1	B	0.69	1/2419 (0.0%)	0.73	1/3278 (0.0%)
1	C	0.50	0/2421	0.62	0/3280
1	F	0.51	1/2412 (0.0%)	0.66	1/3268 (0.0%)
All	All	0.66	5/9661 (0.1%)	0.72	8/13091 (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	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	CYS	CB-SG	-6.50	1.71	1.82
1	A	544	GLU	CG-CD	6.45	1.61	1.51
1	A	529	CYS	CB-SG	-6.00	1.72	1.82
1	A	473	CYS	CB-SG	-5.80	1.72	1.81
1	F	529	CYS	CB-SG	-5.15	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	A	308	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	486	LEU	CA-CB-CG	5.67	128.34	115.30
1	F	429	SER	N-CA-CB	-5.60	102.10	110.50
1	A	308	ARG	CG-CD-NE	5.38	123.10	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	GLY	N-CA-C	-5.37	99.67	113.10
1	A	308	ARG	CD-NE-CZ	5.27	130.97	123.60
1	A	571	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	557	GLY	Peptide
1	C	425	LEU	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	2364	0	2312	64	0
1	B	2374	0	2321	47	0
1	C	2377	0	2327	29	0
1	F	2368	0	2322	33	0
2	A	54	0	0	4	0
2	B	57	0	0	0	0
2	C	14	0	0	2	0
2	F	21	0	0	1	0
All	All	9629	0	9282	171	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 9.

All (171) 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:F:426:LEU:CD1	1:F:427:SER:H	1.59	1.13
1:F:426:LEU:HD13	1:F:427:SER:H	1.35	0.91
1:F:426:LEU:HD12	1:F:427:SER:H	1.37	0.90
1:C:572:LEU:HD22	1:C:576:MET:HE3	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:LEU:CD1	1:F:427:SER:N	2.41	0.82
1:A:519:ILE:HG21	1:A:549:GLN:HE21	1.47	0.80
1:F:426:LEU:HD12	1:F:427:SER:N	1.98	0.78
1:B:536[B]:ARG:NH1	1:B:540:GLU:OE2	2.17	0.78
1:B:304:GLU:HB3	1:B:320:LEU:HD21	1.66	0.77
1:C:572:LEU:HD22	1:C:576:MET:CE	2.18	0.74
1:A:526:GLY:HA3	1:A:542:PHE:CE2	2.23	0.72
1:F:425:LEU:H	1:F:425:LEU:HD23	1.58	0.69
1:A:508:TYR:CZ	1:A:524:ASN:HB3	2.29	0.67
1:A:377[A]:THR:HG23	1:A:463:LEU:HD21	1.77	0.66
1:B:305:GLY:N	1:B:320:LEU:HD23	2.11	0.66
1:A:428:ASP:OD1	1:A:428:ASP:C	2.34	0.66
1:B:536[B]:ARG:HH11	1:B:536[B]:ARG:CG	2.08	0.66
1:A:505:VAL:HG13	1:A:525:LEU:HD11	1.79	0.65
1:A:403:VAL:HG12	1:A:405:PRO:HD2	1.79	0.65
1:A:551:LYS:NZ	1:A:602:GLN:OXT	2.30	0.64
1:A:547:ASN:ND2	1:A:602:GLN:OXT	2.30	0.64
