



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:54 AM UTC

PDB ID : 6CRF / pdb_00006crf
Title : Crystal Structure of Shp2 E76K GOF Mutant in the Open Conformation
Authors : Stams, T.; Fodor, M.
Deposited on : 2018-03-17
Resolution : 2.62 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

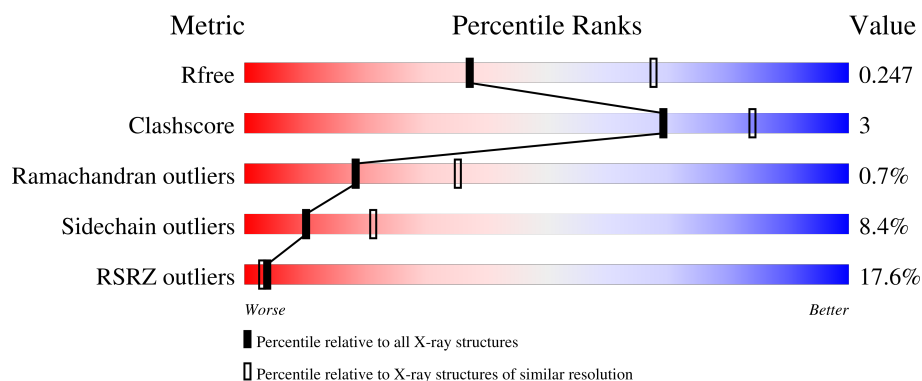
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	526	14% 73% 16% • 10%
1	B	526	17% 74% 10% • 14%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7170 atoms, of which 1 is hydrogen 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.

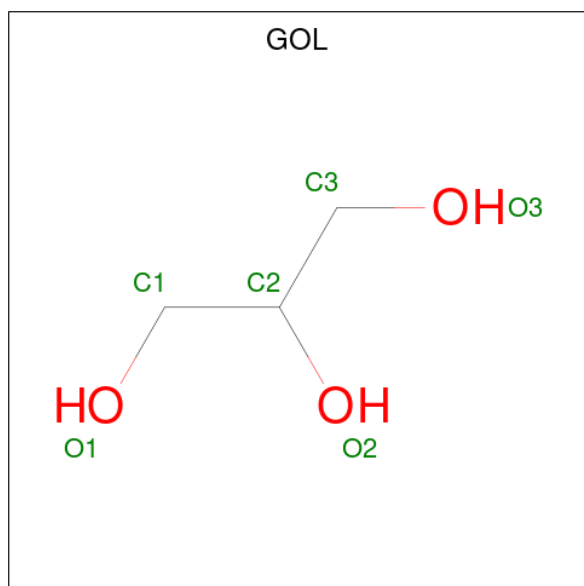
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	475	Total	C	H	N	O	S	0	0	0
			3679	2316	1	659	687	16			
1	B	451	Total	C	N	O	S		0	0	0
			3277	2045	596	621	15				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q06124
A	76	LYS	GLU	engineered mutation	UNP Q06124
B	0	GLY	-	expression tag	UNP Q06124
B	76	LYS	GLU	engineered mutation	UNP Q06124

