



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:30 AM UTC

PDB ID : 6F2G / pdb_00006f2g
Title : Bacterial asc transporter crystal structure in open to in conformation
Authors : Fort, J.; Errasti-Murugarren, E.; Carpena, X.; Palacin, M.; Fita, I.
Deposited on : 2017-11-24
Resolution : 2.92 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
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

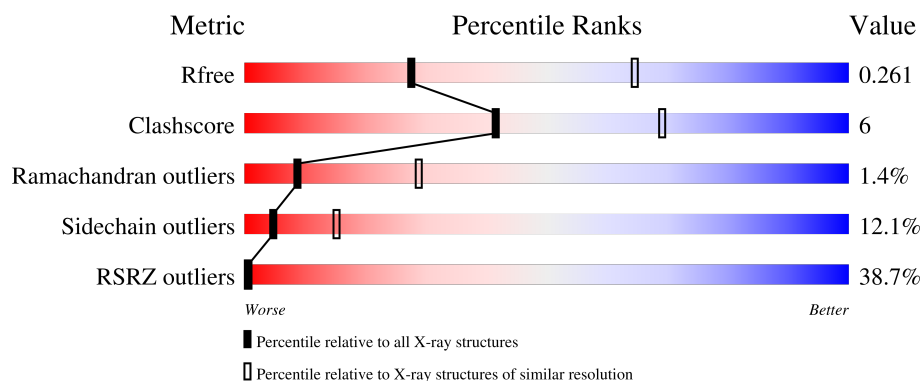
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	444	39% 70% 21% 5% ..
2	B	134	34% 81% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4253 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 Putative amino acid/polyamine transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3258	2200	500	547	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A8UCQ5
A	436	GLY	-	expression tag	UNP A8UCQ5
A	437	GLY	-	expression tag	UNP A8UCQ5
A	438	GLY	-	expression tag	UNP A8UCQ5
A	439	LEU	-	expression tag	UNP A8UCQ5
A	440	GLU	-	expression tag	UNP A8UCQ5
A	441	VAL	-	expression tag	UNP A8UCQ5
A	442	LEU	-	expression tag	UNP A8UCQ5
A	443	PHE	-	expression tag	UNP A8UCQ5
A	444	GLN	-	expression tag	UNP A8UCQ5

- Molecule 2 is a protein called Nanobody 74.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			994	612	186	192	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.83Å 85.83Å 321.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.05 – 2.92 82.93 – 2.92	Depositor EDS
% Data completeness (in resolution range)	74.1 (83.05-2.92) 74.1 (82.93-2.92)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.238 , 0.261 0.240 , 0.261	Depositor DCC
R_{free} test set	972 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	4253	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.20	9/3341 (0.3%)	1.33	12/4569 (0.3%)
2	B	1.20	1/1019 (0.1%)	1.15	2/1381 (0.1%)
All	All	1.20	10/4360 (0.2%)	1.29	14/5950 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ASN	CA-C	-6.29	1.45	1.52
1	A	178	PRO	CA-C	6.28	1.61	1.52
1	A	221	LEU	C-O	-6.15	1.18	1.24
2	B	32	ARG	CA-C	-5.63	1.45	1.52
1	A	338	ILE	CA-CB	5.50	1.61	1.54
1	A	341	GLY	N-CA	5.43	1.50	1.44
1	A	7	ILE	C-O	-5.39	1.17	1.24
1	A	303	THR	C-O	-5.34	1.17	1.24
1	A	49	ILE	CA-CB	5.13	1.60	1.54
1	A	95	TYR	CA-CB	5.05	1.60	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	VAL	CB-CA-C	-7.30	104.63	111.06
1	A	381	VAL	CB-CA-C	-6.31	103.42	110.68
2	B	34	MET	CG-SD-CE	-5.89	87.93	100.90
1	A	177	VAL	CA-C-N	-5.85	112.52	119.84
1	A	177	VAL	C-N-CA	-5.85	112.52	119.84
1	A	168	TYR	CA-C-N	-5.70	113.15	119.19
1	A	168	TYR	C-N-CA	-5.70	113.15	119.19
1	A	126	ILE	N-CA-C	-5.51	105.24	110.42
1	A	53	GLY	CA-C-N	5.30	125.71	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLY	C-N-CA	5.30	125.71	119.94
1	A	315	ARG	CG-CD-NE	-5.28	100.38	112.00
1	A	22	ILE	N-CA-CB	5.25	118.78	110.54
1	A	306	MET	N-CA-C	5.10	121.66	110.80
1	A	380	ARG	NE-CZ-NH2	5.08	123.77	119.20

