



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:04 PM UTC

PDB ID : 3G9W / pdb_00003g9w
Title : Crystal Structure of Talin2 F2-F3 in Complex with the Integrin Beta1D Cytoplasmic Tail
Authors : Anthis, N.J.; Wegener, K.L.; Ye, F.; Kim, C.; Lowe, E.D.; Vakonakis, I.; Bate, N.; Critchley, D.R.; Ginsberg, M.H.; Campbell, I.D.
Deposited on : 2009-02-15
Resolution : 2.17 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

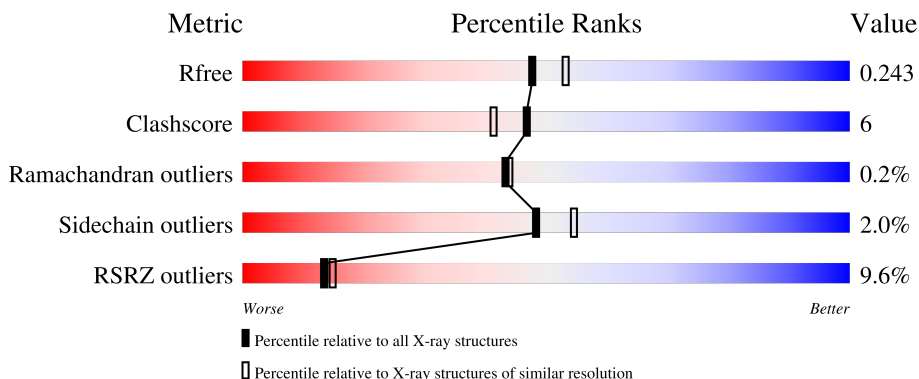
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	223	5% 87% 9% ..
1	B	223	7% 84% 6% 9%
2	C	52	17% 54% 19% 25%
2	D	52	21% 62% 13% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4570 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 Talin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	3	0
			1792	1154	304	329	5			
1	B	204	Total	C	N	O	S	0	1	0
			1667	1070	286	306	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	expression tag	UNP Q71LX4
A	187	ILE	-	expression tag	UNP Q71LX4
A	188	ASP	-	expression tag	UNP Q71LX4
A	189	PRO	-	expression tag	UNP Q71LX4
A	190	PHE	-	expression tag	UNP Q71LX4
A	191	THR	-	expression tag	UNP Q71LX4
A	192	GLY	-	expression tag	UNP Q71LX4
A	193	ILE	-	expression tag	UNP Q71LX4
A	194	ASP	-	expression tag	UNP Q71LX4
A	195	PRO	-	expression tag	UNP Q71LX4
A	196	PHE	-	expression tag	UNP Q71LX4
A	197	THR	-	expression tag	UNP Q71LX4
B	186	GLY	-	expression tag	UNP Q71LX4
B	187	ILE	-	expression tag	UNP Q71LX4
B	188	ASP	-	expression tag	UNP Q71LX4
B	189	PRO	-	expression tag	UNP Q71LX4
B	190	PHE	-	expression tag	UNP Q71LX4
B	191	THR	-	expression tag	UNP Q71LX4
B	192	GLY	-	expression tag	UNP Q71LX4
B	193	ILE	-	expression tag	UNP Q71LX4
B	194	ASP	-	expression tag	UNP Q71LX4
B	195	PRO	-	expression tag	UNP Q71LX4
B	196	PHE	-	expression tag	UNP Q71LX4
B	197	THR	-	expression tag	UNP Q71LX4

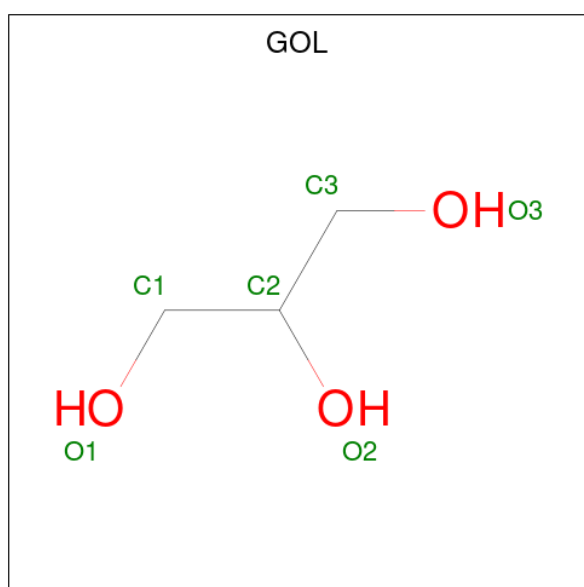
- Molecule 2 is a protein called Integrin beta-1D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	39	Total	C	N	O	S	0	2	0
			341	221	58	58	4			
2	D	40	Total	C	N	O	S	0	0	0
			339	217	60	60	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	750	GLY	-	expression tag	UNP P05556
C	751	PRO	-	expression tag	UNP P05556
D	750	GLY	-	expression tag	UNP P05556
D	751	PRO	-	expression tag	UNP P05556