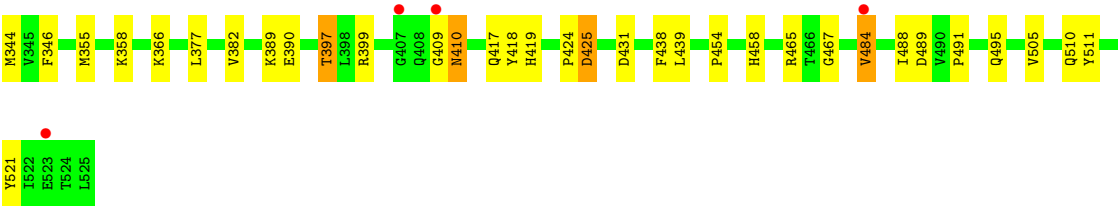
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	118	Total	O	0	0
			118	118		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.10Å 41.73Å 153.85Å 90.00° 125.76° 90.00°	Depositor
Resolution (Å)	124.84 – 2.62 124.84 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.5 (124.84-2.62) 99.8 (124.84-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.198 , 0.237 (Not available) , 0.247	Depositor DCC
R_{free} test set	1936 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.88	2/3751 (0.1%)	1.36	16/5074 (0.3%)
1	B	0.91	0/3332	1.37	20/4517 (0.4%)
All	All	0.89	2/7083 (0.0%)	1.36	36/9591 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	VAL	CA-C	5.57	1.57	1.52
1	A	85	HIS	CA-C	5.08	1.59	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	PRO	CA-C-N	7.38	135.65	121.54
1	B	424	PRO	C-N-CA	7.38	135.65	121.54
1	A	334	LEU	N-CA-C	-7.14	99.96	110.52
1	B	489	ASP	CA-C-N	6.93	125.88	120.33
1	B	489	ASP	C-N-CA	6.93	125.88	120.33
1	A	64	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	334	LEU	N-CA-C	-6.91	100.24	110.46
1	A	303	ASP	CA-CB-CG	6.65	119.25	112.60
1	B	467	GLY	CA-C-N	6.37	128.72	120.44
1	B	467	GLY	C-N-CA	6.37	128.72	120.44
1	A	65	LEU	N-CA-C	-6.06	102.63	111.30
1	A	35	LYS	N-CA-C	-5.96	105.09	112.90
1	B	303	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	222	ASN	N-CA-C	-5.64	100.79	109.76
1	B	409	GLY	CA-C-N	5.50	129.91	120.72
1	B	409	GLY	C-N-CA	5.50	129.91	120.72
1	B	425	ASP	CA-CB-CG	5.44	118.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	GLN	CA-C-N	5.43	127.49	120.44
1	B	510	GLN	C-N-CA	5.43	127.49	120.44
1	B	521	TYR	CA-C-N	5.42	127.39	120.56
1	B	521	TYR	C-N-CA	5.42	127.39	120.56
1	A	133	GLY	CA-C-N	5.40	128.37	120.71
1	A	133	GLY	C-N-CA	5.40	128.37	120.71
1	A	358	LYS	N-CA-C	-5.39	102.50	110.48
1	B	304	TYR	N-CA-C	5.38	118.59	109.76
1	B	358	LYS	N-CA-C	-5.30	102.68	110.52
1	A	432	PRO	CA-C-N	5.27	125.95	119.99
1	A	432	PRO	C-N-CA	5.27	125.95	119.99
1	B	346	PHE	CA-C-N	5.24	127.56	120.38
1	B	346	PHE	C-N-CA	5.24	127.56	120.38
1	A	298	ASN	CA-C-N	5.15	127.57	120.67
1	A	298	ASN	C-N-CA	5.15	127.57	120.67
1	A	509	ALA	CA-C-N	5.15	127.14	120.44
1	A	509	ALA	C-N-CA	5.15	127.14	120.44
1	A	35	LYS	CA-C-N	5.02	127.51	120.28
1	A	35	LYS	C-N-CA	5.02	127.51	120.28

There are no chirality outliers.

There are no planarity outliers.

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	3678	1	3461	29	0
1	B	3277	0	2840	18	0
2	B	6	0	8	0	0
3	A	90	0	0	0	0
3	B	118	0	0	0	0
All	All	7169	1	6309	46	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 3.

