



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:08 AM GMT

PDB ID : 2FTS
Title : Crystal structure of the glycine receptor-gephyrin complex
Authors : Kim, E.Y.; Schindelin, H.
Deposited on : 2006-01-24
Resolution : 2.41 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

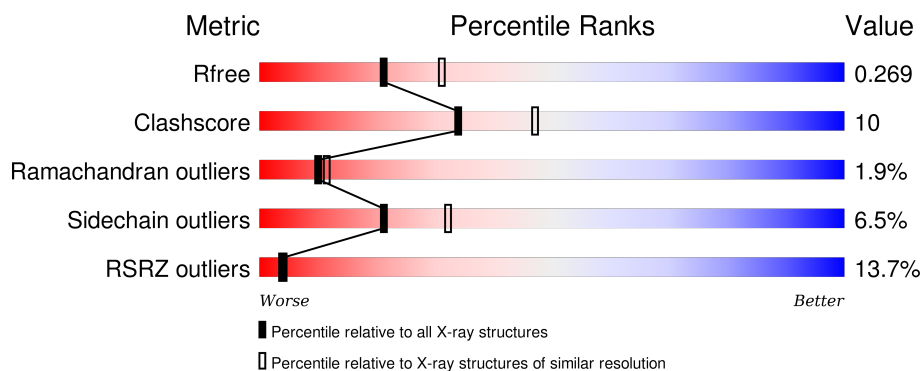
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	419	
2	P	13	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3448 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 gephyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3194	2012	554	607	21			

- Molecule 2 is a protein called Glycine receptor beta chain precursor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	0	0	0
			104	69	16	19			

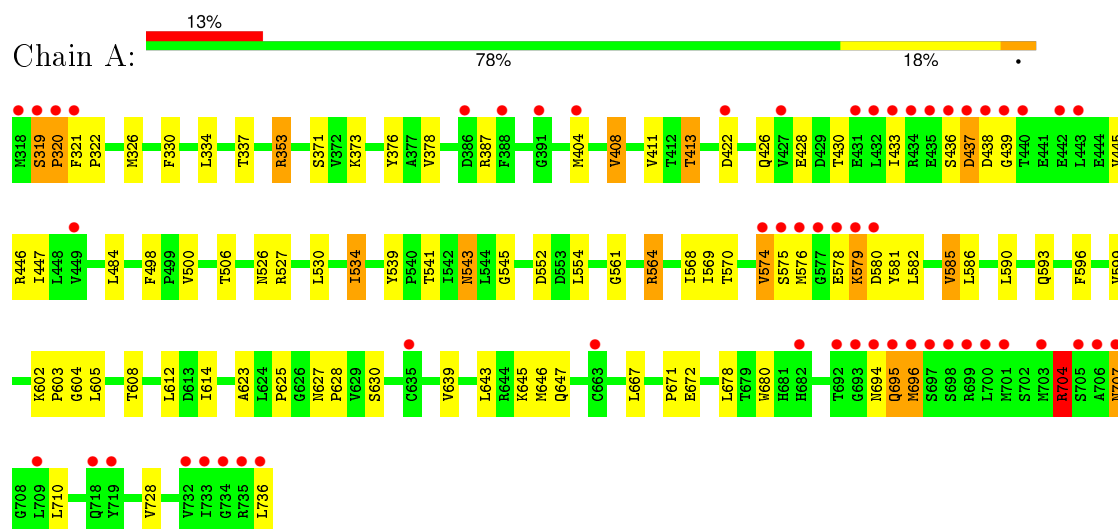
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	P	1	Total	O	0	0
			1	1		

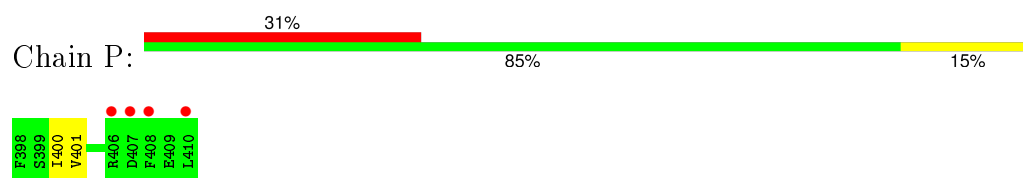
3 Residue-property plots [i](#)

