



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:07 PM GMT

PDB ID : 2J9Q
Title : A NOVEL CONFORMATION FOR THE TPR DOMAIN OF PEX5P
Authors : Stanley, W.A.; Wilmanns, M.; Kursula, P.
Deposited on : 2006-11-15
Resolution : 2.65 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>

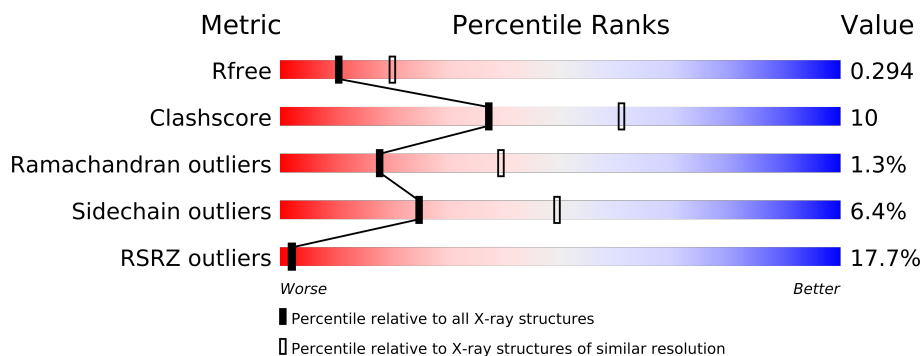
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.65 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	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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	328	
1	B	328	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4468 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	300	Total	C	N	O	S	0	1	0
			2356	1482	409	452	13			
1	B	269	Total	C	N	O	S	0	0	0
			2092	1316	365	400	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	GLY	-	EXPRESSION TAG	UNP P50542
A	313	MET	-	EXPRESSION TAG	UNP P50542
A	314	GLY	-	EXPRESSION TAG	UNP P50542
A	425	ILE	THR	CONFLICT	UNP P50542
B	312	GLY	-	EXPRESSION TAG	UNP P50542
B	313	MET	-	EXPRESSION TAG	UNP P50542
B	314	GLY	-	EXPRESSION TAG	UNP P50542
B	425	ILE	THR	CONFLICT	UNP P50542

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Sr	0	0
			1	1		
2	A	1	Total	Sr	0	0
			1	1		

- Molecule 3 is water.

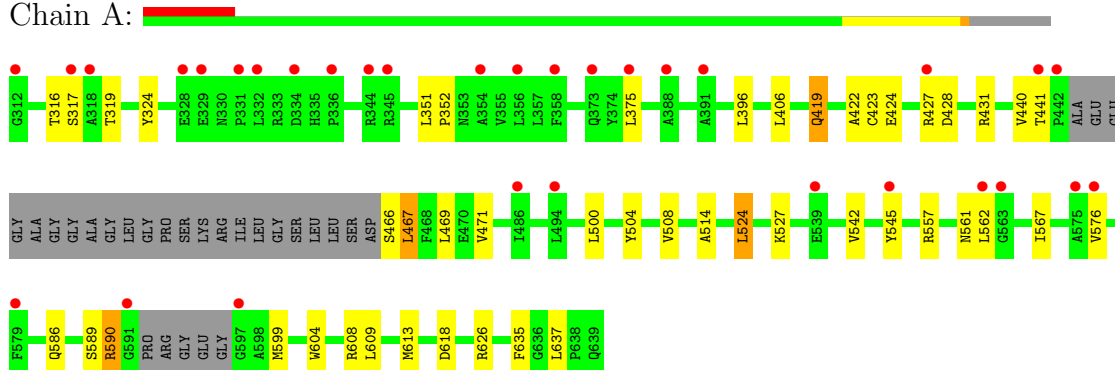
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	5	Total	O	0	0
			5	5		

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.