1:C:581:ASP:N	1:C:581:ASP:OD2	2.32	0.63
1:B:508:TYR:CZ	1:B:524:ASN:HB3	2.34	0.63
1:F:377:THR:CG2	2:F:2004:HOH:O	2.48	0.62
1:B:359:LEU:HD21	1:B:369:LEU:HD12	1.82	0.61
1:C:556:ARG:O	1:C:558:GLU:N	2.34	0.60
1:A:572:LEU:HD23	1:A:576:MET:HE3	1.84	0.59
1:B:304:GLU:HB3	1:B:320:LEU:CD2	2.33	0.59
1:F:377:THR:HG23	1:F:463:LEU:HD21	1.85	0.58
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.68	0.58
1:A:519:ILE:HG21	1:A:549:GLN:NE2	2.17	0.58
1:C:557:GLY:O	1:C:559:GLY:N	2.37	0.57
1:B:298:HIS:CE1	1:B:304:GLU:HG3	2.39	0.57
1:A:298:HIS:CE1	1:A:304:GLU:HG3	2.39	0.57
1:A:428:ASP:O	1:A:432:LEU:HB2	2.04	0.57
1:B:572:LEU:HD23	1:B:576:MET:HE1	1.86	0.56
1:C:508:TYR:CZ	1:C:524:ASN:HB3	2.41	0.56
1:A:382:GLN:NE2	1:A:463:LEU:HD22	2.21	0.56
1:A:508:TYR:CE2	1:A:524:ASN:HB3	2.40	0.56
1:A:572:LEU:HD23	1:A:576:MET:CE	2.36	0.56
1:A:344:GLU:HG3	2:A:2033:HOH:O	2.04	0.56
1:A:363:PRO:HD3	2:A:2016:HOH:O	2.04	0.56
1:C:564:GLU:OE2	1:C:589:ARG:NH2	2.39	0.56
1:A:535:HIS:O	1:A:539:VAL:HG23	2.06	0.56
1:A:522:ARG:HD3	1:A:544:GLU:HB3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG13	1:A:525:LEU:CD1	2.37	0.55
1:B:428:ASP:N	1:B:428:ASP:OD1	2.41	0.54
1:B:536[B]:ARG:HH11	1:B:536[B]:ARG:HG3	1.73	0.54
1:F:580:SER:HA	1:F:583:TYR:CE1	2.42	0.54
1:F:377:THR:HG21	1:F:459:VAL:HG13	1.91	0.53
1:A:508:TYR:CE1	1:A:524:ASN:HB3	2.43	0.53
1:B:553:ARG:HB3	1:B:558:GLU:HG2	1.91	0.53
1:F:382:GLN:CD	1:F:463:LEU:HD22	2.29	0.52
1:A:486:LEU:HD12	1:A:487:LEU:HD23	1.90	0.52
1:C:348:GLU:HG2	1:C:379:GLU:HG2	1.92	0.52
1:B:554:GLY:O	1:B:556:ARG:N	2.42	0.52
1:B:382:GLN:HA	1:B:382:GLN:OE1	2.08	0.52
1:A:567:TRP:CE2	1:A:589:ARG:HG3	2.44	0.52
1:B:382:GLN:OE1	1:B:382:GLN:CA	2.57	0.52
1:A:309:LEU:O	1:A:312:GLY:N	2.35	0.52
1:B:359:LEU:CD2	1:B:369:LEU:HD12	2.40	0.51
1:B:390:ARG:HH22	1:B:405:PRO:HD3	1.74	0.51
1:A:526:GLY:O	1:A:529:CYS:HB2	2.11	0.51
1:B:390:ARG:HH22	1:B:405:PRO:CD	2.24	0.51
1:B:555:PRO:C	1:B:557:GLY:H	2.13	0.51
1:A:364:ASP:OD2	1:A:364:ASP:N	2.38	0.51
1:A:377[B]:THR:HG21	1:A:459:VAL:CG1	2.40	0.51
1:A:393:LEU:CD2	1:A:437:LEU:HB3	2.42	0.49
1:B:523:TYR:CD1	1:B:566:ILE:HG12	2.46	0.49
1:A:523:TYR:CZ	1:A:527:ILE:HD11	2.47	0.49
1:F:298:HIS:CE1	1:F:304:GLU:HG3	2.47	0.49