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

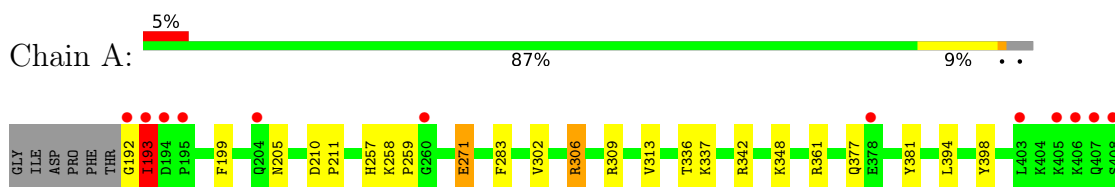
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total	O	0	0
			175	175		
5	B	163	Total	O	0	0
			163	163		
5	C	24	Total	O	0	0
			24	24		
5	D	19	Total	O	0	0
			19	19		

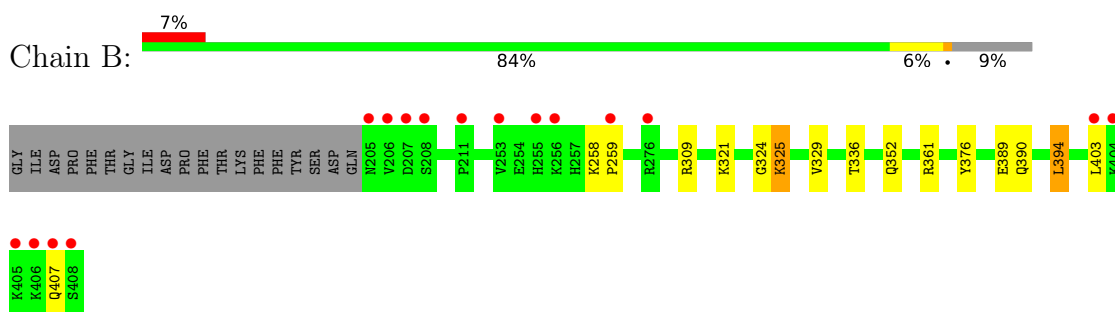
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

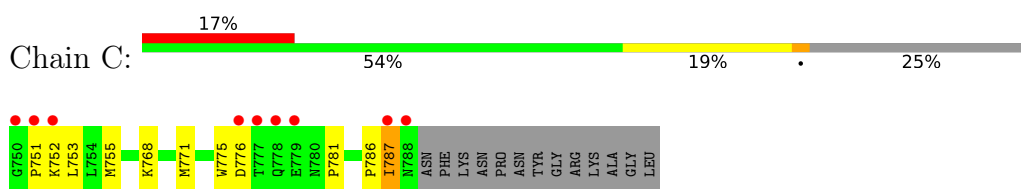
- Molecule 1: Talin-2



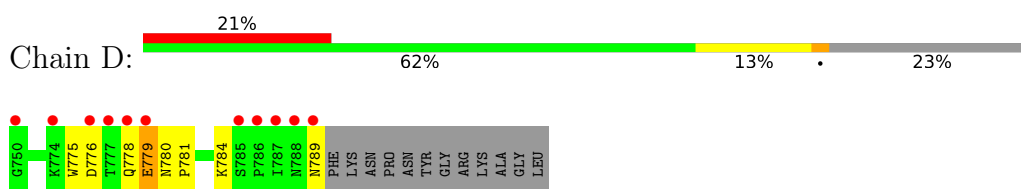
- Molecule 1: Talin-2



- Molecule 2: Integrin beta-1D



- Molecule 2: Integrin beta-1D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.26Å 108.72Å 131.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.94 – 2.17 41.94 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (41.94-2.17) 99.3 (41.94-2.17)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.213 , 0.248 0.203 , 0.243	Depositor DCC
R_{free} test set	2085 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4570	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8367e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.39	0/1841	0.73	2/2472 (0.1%)
1	B	0.38	0/1705	0.73	2/2289 (0.1%)
2	C	0.33	0/355	0.76	0/473
2	D	0.35	0/347	0.72	1/464 (0.2%)
All	All	0.37	0/4248	0.73	5/5698 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASP	CA-C-N	5.28	125.34	119.32
1	A	210	ASP	C-N-CA	5.28	125.34	119.32
1	B	329	VAL	CA-C-N	5.04	124.94	119.85
1	B	329	VAL	C-N-CA	5.04	124.94	119.85
2	D	779	GLU	N-CA-C	5.01	116.03	108.46

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	1792	0	1809	20	0
1	B	1667	0	1692	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	341	0	353	12	0
2	D	339	0	341	5	0
3	A	12	0	16	0	0
3	B	18	0	24	3	0
3	C	6	0	8	1	0
4	A	7	0	10	3	0
4	B	7	0	10	1	0
5	A	175	0	0	4	0
5	B	163	0	0	3	0
5	C	24	0	0	1	0
5	D	19	0	0	0	0
All	All	4570	0	4263	48	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 6.