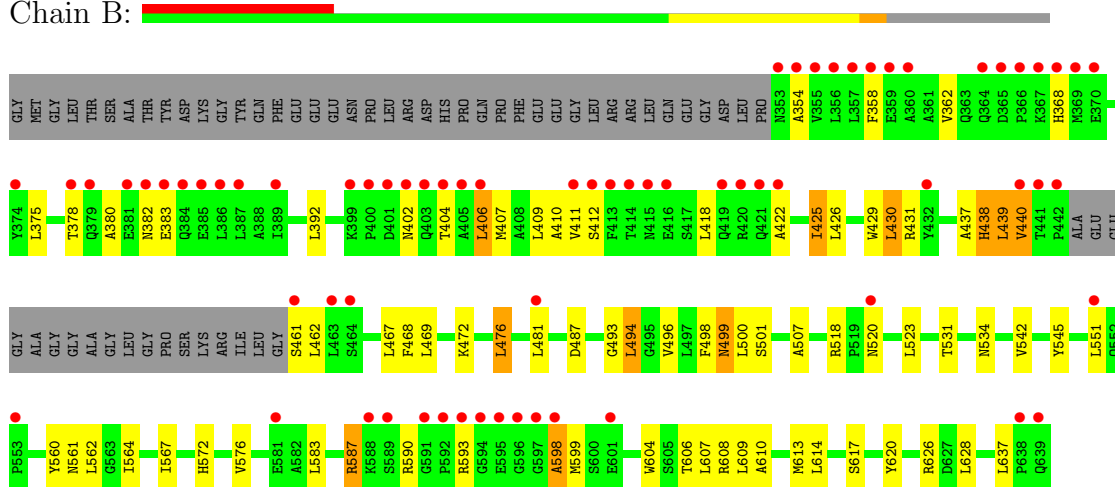
• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

Chain A:



• Molecule 1: PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.67Å 91.41Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.65) 94.0 (19.53-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.300 0.239 , 0.294	Depositor DCC
R_{free} test set	833 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 16659 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4468	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SR

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	0.32	0/2403	0.48	0/3256
1	B	0.32	0/2129	0.49	0/2887
All	All	0.32	0/4532	0.49	0/6143