1:F:426:LEU:HD12	1:F:427:SER:CA	2.42	0.49
1:A:336:GLN:NE2	1:A:365:ASN:HD21	2.10	0.49
1:A:529:CYS:HB3	1:A:538:ALA:HB2	1.94	0.49
1:A:508:TYR:O	1:A:509:ARG:C	2.49	0.49
1:B:336:GLN:HE21	1:B:365:ASN:HD21	1.60	0.49
1:C:382:GLN:CD	1:C:463:LEU:HD22	2.32	0.49
1:F:571:ARG:HD2	1:F:587:ASP:OD1	2.12	0.49
1:B:577:LEU:HD23	1:B:579:GLN:HB2	1.95	0.48
1:B:519:ILE:HG21	1:B:549:GLN:HE21	1.77	0.48
1:C:425:LEU:HB2	1:C:426:LEU:HD23	1.95	0.48
1:B:300:GLN:HE22	1:B:302:PHE:HB3	1.78	0.48
1:C:287:TYR:N	1:C:353:SER:OG	2.26	0.48
1:C:292:GLU:HG3	1:C:292:GLU:O	2.13	0.48
1:A:577:LEU:HD23	1:A:579:GLN:HB2	1.96	0.48
1:A:554:GLY:HA3	1:A:558:GLU:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ARG:NH1	1:B:387:GLU:OE2	2.46	0.47
1:A:394:ARG:HA	1:A:400:ALA:HA	1.95	0.47
1:A:571:ARG:HD2	1:A:587:ASP:OD1	2.15	0.47
1:C:596:THR:HG21	1:F:482:PRO:HB3	1.96	0.47
1:A:522:ARG:O	1:A:525:LEU:HB3	2.13	0.47
1:B:564:GLU:OE2	1:B:589:ARG:NH2	2.47	0.47
1:A:284:ASP:HB2	1:A:356:ARG:NE	2.29	0.47
1:A:403:VAL:HG12	1:A:405:PRO:CD	2.44	0.46
1:F:508:TYR:CZ	1:F:524:ASN:HB3	2.50	0.46
1:F:580:SER:HA	1:F:583:TYR:CD1	2.51	0.46
1:B:471:VAL:HG23	1:B:494:THR:HG22	1.97	0.46
1:B:377:THR:HG23	1:B:463[A]:LEU:HD21	1.98	0.46
1:A:580:SER:HA	1:A:583:TYR:CE1	2.51	0.46
1:F:471:VAL:O	1:F:472:ASP:C	2.54	0.46
1:F:352:ILE:HG23	1:F:372:LEU:HD11	1.99	0.45
1:A:492:GLY:HA3	1:A:508:TYR:CE2	2.51	0.45
1:B:305:GLY:CA	1:B:320:LEU:HD23	2.46	0.45
1:A:536[B]:ARG:CZ	1:A:598:PHE:HD2	2.30	0.45
1:B:463[B]:LEU:HD12	1:B:463[B]:LEU:C	2.37	0.45
1:B:523:TYR:CE1	1:B:566:ILE:HG12	2.51	0.45
1:A:287:TYR:CD2	1:A:287:TYR:C	2.90	0.45
1:A:404:THR:N	1:A:405:PRO:CD	2.80	0.45
1:C:590:ASP:OD2	1:C:593:THR:OG1	2.30	0.45
1:F:581:ASP:OD2	1:F:581:ASP:N	2.46	0.45
1:A:307:ARG:HD2	1:C:383:ARG:NH2	2.32	0.44
1:A:317:ALA:O	1:A:321:PHE:CD1	2.70	0.44
1:B:403:VAL:CG1	1:B:405:PRO:HD2	2.46	0.44
1:F:421:ILE:HG22	1:F:422:LEU:N	2.32	0.44
1:A:524:ASN:CG	2:A:2037:HOH:O	2.56	0.44
1:F:348:GLU:HG2	1:F:379:GLU:HG2	1.99	0.44
1:A:435:LYS:HA	1:A:460:LEU:HD13	1.98	0.44
1:F:425:LEU:HD23	1:F:425:LEU:N	2.30	0.44
1:C:377:THR:HG23	2:C:2003:HOH:O	2.17	0.44
1:A:396:THR:O	1:A:399:TYR:N	2.47	0.44
1:C:452:ASP:OD2	1:C:481:ARG:NH2	2.51	0.44