All (46) 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:B:390:GLU:HG2	1:B:399:ARG:HG2	1.73	0.69
1:A:201:PRO:HB3	1:A:211:GLN:HA	1.75	0.68
1:A:518:VAL:O	1:A:522:ILE:HG12	2.00	0.61
1:A:1:MET:HB3	1:A:79:GLN:OE1	2.03	0.58
1:A:418:TYR:HB3	1:A:438:PHE:CE1	2.39	0.58
1:A:224:ALA:HB2	1:A:484:VAL:HG13	1.87	0.57
1:A:57:GLN:HE22	1:B:271:GLN:HE21	1.53	0.55
1:A:358:LYS:HB2	1:A:361:GLU:HG3	1.90	0.54
1:A:397:THR:HG22	1:A:421:ARG:HD3	1.90	0.53
1:A:273:ASN:HA	1:A:276:LYS:HD2	1.91	0.51
1:B:491:PRO:HG3	1:B:511:TYR:OH	2.10	0.51
1:B:410:ASN:ND2	1:B:410:ASN:H	2.08	0.51
1:B:399:ARG:HD2	1:B:417:GLN:OE1	2.11	0.50
1:B:418:TYR:HB3	1:B:438:PHE:CE1	2.46	0.50
1:A:26:ASP:HA	1:A:46:ARG:HG2	1.94	0.50
1:A:369:LYS:HD3	1:A:371:TRP:O	2.11	0.49
1:B:6:TRP:HZ2	1:B:75:ALA:HA	1.78	0.49
1:A:134:SER:HA	1:A:214:GLN:O	2.13	0.49
1:A:390:GLU:HG2	1:A:399:ARG:HG2	1.93	0.49
1:B:150:SER:HA	1:B:169:HIS:HA	1.94	0.48
1:B:397:THR:HG23	1:B:419:HIS:HB3	1.95	0.48
1:B:290:VAL:HG11	1:B:344:MET:HG3	1.96	0.48
1:B:309:ILE:HD13	1:B:328:ILE:HG12	1.96	0.48
1:B:355:MET:HG3	1:B:458:HIS:CE1	2.49	0.47
1:A:475:LEU:HA	1:A:478:ILE:HD12	1.96	0.47
1:A:247:PHE:CG	1:A:512:ARG:HG2	2.50	0.46
1:A:418:TYR:HB3	1:A:438:PHE:HE1	1.79	0.46
1:B:418:TYR:HB3	1:B:438:PHE:HE1	1.81	0.46
1:A:47:ARG:HH22	1:A:89:LYS:HZ2	1.64	0.45
1:B:328:ILE:HG13	1:B:454:PRO:HB2	1.98	0.45
1:A:43:LEU:HD21	1:A:98:LEU:HD21	1.99	0.44
1:A:248:TRP:CE2	1:A:252:GLU:HG3	2.53	0.44
1:A:403:LEU:O	1:A:412:GLU:HA	2.17	0.44
1:A:3:SER:HB2	1:A:5:ARG:HG3	2.00	0.43
1:A:81:TYR:CD1	1:A:87:GLN:HG2	2.52	0.43
1:B:261:LEU:HD22	1:B:495:GLN:NE2	2.33	0.43
1:B:223:ALA:HB3	1:B:484:VAL:O	2.19	0.42
1:A:226:ILE:HD13	1:A:488:ILE:HD11	2.01	0.42
1:A:233:LEU:HA	1:A:246:GLY:HA3	2.01	0.42
1:A:450:MET:HE2	1:A:450:MET:HB3	1.88	0.42
1:B:77:LEU:HD13	1:B:77:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD11	1:A:344:MET:HB2	2.02	0.41
1:B:65:LEU:HD13	1:B:77:LEU:HD21	2.02	0.41
1:A:355:MET:HG3	1:A:458:HIS:CE1	2.55	0.41
1:A:396:TYR:OH	1:A:441:GLU:HG2	2.22	0.40
1:A:446:GLN:HG3	1:A:455:VAL:CG2	2.52	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	459/526 (87%)	440 (96%)	16 (4%)	3 (1%)	18	35
1	B	425/526 (81%)	395 (93%)	27 (6%)	3 (1%)	18	35
All	All	884/1052 (84%)	835 (94%)	43 (5%)	6 (1%)	18	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	VAL
1	B	108	THR
1	A	217	ASN
1	B	59	THR
1	B	505	VAL
1	A	464	GLY

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	373/467 (80%)	340 (91%)	33 (9%)	9	19
1	B	292/467 (62%)	269 (92%)	23 (8%)	11	24
All	All	665/934 (71%)	609 (92%)	56 (8%)	10	21