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: gephyrin



• Molecule 2: Glycine receptor beta chain precursor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.30Å 123.54Å 155.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.41 40.43 – 2.41	Depositor EDS
% Data completeness (in resolution range)	93.2 (20.00-2.41) 93.2 (40.43-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.192 , 0.272 0.206 , 0.269	Depositor DCC
R_{free} test set	934 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18221 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3448	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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 [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	0.87	1/3255 (0.0%)	0.79	3/4427 (0.1%)
2	P	0.83	0/106	0.49	0/142
All	All	0.87	1/3361 (0.0%)	0.78	3/4569 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ASP	CB-CG	6.94	1.66	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	704	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	439	GLY	N-CA-C	-5.22	100.06	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3194	0	3235	67	0
2	P	104	0	102	4	0
3	A	149	0	0	3	1
3	P	1	0	0	0	0
All	All	3448	0	3337	67	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 (67) 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:A:678:LEU:H	1:A:707:ASN:HD21	1.15	0.94
1:A:643:LEU:HD23	1:A:646:MET:HE3	1.63	0.80
1:A:527:ARG:HH11	1:A:543:ASN:HD21	1.28	0.79
1:A:608:THR:HB	1:A:623:ALA:HB3	1.69	0.74
1:A:433:ILE:HD11	1:A:446:ARG:HG2	1.71	0.72
1:A:564:ARG:HH11	1:A:564:ARG:HG2	1.56	0.71
1:A:581:TYR:O	1:A:585:VAL:HG12	1.92	0.69
1:A:321:PHE:HB3	1:A:322:PRO:HD2	1.74	0.68
1:A:319:SER:O	1:A:320:PRO:C	2.35	0.65
1:A:602:LYS:O	1:A:672:GLU:HA	1.98	0.64
1:A:534:ILE:HD11	1:A:541:THR:CG2	2.29	0.62
1:A:707:ASN:HD22	1:A:707:ASN:H	1.47	0.62
1:A:371:SER:O	1:A:413:THR:O	2.18	0.61
1:A:437:ASP:OD2	1:A:438:ASP:N	2.34	0.60
1:A:426:GLN:HE21	1:A:428:GLU:HB2	1.67	0.60
1:A:436:SER:O	1:A:437:ASP:C	2.40	0.59
1:A:543:ASN:HD22	1:A:545:GLY:H	1.50	0.59
1:A:530:LEU:O	1:A:534:ILE:HG23	2.04	0.57
1:A:319:SER:HB3	1:A:320:PRO:HD2	1.87	0.56
1:A:704:ARG:HG2	1:A:704:ARG:HH11	1.71	0.56
1:A:671:PRO:HB3	2:P:401:VAL:HG13	1.87	0.55
1:A:526:ASN:HD21	1:A:628:PRO:HA	1.70	0.55
1:A:604:GLY:HA2	1:A:625:PRO:HG2	1.89	0.54
1:A:543:ASN:ND2	1:A:545:GLY:H	2.05	0.54
1:A:321:PHE:HB3	1:A:322:PRO:CD	2.39	0.53
1:A:404:MET:HE2	3:A:9:HOH:O	2.08	0.53
1:A:353:ARG:HD2	1:A:498:PHE:CE1	2.44	0.53
1:A:554:LEU:HD12	1:A:582:LEU:HD13	1.91	0.51
1:A:704:ARG:HH11	1:A:704:ARG:CG	2.23	0.51
1:A:581:TYR:O	1:A:585:VAL:CG1	2.60	0.50
1:A:373:LYS:HD3	1:A:426:GLN:HB3	1.94	0.49
1:A:678:LEU:N	1:A:707:ASN:HD21	1.98	0.48
1:A:695:GLN:O	1:A:696:MET:HB2	2.13	0.48
1:A:627:ASN:HD22	1:A:630:SER:H	1.60	0.48
1:A:643:LEU:HD23	1:A:646:MET:CE	2.41	0.48
1:A:446:ARG:HG3	3:A:79:HOH:O	2.12	0.47
1:A:534:ILE:HD11	1:A:541:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LEU:HD11	1:A:728:VAL:HG21	1.95	0.47
1:A:534:ILE:HD11	1:A:541:THR:HG22	1.96	0.47
1:A:578:GLU:O	1:A:579:LYS:HB3	2.15	0.47
1:A:322:PRO:HG2	1:A:596:PHE:HA	1.96	0.47
1:A:326:MET:CE	2:P:400:ILE:HD12	2.46	0.45
1:A:543:ASN:C	1:A:543:ASN:HD22	2.19	0.45
1:A:334:LEU:O	1:A:645:LYS:HE3	2.17	0.45
1:A:695:GLN:O	1:A:696:MET:CB	2.65	0.44
1:A:569:ILE:HD11	1:A:639:VAL:HG11	1.99	0.44
1:A:570:THR:HG21	1:A:582:LEU:CD2	2.48	0.43
1:A:376:TYR:CE1	1:A:430:THR:HG21	2.54	0.43
1:A:319:SER:O	1:A:321:PHE:N	2.52	0.43
1:A:603:PRO:HB2	1:A:630:SER:OG	2.18	0.42
1:A:570:THR:HG21	1:A:582:LEU:HD21	2.00	0.42
1:A:561:GLY:HA3	1:A:568:ILE:HD11	2.01	0.42
1:A:353:ARG:HD3	3:A:35:HOH:O	2.20	0.42
1:A:330:PHE:HB2	2:P:400:ILE:HD11	2.00	0.42
1:A:408:VAL:HG21	1:A:447:ILE:HD11	2.01	0.42
1:A:680:TRP:CH2	1:A:736:LEU:HD13	2.55	0.42
1:A:337:THR:O	1:A:645:LYS:HE3	2.20	0.41
1:A:534:ILE:HD12	1:A:539:TYR:HB2	2.01	0.41
1:A:576:MET:SD	1:A:576:MET:N	2.93	0.41
1:A:506:THR:HG21	1:A:554:LEU:HD11	2.01	0.41
1:A:707:ASN:HD22	1:A:707:ASN:N	2.09	0.41
1:A:330:PHE:HB2	2:P:400:ILE:CD1	2.51	0.41
1:A:574:VAL:HG12	1:A:579:LYS:HA	2.03	0.41
1:A:376:TYR:HB3	1:A:408:VAL:HG13	2.02	0.40
1:A:408:VAL:HG21	1:A:447:ILE:CD1	2.51	0.40
1:A:586:LEU:HD23	1:A:590:LEU:HD12	2.03	0.40
1:A:707:ASN:ND2	1:A:707:ASN:H	2.16	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:A:125:HOH:O	3:A:126:HOH:O[3_554]	1.92	0.28