1:B:536[B]:ARG:NH1	1:B:536[B]:ARG:CG	2.75	0.44
1:B:553:ARG:HD2	1:B:558:GLU:HG2	1.99	0.44
1:F:468:ASP:N	1:F:468:ASP:OD1	2.51	0.44
1:C:394:ARG:HA	1:C:400:ALA:HA	1.99	0.44
1:A:529:CYS:CB	1:A:538:ALA:HB2	2.47	0.44
1:A:365:ASN:OD1	1:A:365:ASN:C	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ASP:OD1	1:B:486:LEU:HB3	2.18	0.43
1:B:307:ARG:O	1:B:308:ARG:C	2.57	0.43
1:A:437:LEU:O	1:A:440:ALA:HB3	2.19	0.43
1:B:519:ILE:HG21	1:B:549:GLN:NE2	2.34	0.43
1:C:377:THR:OG1	1:C:459:VAL:HG13	2.19	0.43
1:C:298:HIS:CE1	1:C:304:GLU:HG3	2.53	0.43
1:F:478:LEU:HD22	1:F:488:TRP:NE1	2.32	0.43
1:F:505:VAL:HG13	1:F:525:LEU:HD11	2.01	0.43
1:A:445:ASP:OD2	1:A:448:SER:OG	2.37	0.43
1:B:536[B]:ARG:HE	1:B:598:PHE:HD2	1.67	0.43
1:B:431:PHE:CE2	1:B:432:LEU:HD12	2.54	0.43
1:C:535:HIS:O	1:C:539:VAL:HG23	2.19	0.43
1:C:377:THR:OG1	1:C:459:VAL:CG1	2.67	0.42
1:C:470:ALA:HB3	1:C:494:THR:HG21	2.01	0.42
1:F:570:LEU:O	1:F:571:ARG:C	2.57	0.42
1:B:470:ALA:HB3	1:B:494:THR:HG21	2.00	0.42
1:A:568:SER:HA	2:A:2049:HOH:O	2.20	0.42
1:A:502:GLU:O	1:A:505:VAL:HB	2.19	0.42
1:C:478:LEU:HD22	1:C:488:TRP:NE1	2.34	0.42
1:C:364:ASP:HB3	1:C:395:TYR:CD2	2.55	0.42
1:F:431:PHE:CZ	1:F:464:SER:HB3	2.54	0.42
1:B:536[B]:ARG:HG3	1:B:536[B]:ARG:NH1	2.33	0.42
1:A:300:GLN:HE22	1:A:302:PHE:HB3	1.84	0.41
1:B:441:ALA:O	1:B:442:VAL:C	2.59	0.41
1:F:336:GLN:N	1:F:358:CYS:SG	2.93	0.41
1:F:503:GLU:N	1:F:503:GLU:OE1	2.51	0.41
1:C:421:ILE:HG22	1:C:422:LEU:N	2.34	0.41
1:A:307:ARG:O	1:A:308:ARG:C	2.58	0.41
1:A:571:ARG:CD	1:A:587:ASP:OD1	2.68	0.41
1:B:317:ALA:O	1:B:321:PHE:CD1	2.73	0.41
1:A:428:ASP:OD1	1:A:429:SER:N	2.53	0.41
1:A:554:GLY:CA	1:A:558:GLU:HB2	2.50	0.41
1:B:567:TRP:CE2	1:B:589:ARG:HG3	2.56	0.41
1:A:314:LEU:O	1:A:315:PRO:C	2.59	0.41
1:F:423:GLY:O	1:F:424:SER:OG	2.33	0.41
1:F:523:TYR:O	1:F:526:GLY:N	2.54	0.41
1:B:551:LYS:NZ	1:B:602:GLN:OXT	2.53	0.41
1:B:451:PRO:HG2	1:B:481[B]:ARG:HE	1.86	0.41
1:B:336:GLN:NE2	1:B:365:ASN:HD21	2.18	0.41
1:C:489:ASN:HB3	2:C:2007:HOH:O	2.21	0.41
1:A:572:LEU:CD2	1:A:576:MET:CE	2.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:HG3	1:C:320:LEU:CD1	2.51	0.40
1:C:352:ILE:HG23	1:C:372:LEU:HD11	2.03	0.40