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	LYS
1	A	36	SER
1	A	52	THR
1	A	61	ASP
1	A	65	LEU
1	A	87	GLN
1	A	88	LEU
1	A	95	VAL
1	A	108	THR
1	A	117	LEU
1	A	121	GLU
1	A	258	GLU
1	A	261	LEU
1	A	271	GLN
1	A	275	ASN
1	A	292	LEU
1	A	294	ASP
1	A	303	ASP
1	A	362	ARG
1	A	369	LYS
1	A	373	ASP
1	A	389	LYS
1	A	391	SER
1	A	408	GLN
1	A	439	LEU
1	A	450	MET
1	A	481	GLU
1	A	484	VAL
1	A	485	ASP
1	A	516	MET
1	A	523	GLU
1	A	525	LEU

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Mol	Chain	Res	Type
1	B	65	LEU
1	B	77	LEU
1	B	221	ILE
1	B	226	ILE
1	B	228	SER
1	B	272	GLU
1	B	280	LYS
1	B	292	LEU
1	B	299	GLU
1	B	303	ASP
1	B	335	GLN
1	B	366	LYS
1	B	377	LEU
1	B	382	VAL
1	B	389	LYS
1	B	397	THR
1	B	410	ASN
1	B	425	ASP
1	B	431	ASP
1	B	439	LEU
1	B	465	ARG
1	B	484	VAL
1	B	488	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	37	ASN
1	A	114	HIS
1	A	271	GLN
1	A	339	ASN
1	A	410	ASN
1	A	443	HIS
1	A	446	GLN
1	A	519	GLN
1	B	114	HIS
1	B	245	GLN
1	B	257	GLN
1	B	271	GLN
1	B	293	HIS
1	B	335	GLN

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Mol	Chain	Res	Type
1	B	446	GLN
1	B	495	GLN
1	B	506	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	601	-	5,5,5	0.10	0	5,5,5	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	601	-	-	0/4/4/4	-

