



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:29 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 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>

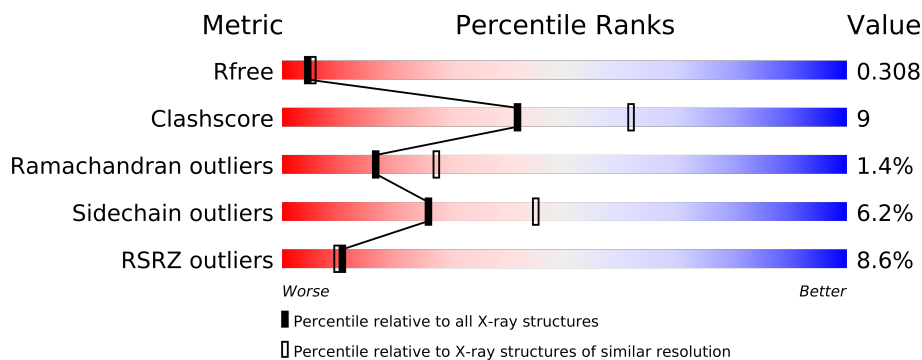
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. 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	319	
1	B	319	
1	C	319	
1	F	319	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9629 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 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			

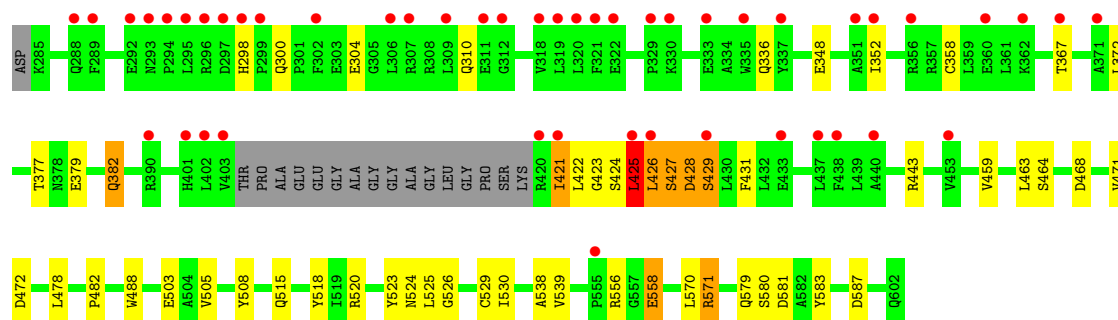
There are 4 discrepancies between the modelled and reference sequences:

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

Chain F: 

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) 89.6 (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)	0.30 , -3.0	EDS
Estimated twinning fraction	0.229 for h,h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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.

5 Model quality i

5.1 Standard geometry i

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

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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 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	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

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 9.

All (171) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:F:426:LEU:CD1	1:F:427:SER:N	2.41	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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	296/319 (93%)	263 (89%)	29 (10%)	4 (1%)	16	27
1	B	297/319 (93%)	276 (93%)	21 (7%)	0	100	100
1	C	299/319 (94%)	275 (92%)	18 (6%)	6 (2%)	11	17
1	F	298/319 (93%)	269 (90%)	23 (8%)	6 (2%)	11	17
All	All	1190/1276 (93%)	1083 (91%)	91 (8%)	16 (1%)	16	29

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
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%)	24	42
1	B	249/258 (96%)	232 (93%)	17 (7%)	22	39
1	C	249/258 (96%)	237 (95%)	12 (5%)	35	60
1	F	248/258 (96%)	232 (94%)	16 (6%)	24	42
All	All	994/1032 (96%)	933 (94%)	61 (6%)	26	46

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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	297/319 (93%)	0.41	2 (0%) 84 86	13, 22, 26, 29	0
1	B	297/319 (93%)	0.46	4 (1%) 74 76	17, 23, 27, 31	0
1	C	302/319 (94%)	0.93	49 (16%) 2 2	20, 23, 25, 28	1 (0%)
1	F	302/319 (94%)	0.88	48 (15%) 3 2	20, 23, 25, 28	0
All	All	1198/1276 (93%)	0.67	103 (8%) 11 10	13, 23, 26, 31	1 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	LEU	5.9
1	C	337	TYR	5.7
1	F	402	LEU	5.3
1	C	403	VAL	5.2
1	C	335	TRP	5.0
1	C	421	ILE	4.6
1	F	429	SER	4.4
1	C	301	PRO	4.3
1	F	555	PRO	4.3
1	F	367	THR	4.2
1	C	367	THR	4.2
1	F	330	LYS	4.1
1	F	426	LEU	4.0
1	F	298	HIS	3.9
1	C	286	GLY	3.9
1	C	294	PRO	3.9
1	C	318	VAL	3.9
1	C	420	ARG	3.9
1	C	299	PRO	3.9
1	F	337	TYR	3.8
1	F	309	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	402	LEU	3.8
1	F	421	ILE	3.8
1	C	425	LEU	3.7
1	C	444	LEU	3.7
1	F	296	ARG	3.6
1	F	420	ARG	3.5
1	C	391	ASP	3.4
1	C	307	ARG	3.4
1	F	289	PHE	3.3
1	F	294	PRO	3.2
1	C	429	SER	3.2
1	F	312	GLY	3.2
1	F	425	LEU	3.2
1	F	297	ASP	3.2
1	C	556	ARG	3.1
1	C	554	GLY	3.1
1	C	330	LYS	3.1
1	C	309	LEU	3.1
1	C	296	ARG	3.0
1	F	318	VAL	3.0
1	C	555	PRO	3.0
1	F	293	ASN	3.0
1	C	288	GLN	3.0
1	C	356	ARG	3.0
1	C	401	HIS	3.0
1	F	433	GLU	3.0
1	F	320	LEU	3.0
1	F	356	ARG	3.0
1	F	351	ALA	2.9
1	C	394	ARG	2.9
1	F	288	GLN	2.8
1	C	392	TRP	2.8
1	C	426	LEU	2.8
1	F	335	TRP	2.7
1	B	447	THR	2.7
1	F	307	ARG	2.6
1	F	362	LYS	2.6
1	F	321	PHE	2.6
1	C	315	PRO	2.6
1	C	395	TYR	2.6
1	F	292	GLU	2.6
1	F	360	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	404	THR	2.6
1	C	326	GLN	2.5
1	C	327	GLN	2.5
1	C	427	SER	2.5
1	C	431	PHE	2.5
1	F	311	GLU	2.5
1	F	302	PHE	2.5
1	F	403	VAL	2.5
1	F	390	ARG	2.5
1	F	371	ALA	2.4
1	B	286	GLY	2.4
1	C	314	LEU	2.4
1	C	558	GLU	2.4
1	C	291	GLU	2.4
1	F	329	PRO	2.4
1	A	285	LYS	2.4
1	F	295	LEU	2.3
1	C	390	ARG	2.3
1	A	404	THR	2.3
1	F	453	VAL	2.3
1	C	302	PHE	2.3
1	B	405	PRO	2.3
1	F	319	LEU	2.3
1	F	322	GLU	2.3
1	C	359	LEU	2.3
1	C	358	CYS	2.2
1	C	376	PHE	2.2
1	F	401	HIS	2.2
1	F	306	LEU	2.2
1	F	437	LEU	2.2
1	F	438	PHE	2.2
1	C	433	GLU	2.2
1	F	333	GLU	2.2
1	C	438	PHE	2.2
1	F	440	ALA	2.1
1	C	460	LEU	2.1
1	C	305	GLY	2.1
1	C	293	ASN	2.1
1	F	299	PRO	2.1
1	F	352	ILE	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.