The worst 5 of 48 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:377:GLN:HE22	4:A:410:PEG:H41	1.41	0.83
1:B:321:LYS:NZ	3:B:409:GOL:H32	1.94	0.82
4:A:410:PEG:H32	5:A:565:HOH:O	1.83	0.79
1:A:192:GLY:O	1:A:193:ILE:HG12	1.93	0.69
1:B:389:GLU:HG2	5:B:522:HOH:O	1.92	0.68

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	218/223 (98%)	215 (99%)	2 (1%)	1 (0%)	24 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	203/223 (91%)	201 (99%)	2 (1%)	0	100	100
2	C	39/52 (75%)	37 (95%)	2 (5%)	0	100	100
2	D	38/52 (73%)	37 (97%)	1 (3%)	0	100	100
All	All	498/550 (90%)	490 (98%)	7 (1%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ILE

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	197/199 (99%)	193 (98%)	4 (2%)	48	54
1	B	183/199 (92%)	180 (98%)	3 (2%)	55	61
2	C	38/46 (83%)	36 (95%)	2 (5%)	20	17
2	D	37/46 (80%)	37 (100%)	0	100	100
All	All	455/490 (93%)	446 (98%)	9 (2%)	48	54

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	753	LEU
2	C	787	ILE
1	A	394	LEU
1	B	325	LYS
1	B	336	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	GLN
1	B	244	GLN
1	B	248	GLN
1	A	244	GLN
1	A	205	ASN

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](#)

8 ligands are 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	$\# Z > 2$
3	GOL	C	1	-	5,5,5	0.36	0	5,5,5	0.30	0
4	PEG	A	410	-	6,6,6	0.50	0	5,5,5	0.25	0
3	GOL	A	1	-	5,5,5	0.41	0	5,5,5	0.21	0
4	PEG	B	410	-	6,6,6	0.44	0	5,5,5	0.31	0
3	GOL	B	411	-	5,5,5	0.39	0	5,5,5	0.49	0
3	GOL	B	409	-	5,5,5	0.39	0	5,5,5	0.38	0
3	GOL	B	1	-	5,5,5	0.37	0	5,5,5	0.19	0
3	GOL	A	409	-	5,5,5	0.43	0	5,5,5	0.42	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
3	GOL	C	1	-	-	2/4/4/4	-
4	PEG	A	410	-	-	3/4/4/4	-
3	GOL	A	1	-	-	0/4/4/4	-
4	PEG	B	410	-	-	2/4/4/4	-
3	GOL	B	411	-	-	2/4/4/4	-
3	GOL	B	409	-	-	3/4/4/4	-
3	GOL	B	1	-	-	0/4/4/4	-
3	GOL	A	409	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	409	GOL	O1-C1-C2-C3
3	B	409	GOL	C1-C2-C3-O3
3	B	411	GOL	C1-C2-C3-O3
3	C	1	GOL	O1-C1-C2-C3
3	B	411	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GOL	1	0
4	A	410	PEG	3	0
4	B	410	PEG	1	0
3	B	409	GOL	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	217/223 (97%)	0.18	12 (5%) 30 34	10, 23, 58, 127	6 (2%)
1	B	204/223 (91%)	0.26	16 (7%) 19 21	11, 26, 72, 143	6 (2%)
2	C	39/52 (75%)	1.06	9 (23%) 2 2	17, 33, 85, 108	3 (7%)
2	D	40/52 (76%)	1.19	11 (27%) 1 1	21, 36, 87, 91	1 (2%)
All	All	500/550 (90%)	0.37	48 (9%) 13 15	10, 27, 76, 143	16 (3%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	6.1
2	D	787	ILE	6.0
1	A	193	ILE	5.9
2	D	789	ASN	5.4
1	A	405	LYS	5.3

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
4	PEG	A	410	7/7	0.81	0.19	52,58,63,64	0
4	PEG	B	410	7/7	0.81	0.24	48,58,71,71	0
3	GOL	B	409	6/6	0.82	0.20	54,62,63,66	0
3	GOL	B	411	6/6	0.84	0.16	35,40,47,48	0
3	GOL	C	1	6/6	0.90	0.12	49,55,56,56	0
3	GOL	A	409	6/6	0.93	0.11	30,35,38,38	0
3	GOL	B	1	6/6	0.96	0.07	23,29,30,32	0
3	GOL	A	1	6/6	0.96	0.08	21,26,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.