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2356	0	2308	38	0
1	B	2092	0	2068	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	0	1	0
3	B	5	0	0	0	0
All	All	4468	0	4376	89	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 10.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:468:PHE:CE1	1:B:500:LEU:HD11	1.96	0.99
1:B:411:VAL:HG11	1:B:523:LEU:HD22	1.66	0.78
1:A:440:VAL:HG12	1:A:441:THR:H	1.51	0.76
1:A:609:LEU:HD23	1:B:609:LEU:HD23	1.70	0.72
1:B:392:LEU:HD13	1:B:409:LEU:HB3	1.74	0.70
1:B:409:LEU:HD12	1:B:410:ALA:N	2.07	0.70
1:A:609:LEU:HD21	1:B:606:THR:HG23	1.73	0.69
1:A:422:ALA:HB3	1:A:500:LEU:HD11	1.76	0.68
1:B:468:PHE:CD1	1:B:500:LEU:HD11	2.30	0.66
1:B:410:ALA:HB2	1:B:426:LEU:HD21	1.81	0.63
1:B:422:ALA:O	1:B:425:ILE:HG22	1.99	0.63
1:B:392:LEU:HD13	1:B:409:LEU:CB	2.30	0.60
1:B:418:LEU:O	1:B:422:ALA:HB3	2.01	0.60
1:B:520:ASN:O	1:B:551:LEU:HD13	2.02	0.59
1:A:604:TRP:CE2	1:A:626:ARG:HG3	2.37	0.59
1:B:499:ASN:HD21	1:B:534:ASN:HD22	1.50	0.59
1:B:380:ALA:HB1	1:B:412:SER:CB	2.33	0.59
1:A:316:THR:HG22	1:A:317:SER:H	1.69	0.57
1:A:567:ILE:CG2	1:B:613:MET:CE	2.83	0.57
1:A:567:ILE:HG21	1:B:613:MET:CE	2.35	0.57
1:B:576:VAL:HG13	1:B:607:LEU:HD11	1.87	0.56
1:B:500:LEU:HD12	1:B:500:LEU:C	2.26	0.56
1:B:429:TRP:HE3	1:B:430:LEU:HD12	1.71	0.55
1:B:567:ILE:HD11	1:B:610:ALA:HB2	1.87	0.55
1:B:439:LEU:HD22	1:B:440:VAL:N	2.23	0.54
1:B:410:ALA:CB	1:B:426:LEU:HD21	2.37	0.54
1:A:567:ILE:CG2	1:B:613:MET:HE2	2.38	0.53
1:B:406:LEU:HD13	1:B:429:TRP:HE1	1.72	0.53
1:B:545:TYR:CZ	1:B:561:ASN:HB3	2.44	0.53
1:A:419:GLN:NE2	3:A:2005:HOH:O	2.42	0.52
1:B:583:LEU:HD13	1:B:604:TRP:CZ2	2.44	0.52
1:A:613:MET:CE	1:B:613:MET:CE	2.88	0.52
1:B:476:LEU:HD13	1:B:494:LEU:HD11	1.91	0.52
1:A:567:ILE:HG21	1:B:613:MET:HE3	1.92	0.52
1:A:545:TYR:CZ	1:A:561:ASN:HB3	2.46	0.51
1:B:587:ARG:HG3	1:B:628:LEU:HD23	1.92	0.51
1:B:494:LEU:HD22	1:B:498:PHE:CD2	2.46	0.50
1:A:576:VAL:HG11	1:A:635:PHE:CE2	2.46	0.50
1:B:409:LEU:HD12	1:B:410:ALA:HB2	1.93	0.49
1:B:358:PHE:HB2	1:B:375:LEU:HD13	1.93	0.49
1:B:383:GLU:CD	1:B:598:ALA:HB1	2.31	0.49
1:B:500:LEU:HD12	1:B:501:SER:N	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:428:ASP:HA	1:A:431:ARG:HG2	1.94	0.49
1:B:499:ASN:HD21	1:B:534:ASN:ND2	2.11	0.49
1:B:407:MET:CE	1:B:410:ALA:HB3	2.44	0.48