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	117:LEU	C	118:SER	N	3.28

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	475/526 (90%)	0.71	72 (15%) 5 4	38, 66, 135, 164	0
1	B	451/526 (85%)	0.81	91 (20%) 3 2	29, 62, 164, 203	0
All	All	926/1052 (88%)	0.76	163 (17%) 4 3	29, 66, 150, 203	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	VAL	7.0
1	A	149	LEU	6.1
1	B	107	PRO	6.0
1	A	168	THR	5.8
1	B	168	THR	5.4
1	A	151	VAL	5.4
1	A	174	CYS	4.8
1	A	236	LEU	4.8
1	A	179	TYR	4.7
1	B	148	VAL	4.7
1	A	409	GLY	4.4
1	B	169	HIS	4.0
1	B	147	PHE	4.0
1	A	181	VAL	3.9
1	B	191	THR	3.9
1	B	201	PRO	3.9
1	B	234	SER	3.9
1	B	171	MET	3.9
1	A	150	SER	3.8
1	A	178	LYS	3.8
1	A	171	MET	3.7
1	A	93	GLY	3.6
1	B	86	GLY	3.5
1	A	202	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	108	THR	3.5
1	A	187	PHE	3.4
1	B	150	SER	3.4
1	A	190	LEU	3.4
1	A	169	HIS	3.4
1	B	146	ASP	3.4
1	B	181	VAL	3.4
1	B	112	TRP	3.3
1	A	136	LEU	3.3
1	B	10	ASN	3.3
1	A	85	HIS	3.3
1	B	185	GLU	3.3
1	B	26	ASP	3.3
1	A	108	THR	3.3
1	A	167	VAL	3.3
1	A	134	SER	3.2
1	A	148	VAL	3.2
1	A	259	CYS	3.2
1	A	426	HIS	3.1
1	A	194	VAL	3.1
1	B	29	PHE	3.1
1	B	145	GLY	3.1
1	B	223	ALA	3.1
1	B	188	ASP	3.1
1	B	59	THR	3.1
1	B	192	ASP	3.1
1	B	144	PRO	3.1
1	A	188	ASP	3.0
1	A	86	GLY	3.0
1	B	149	LEU	3.0
1	A	146	ASP	3.0
1	B	172	ILE	3.0
1	B	167	VAL	3.0
1	B	132	HIS	3.0
1	B	170	VAL	3.0
1	B	85	HIS	3.0
1	A	256	GLN	2.9
1	B	57	GLN	2.9
1	B	37	ASN	2.9
1	A	153	THR	2.9
1	A	180	ASP	2.9
1	B	180	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	197	TYR	2.9
1	B	98	LEU	2.9
1	A	211	GLN	2.8
1	B	6	TRP	2.8
1	B	54	ILE	2.8
1	A	128	GLU	2.8
1	A	424	PRO	2.8
1	A	193	LEU	2.8
1	A	525	LEU	2.8
1	B	194	VAL	2.8
1	A	126	LEU	2.8
1	B	65	LEU	2.7
1	B	51	VAL	2.7
1	A	428	VAL	2.7
1	A	172	ILE	2.7
1	B	46	ARG	2.7
1	B	44	SER	2.7
1	B	96	ILE	2.6
1	B	30	LEU	2.6
1	B	227	GLU	2.6
1	B	484	VAL	2.6
1	B	153	THR	2.6
1	B	523	GLU	2.6
1	B	151	VAL	2.6
1	B	190	LEU	2.5
1	A	199	LYS	2.5
1	B	110	GLU	2.5
1	A	152	ARG	2.5
1	A	216	LEU	2.5
1	B	186	ARG	2.5
1	A	137	VAL	2.5
1	A	212	LEU	2.5
1	A	132	HIS	2.5
1	A	139	GLU	2.5
1	B	187	PHE	2.5
1	B	58	ASN	2.5
1	A	186	ARG	2.5
1	B	4	ARG	2.5
1	B	143	HIS	2.5
1	B	115	GLY	2.5
1	B	215	PRO	2.4
1	A	117	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	117	LEU	2.4
1	A	2	THR	2.4
1	B	136	LEU	2.4
1	A	451	ASP	2.4
1	A	469	PHE	2.4
1	B	100	TYR	2.4
1	B	213	LYS	2.4
1	A	407	GLY	2.4
1	A	185	GLU	2.3
1	A	192	ASP	2.3
1	B	248	TRP	2.3
1	B	409	GLY	2.3
1	A	147	PHE	2.3
1	B	53	HIS	2.3
1	B	135	PHE	2.3
1	A	195	GLU	2.3
1	A	106	ASP	2.3
1	A	201	PRO	2.3
1	B	303	ASP	2.3
1	A	191	THR	2.3
1	B	179	TYR	2.3
1	B	217	ASN	2.3
1	B	142	SER	2.3
1	A	135	PHE	2.3
1	B	56	ILE	2.2
1	A	293	HIS	2.2
1	B	17	GLU	2.2
1	B	66	TYR	2.2
1	B	109	SER	2.2
1	B	103	ASN	2.2
1	B	119	GLY	2.2
1	B	267	GLU	2.2
1	A	325	LYS	2.2
1	B	118	SER	2.2
1	B	75	ALA	2.1
1	A	107	PRO	2.1
1	B	245	GLN	2.1
1	B	407	GLY	2.1
1	A	166	LYS	2.1
1	B	82	MET	2.1
1	A	0	GLY	2.1
1	B	23	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	31	ALA	2.1
1	A	210	LEU	2.1
1	B	7	PHE	2.1
1	B	128	GLU	2.0
1	A	214	GLN	2.0
1	A	505	VAL	2.0
1	B	113	PHE	2.0
1	B	61	ASP	2.0
1	A	189	SER	2.0
1	B	42	THR	2.0
1	B	20	LEU	2.0
1	B	84	HIS	2.0
1	A	200	ASN	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](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	601	6/6	0.89	0.14	77,80,83,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.