1:F:538:ALA:O	1:F:539:VAL:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/319 (93%)	263 (89%)	29 (10%)	4 (1%)	14	24
1	B	297/319 (93%)	276 (93%)	21 (7%)	0	100	100
1	C	299/319 (94%)	275 (92%)	18 (6%)	6 (2%)	9	15
1	F	298/319 (93%)	269 (90%)	23 (8%)	6 (2%)	9	15
All	All	1190/1276 (93%)	1083 (91%)	91 (8%)	16 (1%)	14	26

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	287	TYR
1	C	557	GLY
1	C	558	GLU
1	F	425	LEU
1	F	427	SER
1	F	558	GLU
1	C	421	ILE
1	C	423	GLY
1	F	421	ILE
1	A	558	GLU
1	C	427	SER
1	F	428	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	429	SER
1	A	559	GLY
1	A	397	PRO
1	A	404	THR

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	248/258 (96%)	232 (94%)	16 (6%)	21	39
1	B	249/258 (96%)	232 (93%)	17 (7%)	20	36
1	C	249/258 (96%)	237 (95%)	12 (5%)	31	55
1	F	248/258 (96%)	232 (94%)	16 (6%)	21	39
All	All	994/1032 (96%)	933 (94%)	61 (6%)	23	42

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	A	292	GLU
1	A	308	ARG
1	A	310	GLN
1	A	404	THR
1	A	428	ASP
1	A	448	SER
1	A	486	LEU
1	A	515	GLN
1	A	520	ARG
1	A	552	SER
1	A	556	ARG
1	A	558	GLU
1	A	571	ARG
1	A	579	GLN
1	A	600	LEU
1	B	284	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291	GLU
1	B	292	GLU
1	B	303	GLU
1	B	320	LEU
1	B	367	THR
1	B	382	GLN
1	B	404	THR
1	B	428	ASP
1	B	432	LEU
1	B	500	GLN
1	B	515	GLN
1	B	520	ARG
1	B	571	ARG
1	B	579	GLN
1	B	600	LEU
1	B	602	GLN
1	C	291	GLU
1	C	292	GLU
1	C	308	ARG
1	C	431	PHE
1	C	500	GLN
1	C	515	GLN
1	C	518	TYR
1	C	520	ARG
1	C	530	ILE
1	C	571	ARG
1	C	572	LEU
1	C	579	GLN
1	F	300	GLN
1	F	310	GLN
1	F	367	THR
1	F	382	GLN
1	F	425	LEU
1	F	426	LEU
1	F	428	ASP
1	F	443	ARG
1	F	515	GLN
1	F	518	TYR
1	F	520	ARG
1	F	530	ILE
1	F	556	ARG
1	F	558	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	571	ARG
1	F	579	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	336	GLN
1	A	347	GLN
1	A	366	GLN
1	A	489	ASN
1	A	524	ASN
1	B	298	HIS
1	B	326	GLN
1	B	331	HIS
1	B	336	GLN
1	C	298	HIS
1	C	336	GLN
1	C	489	ASN
1	C	524	ASN
1	F	298	HIS
1	F	336	GLN
1	F	489	ASN
1	F	524	ASN
1	F	579	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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	297/319 (93%)	0.39	3 (1%) 84 86	13, 22, 26, 29	0
1	B	297/319 (93%)	0.42	6 (2%) 68 72	17, 23, 27, 31	0