1:B:542:VAL:HG13	1:B:562:LEU:HD11	1.95	0.48
1:A:467:LEU:HD22	1:A:471:VAL:HG23	1.95	0.48
1:B:378:THR:O	1:B:378:THR:HG22	2.14	0.47
1:A:422:ALA:CB	1:A:500:LEU:HD11	2.44	0.47
1:A:557:ARG:HA	1:A:599:MET:HE1	1.96	0.47
1:A:351:LEU:N	1:A:352:PRO:CD	2.78	0.47
1:A:316:THR:HG22	1:A:317:SER:N	2.29	0.47
1:B:493:GLY:O	1:B:496:VAL:HG22	2.15	0.47
1:B:358:PHE:O	1:B:362:VAL:HG13	2.14	0.46
1:B:617:SER:HA	1:B:620:TYR:CE1	2.51	0.46
1:A:419:GLN:HB3	1:A:500:LEU:HD22	1.98	0.46
1:A:324:TYR:OH	1:A:375:LEU:HD11	2.16	0.45
1:A:424:GLU:HG3	1:A:467:LEU:HD11	1.98	0.45
1:B:409:LEU:HD13	1:B:425:ILE:HG23	2.00	0.44
1:B:380:ALA:HB1	1:B:412:SER:OG	2.17	0.44
1:B:437:ALA:O	1:B:439:LEU:HD12	2.19	0.43
1:A:466:SER:OG	1:A:469:LEU:HD13	2.18	0.43
1:A:423:CYS:HB3	1:A:471:VAL:HG21	2.01	0.43
1:A:504:TYR:O	1:A:508:VAL:HG23	2.18	0.43
1:A:604:TRP:CZ2	1:A:626:ARG:HG3	2.53	0.43
1:A:586:GLN:O	1:A:590:ARG:HG3	2.18	0.43
1:B:572:HIS:HB2	1:B:614:LEU:HD13	2.00	0.43
1:B:354:ALA:CB	1:B:378:THR:HG21	2.49	0.42
1:A:567:ILE:CG2	1:B:613:MET:HE3	2.48	0.42
1:B:507:ALA:HB3	1:B:531:THR:HG21	2.02	0.42
1:B:467:LEU:HD13	1:B:467:LEU:C	2.40	0.42
1:B:468:PHE:CZ	1:B:501:SER:HB3	2.55	0.42
1:A:514:ALA:CB	1:A:524:LEU:HD11	2.50	0.41
1:A:396:LEU:HD21	1:A:406:LEU:HG	2.02	0.41
1:B:560:TYR:CZ	1:B:564:ILE:HD11	2.55	0.41
1:A:431:ARG:HB3	1:A:440:VAL:HG21	2.02	0.41
1:B:609:LEU:HG	1:B:613:MET:CE	2.50	0.41
1:A:542:VAL:HG13	1:A:562:LEU:HD11	2.03	0.41
1:B:407:MET:HE1	1:B:410:ALA:HB3	2.02	0.41
1:A:467:LEU:HD22	1:A:471:VAL:CG2	2.51	0.41
1:B:438:HIS:CG	1:B:438:HIS:O	2.74	0.41
1:A:423:CYS:HB2	1:A:467:LEU:HD13	2.03	0.41
1:A:613:MET:HE1	1:B:613:MET:HE2	2.04	0.40
1:B:409:LEU:HD22	1:B:425:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:618:ASP:OD2	1:A:618:ASP:N	2.54	0.40
1:B:469:LEU:HD12	1:B:472:LYS:HE3	2.03	0.40
1:B:437:ALA:O	1:B:439:LEU:N	2.54	0.40
1:A:613:MET:CE	1:B:613:MET:HE2	2.51	0.40
1:B:609:LEU:HG	1:B:613:MET:HE3	2.03	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	295/328 (90%)	280 (95%)	13 (4%)	2 (1%)	30	59
1	B	265/328 (81%)	236 (89%)	24 (9%)	5 (2%)	12	26
All	All	560/656 (85%)	516 (92%)	37 (7%)	7 (1%)	18	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	589	SER
1	A	590	ARG
1	B	368	HIS
1	B	402	ASN
1	B	438	HIS
1	B	598	ALA
1	B	440	VAL