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	3258	0	3457	49	0
2	B	994	0	928	9	0
3	B	1	0	0	0	0
All	All	4253	0	4385	55	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.

All (55) 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:316:ILE:HD13	2:B:108:PRO:HG2	1.79	0.65
1:A:74:LEU:HD12	1:A:86:VAL:HG21	1.81	0.63
1:A:109:GLN:HE22	1:A:260:ALA:HB2	1.64	0.61
2:B:29:PHE:HB3	2:B:77:ASN:HD22	1.67	0.60
1:A:74:LEU:HD12	1:A:86:VAL:CG2	2.34	0.57
1:A:143:SER:HB3	1:A:292:ILE:HD11	1.86	0.57
1:A:355:TRP:HB3	1:A:398:ILE:HD11	1.85	0.57
1:A:389:LEU:HA	1:A:392:ILE:HG22	1.88	0.56
1:A:47:GLY:HA3	1:A:233:MET:HG3	1.86	0.56
2:B:127:HIS:O	2:B:128:HIS:HB2	2.04	0.56
1:A:276:THR:HA	1:A:279:ILE:HD12	1.87	0.56
1:A:343:PHE:O	1:A:347:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HA	1:A:390:ILE:HD12	1.89	0.54
1:A:104:ILE:HD11	1:A:338:ILE:HA	1.90	0.54
1:A:158:LEU:HD22	1:A:239:THR:HG21	1.90	0.54
2:B:131:GLU:N	2:B:131:GLU:OE1	2.41	0.53
1:A:347:THR:O	1:A:351:VAL:HG23	2.09	0.53
1:A:181:VAL:HG12	1:A:183:THR:HG22	1.91	0.53
1:A:108:THR:HA	1:A:121:ILE:HD12	1.91	0.52
1:A:20:ALA:HB1	1:A:283:VAL:HG22	1.91	0.52
1:A:96:PRO:HG3	1:A:330:MET:HG3	1.93	0.51
1:A:298:PRO:HA	1:A:301:LEU:HD12	1.92	0.51
1:A:174:ILE:HA	1:A:177:VAL:HG13	1.92	0.50
1:A:135:VAL:HA	1:A:138:LEU:HD12	1.93	0.49
1:A:195:ILE:O	1:A:351:VAL:HG21	2.11	0.49
1:A:62:THR:HG21	1:A:379:TYR:HB3	1.93	0.49
1:A:351:VAL:O	1:A:355:TRP:HB2	2.12	0.49
1:A:69:GLY:C	1:A:71:MET:H	2.20	0.49
1:A:24:PHE:CD1	1:A:105:ILE:HG13	2.49	0.48
1:A:218:GLY:O	1:A:222:PRO:HD3	2.14	0.48
1:A:82:LEU:O	1:A:86:VAL:HG23	2.15	0.47
1:A:357:PHE:HA	1:A:360:LEU:HD12	1.97	0.46
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.97	0.46
1:A:33:ALA:HB1	1:A:38:LEU:HB3	1.98	0.46
1:A:213:GLU:OE2	2:B:99:LYS:NZ	2.49	0.45
1:A:385:PRO:O	1:A:389:LEU:HD13	2.17	0.45
1:A:219:LYS:O	1:A:220:MET:CB	2.64	0.45
1:A:409:ASN:HA	1:A:412:ILE:HD12	1.99	0.44
1:A:90:GLN:HA	1:A:94:TYR:HB3	1.98	0.44
1:A:219:LYS:O	1:A:219:LYS:HG3	2.17	0.44
1:A:221:LEU:O	1:A:224:VAL:HG12	2.18	0.44
1:A:355:TRP:HB3	1:A:398:ILE:CD1	2.47	0.43
1:A:181:VAL:CG1	1:A:183:THR:HG22	2.49	0.43
1:A:84:PHE:CE2	1:A:424:TYR:HB2	2.53	0.43
1:A:304:GLN:HA	2:B:62:ASP:HB2	2.00	0.43
1:A:136:ASN:HD21	1:A:288:ASN:ND2	2.16	0.42
1:A:22:ILE:HD13	1:A:158:LEU:HD21	2.02	0.42
1:A:209:THR:O	1:A:213:GLU:HB2	2.20	0.42
1:A:34:GLY:HA3	1:A:184:HIS:CD2	2.56	0.41
1:A:183:THR:HG23	1:A:184:HIS:CD2	2.55	0.41
2:B:12:VAL:HG21	2:B:86:LEU:HD13	2.03	0.41
2:B:91:THR:HG23	2:B:121:THR:HA	2.03	0.41
1:A:221:LEU:O	1:A:225:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:PHE:HB3	2:B:77:ASN:ND2	2.33	0.40
1:A:106:PHE:CE2	1:A:128:THR:HG21	2.57	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	428/444 (96%)	401 (94%)	22 (5%)	5 (1%)	10	32
2	B	129/134 (96%)	120 (93%)	6 (5%)	3 (2%)	5	18
All	All	557/578 (96%)	521 (94%)	28 (5%)	8 (1%)	9	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	128	HIS
1	A	206	ASN
1	A	217	PRO
1	A	306	MET
2	B	129	HIS
1	A	218	GLY
1	A	220	MET
2	B	130	HIS