1	C	302/319 (94%)	0.92	50 (16%) 2 2	20, 23, 25, 28	1 (0%)
1	F	302/319 (94%)	0.85	48 (15%) 3 2	20, 23, 25, 28	0
All	All	1198/1276 (93%)	0.65	107 (8%) 12 13	13, 23, 26, 31	1 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	LEU	6.2
1	C	403	VAL	5.8
1	C	337	TYR	5.6
1	F	402	LEU	5.4
1	C	335	TRP	4.9
1	F	429	SER	4.8
1	C	421	ILE	4.8
1	F	555	PRO	4.6
1	C	301	PRO	4.6
1	C	367	THR	4.5
1	C	318	VAL	4.2
1	C	299	PRO	4.2
1	F	330	LYS	4.2
1	C	294	PRO	4.1
1	F	426	LEU	4.1
1	F	367	THR	4.1
1	C	286	GLY	4.1
1	C	420	ARG	4.1
1	F	298	HIS	4.0
1	F	420	ARG	3.9
1	C	425	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	402	LEU	3.9
1	F	296	ARG	3.8
1	F	309	LEU	3.8
1	F	337	TYR	3.8
1	C	307	ARG	3.7
1	C	444	LEU	3.7
1	F	421	ILE	3.6
1	C	330	LYS	3.6
1	C	391	ASP	3.5
1	F	312	GLY	3.4
1	C	296	ARG	3.4
1	C	309	LEU	3.4
1	F	294	PRO	3.4
1	C	356	ARG	3.3
1	C	556	ARG	3.3
1	F	297	ASP	3.3
1	F	289	PHE	3.3
1	F	425	LEU	3.3
1	C	554	GLY	3.3
1	F	318	VAL	3.3
1	C	555	PRO	3.2
1	C	429	SER	3.2
1	F	356	ARG	3.2
1	C	401	HIS	3.2
1	F	351	ALA	3.1
1	F	293	ASN	3.0
1	C	288	GLN	3.0
1	C	394	ARG	3.0
1	F	320	LEU	2.9
1	F	433	GLU	2.9
1	F	288	GLN	2.9
1	C	426	LEU	2.9
1	B	447	THR	2.9
1	F	307	ARG	2.8
1	C	392	TRP	2.8
1	C	315	PRO	2.7
1	F	390	ARG	2.7
1	C	431	PHE	2.7
1	F	335	TRP	2.7
1	F	311	GLU	2.7
1	B	404	THR	2.7
1	F	360	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	329	PRO	2.6
1	C	326	GLN	2.6
1	C	327	GLN	2.5
1	C	395	TYR	2.5
1	F	292	GLU	2.5
1	C	558	GLU	2.5
1	C	376	PHE	2.5
1	F	403	VAL	2.5
1	F	453	VAL	2.5
1	F	362	LYS	2.5
1	C	390	ARG	2.5
1	B	286	GLY	2.5
1	F	306	LEU	2.5
1	C	427	SER	2.5
1	C	359	LEU	2.4
1	C	302	PHE	2.4
1	F	401	HIS	2.4
1	B	405	PRO	2.4
1	F	321	PHE	2.4
1	A	285	LYS	2.4
1	F	302	PHE	2.4
1	C	291	GLU	2.4
1	F	371	ALA	2.4
1	C	314	LEU	2.3
1	C	358	CYS	2.3
1	F	440	ALA	2.2
1	F	299	PRO	2.2
1	F	333	GLU	2.2
1	F	437	LEU	2.2
1	F	322	GLU	2.2
1	A	404	THR	2.2
1	C	305	GLY	2.1
1	C	433	GLU	2.1
1	F	295	LEU	2.1
1	B	446	PRO	2.1
1	C	385	ALA	2.1
1	F	438	PHE	2.1
1	F	352	ILE	2.1
1	C	372	LEU	2.1
1	C	293	ASN	2.0
1	C	446	PRO	2.0
1	F	319	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	536[A]	ARG	2.0
1	A	572	LEU	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.