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	248/264 (94%)	240 (97%)	8 (3%)	51	81
1	B	220/264 (83%)	198 (90%)	22 (10%)	11	23
All	All	468/528 (89%)	438 (94%)	30 (6%)	25	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	THR
1	A	419	GLN
1	A	427	ARG
1	A	467	LEU
1	A	524	LEU
1	A	527	LYS
1	A	608	ARG
1	A	637	LEU
1	B	382	ASN
1	B	404	THR
1	B	406	LEU
1	B	425	ILE
1	B	430	LEU
1	B	431	ARG
1	B	439	LEU
1	B	461	SER
1	B	462	LEU
1	B	476	LEU
1	B	481	LEU
1	B	487	ASP
1	B	494	LEU
1	B	499	ASN
1	B	518	ARG
1	B	587	ARG
1	B	590	ARG
1	B	593	ARG
1	B	599	MET
1	B	608	ARG
1	B	626	ARG
1	B	637	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	B	353	ASN
1	B	382	ASN
1	B	415	ASN
1	B	499	ASN
1	B	616	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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	300/328 (91%)	0.90	32 (10%) 6 6	39, 44, 47, 52	0
1	B	269/328 (82%)	1.38	69 (25%) 1 1	39, 44, 50, 57	0
All	All	569/656 (86%)	1.13	101 (17%) 2 2	39, 44, 48, 57	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ASP	8.0
1	B	594	GLY	7.7
1	B	386	LEU	6.4
1	B	593	ARG	5.8
1	A	441	THR	5.5
1	B	442	PRO	5.4
1	A	591	GLY	5.3
1	B	357	LEU	5.3
1	B	356	LEU	5.1
1	B	353	ASN	5.0
1	B	403	GLN	4.9
1	B	402	ASN	4.9
1	B	414	THR	4.9
1	B	595	GLU	4.9
1	B	415	ASN	4.6
1	B	404	THR	4.6
1	B	383	GLU	4.3
1	B	411	VAL	4.2
1	B	440	VAL	4.2
1	A	312	GLY	4.0
1	B	355	VAL	4.0
1	B	374	TYR	4.0
1	B	381	GLU	4.0
1	B	405	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	389	ILE	3.9
1	B	400	PRO	3.9
1	B	432	TYR	3.8
1	B	354	ALA	3.8
1	B	591	GLY	3.8
1	B	441	THR	3.6
1	B	413	PHE	3.6
1	A	579	PHE	3.5
1	A	331	PRO	3.5
1	A	563	GLY	3.5
1	B	592	PRO	3.4
1	A	332	LEU	3.4
1	B	416	GLU	3.4
1	B	638	PRO	3.3
1	B	367	LYS	3.3
1	A	318	ALA	3.3
1	B	387	LEU	3.3
1	A	329	GLU	3.3
1	B	382	ASN	3.3
1	B	369	MET	3.2
1	B	419	GLN	3.2
1	A	391	ALA	3.1
1	B	596	GLY	3.1
1	B	598	ALA	3.1
1	B	358	PHE	3.1
1	A	597	GLY	3.0
1	B	365	ASP	3.0
1	B	379	GLN	2.9
1	B	370	GLU	2.9
1	B	384	GLN	2.9
1	B	601	GLU	2.8
1	B	420	ARG	2.8
1	B	422	ALA	2.8
1	B	461	SER	2.8
1	B	399	LYS	2.8
1	A	317	SER	2.8
1	A	562	LEU	2.7
1	B	421	GLN	2.7
1	B	360	ALA	2.7
1	A	328	GLU	2.6
1	A	442	PRO	2.6
1	A	388	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	597	GLY	2.5
1	B	385	GLU	2.5
1	A	545	TYR	2.5
1	B	364	GLN	2.4
1	B	520	ASN	2.4
1	B	481	LEU	2.4
1	A	576	VAL	2.4
1	A	345	ARG	2.4
1	A	539	GLU	2.4
1	A	375	LEU	2.4
1	A	427	ARG	2.4
1	A	356	LEU	2.4
1	A	336	PRO	2.3
1	A	373	GLN	2.3
1	B	639	GLN	2.3
1	A	494	LEU	2.3
1	B	378	THR	2.3
1	B	366	PRO	2.3
1	B	589	SER	2.3
1	A	344	ARG	2.3
1	A	334	ASP	2.3
1	B	581	GLU	2.2
1	B	359	GLU	2.2
1	A	358	PHE	2.2
1	B	464	SER	2.2
1	B	588	LYS	2.1
1	B	463	LEU	2.1
1	B	551	LEU	2.1
1	A	486	ILE	2.1
1	B	412	SER	2.1
1	B	368	HIS	2.1
1	B	406	LEU	2.1
1	A	575	ALA	2.0
1	B	553	PRO	2.0
1	A	354	ALA	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SR	B	1640	1/1	0.10	-1.68	44,44,44,44	0
2	SR	A	1640	1/1	0.10	-1.76	47,47,47,47	0

6.5 Other polymers

There are no such residues in this entry.