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	417/419 (100%)	396 (95%)	13 (3%)	8 (2%)	10	11
2	P	11/13 (85%)	11 (100%)	0	0	100	100
All	All	428/432 (99%)	407 (95%)	13 (3%)	8 (2%)	10	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	SER
1	A	580	ASP
1	A	696	MET
1	A	579	LYS
1	A	695	GLN
1	A	319	SER
1	A	320	PRO
1	A	437	ASP

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	356/356 (100%)	332 (93%)	24 (7%)	20	31
2	P	12/12 (100%)	12 (100%)	0	100	100
All	All	368/368 (100%)	344 (94%)	24 (6%)	21	32

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	VAL
1	A	387	ARG
1	A	408	VAL
1	A	411	VAL
1	A	413	THR
1	A	445	VAL
1	A	484	LEU
1	A	500	VAL
1	A	534	ILE
1	A	543	ASN
1	A	552	ASP
1	A	564	ARG
1	A	574	VAL
1	A	585	VAL
1	A	593	GLN
1	A	599	VAL
1	A	605	LEU
1	A	612	LEU
1	A	614	ILE
1	A	647	GLN
1	A	667	LEU
1	A	694	ASN
1	A	704	ARG
1	A	707	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	GLN
1	A	508	ASN
1	A	526	ASN
1	A	537	HIS
1	A	543	ASN
1	A	550	ASN
1	A	627	ASN
1	A	681	HIS
1	A	707	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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

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	419/419 (100%)	0.91	55 (13%) 5 4	39, 46, 52, 71	0
2	P	13/13 (100%)	1.83	4 (30%) 1 0	52, 56, 80, 81	0
All	All	432/432 (100%)	0.94	59 (13%) 4 4	39, 46, 53, 81	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	440	THR	11.5
1	A	577	GLY	8.9
1	A	693	GLY	8.5
1	A	700	LEU	7.7
1	A	436	SER	7.4
1	A	575	SER	7.3
2	P	406	ARG	6.6
1	A	574	VAL	5.8
1	A	319	SER	5.2
1	A	576	MET	4.8
1	A	698	SER	4.8
1	A	694	ASN	4.6
2	P	407	ASP	4.5
1	A	437	ASP	4.4
1	A	699	ARG	4.3
2	P	408	PHE	4.3
1	A	320	PRO	4.3
1	A	443	LEU	4.2
1	A	735	ARG	4.1
1	A	318	MET	4.0
1	A	733	ILE	4.0
1	A	435	GLU	4.0
1	A	432	LEU	3.8
1	A	388	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	433	ILE	3.8
1	A	578	GLU	3.7
1	A	404	MET	3.7
1	A	734	GLY	3.6
1	A	321	PHE	3.5
1	A	579	LYS	3.4
1	A	580	ASP	3.2
1	A	692	THR	3.2
1	A	701	MET	3.1
1	A	696	MET	3.1
1	A	697	SER	3.1
1	A	732	VAL	2.9
1	A	439	GLY	2.9
1	A	736	LEU	2.8
1	A	718	GLN	2.8
1	A	705	SER	2.7
1	A	438	ASP	2.7
1	A	719	TYR	2.6
2	P	410	LEU	2.6
1	A	703	MET	2.6
1	A	635	CYS	2.6
1	A	442	GLU	2.5
1	A	434	ARG	2.5
1	A	695	GLN	2.5
1	A	422	ASP	2.4
1	A	391	GLY	2.4
1	A	682	HIS	2.3
1	A	427	VAL	2.3
1	A	386	ASP	2.3
1	A	663	CYS	2.2
1	A	706	ALA	2.2
1	A	449	VAL	2.1
1	A	431	GLU	2.1
1	A	707	ASN	2.0
1	A	709	LEU	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 [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.