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	344/356 (97%)	299 (87%)	45 (13%)	4	12
2	B	102/104 (98%)	93 (91%)	9 (9%)	9	28
All	All	446/460 (97%)	392 (88%)	54 (12%)	5	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	22	ILE
1	A	38	LEU
1	A	49	ILE
1	A	66	GLN
1	A	71	MET
1	A	82	LEU
1	A	86	VAL
1	A	105	ILE
1	A	127	LEU
1	A	145	TRP
1	A	149	LEU
1	A	155	LEU
1	A	160	VAL
1	A	176	LEU
1	A	183	THR
1	A	187	LEU
1	A	195	ILE
1	A	202	ASP
1	A	205	ILE
1	A	207	VAL
1	A	210	LEU
1	A	219	LYS
1	A	220	MET
1	A	224	VAL
1	A	273	LYS
1	A	303	THR
1	A	305	LYS
1	A	316	ILE
1	A	321	ASN
1	A	324	ILE
1	A	330	MET
1	A	338	ILE
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	349	LEU
1	A	354	ILE
1	A	368	LEU
1	A	380	ARG
1	A	387	ILE
1	A	398	ILE
1	A	399	ILE
1	A	408	LYS
1	A	411	PHE
1	A	428	LYS
1	A	429	LYS
2	B	12	VAL
2	B	13	GLN
2	B	43	GLU
2	B	65	LYS
2	B	76	LYS
2	B	82	GLN
2	B	112	VAL
2	B	126	HIS
2	B	130	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	109	GLN
1	A	136	ASN
1	A	147	GLN
1	A	184	HIS
1	A	321	ASN
1	A	325	ASN
1	A	345	GLN
1	A	409	ASN
2	B	77	ASN
2	B	106	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

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](#)

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	430/444 (96%)	2.02	172 (40%) ⓘ ⓘ	85, 120, 167, 203	1 (0%)
2	B	131/134 (97%)	1.46	45 (34%) ⓘ ⓘ	69, 98, 159, 227	0
All	All	561/578 (97%)	1.89	217 (38%) ⓘ ⓘ	69, 114, 165, 227	1 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	18.4
2	B	39	GLN	13.1
1	A	203	GLY	12.8
2	B	41	PRO	12.4
1	A	390	ILE	10.5
1	A	205	ILE	10.5
2	B	40	ALA	10.1
1	A	70	MET	9.8
1	A	386	VAL	9.8
1	A	354	ILE	9.1
1	A	202	ASP	8.6
1	A	339	LEU	8.5
1	A	16	THR	8.3
1	A	226	ILE	8.1
1	A	318	PRO	7.9
1	A	204	TRP	7.8
1	A	48	ILE	7.8
1	A	127	LEU	7.8
1	A	50	THR	7.7
1	A	94	TYR	7.5
1	A	52	ALA	7.1
1	A	174	ILE	7.1
2	B	75	ALA	7.0
1	A	357	PHE	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	156	ILE	6.8
1	A	17	VAL	6.7
1	A	90	GLN	6.5
1	A	49	ILE	6.5
1	A	363	ILE	6.3
2	B	112	VAL	6.2
1	A	45	VAL	6.1
1	A	4	VAL	6.0
1	A	367	ILE	6.0
1	A	78	TYR	5.9
1	A	274	LEU	5.9
1	A	86	VAL	5.8
1	A	229	LEU	5.8
1	A	71	MET	5.8
1	A	51	ILE	5.7
1	A	44	PHE	5.7
1	A	12	VAL	5.7
1	A	69	GLY	5.7
1	A	228	GLY	5.7
2	B	76	LYS	5.6
1	A	18	ILE	5.5
1	A	14	VAL	5.5
1	A	170	GLY	5.5
1	A	356	PHE	5.5
1	A	353	VAL	5.4
1	A	340	THR	5.3
1	A	246	VAL	5.3
1	A	83	GLY	5.1
1	A	227	GLY	5.1
2	B	45	ARG	5.0
1	A	389	LEU	5.0
2	B	128	HIS	5.0
1	A	370	LYS	4.9
2	B	9	GLY	4.8
1	A	123	PRO	4.8
2	B	100	ASN	4.7
1	A	87	GLY	4.7
1	A	366	ILE	4.7
2	B	13	GLN	4.6
1	A	230	SER	4.6
1	A	28	ALA	4.5
1	A	225	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLY	4.5
1	A	192	SER	4.5
2	B	126	HIS	4.5
1	A	81	TRP	4.4
1	A	232	VAL	4.3
1	A	355	TRP	4.3
1	A	80	ARG	4.3
1	A	201	TYR	4.3
1	A	13	VAL	4.2
1	A	391	ALA	4.2
1	A	41	LEU	4.2
1	A	142	TYR	4.2
1	A	145	TRP	4.1
1	A	245	PHE	4.1
1	A	319	LYS	4.1
1	A	11	THR	4.1
1	A	196	ALA	4.1
1	A	153	LEU	4.0
1	A	270	ILE	4.0
2	B	109	ASN	4.0
2	B	8	GLY	4.0
1	A	358	ILE	4.0
1	A	95	TYR	4.0
2	B	46	GLU	4.0
1	A	168	TYR	4.0
1	A	209	THR	4.0
1	A	193	ALA	3.9
1	A	75	GLU	3.9
2	B	42	GLY	3.8
2	B	44	GLY	3.8
1	A	248	ASP	3.8
1	A	89	ALA	3.8
2	B	56	SER	3.8
1	A	235	VAL	3.8
2	B	19	ARG	3.8
1	A	165	GLY	3.8
1	A	130	ILE	3.7
1	A	344	ASN	3.7
1	A	383	PHE	3.7
1	A	143	SER	3.7
1	A	224	VAL	3.7
1	A	155	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	26	GLY	3.7
1	A	82	LEU	3.6
1	A	433	SER	3.6
2	B	1	GLN	3.6
2	B	57	TYR	3.6
1	A	85	LEU	3.6
2	B	129	HIS	3.5
1	A	74	LEU	3.5
1	A	175	ARG	3.4
2	B	123	SER	3.4
1	A	242	ALA	3.4
1	A	406	GLN	3.4
1	A	407	PRO	3.4
1	A	247	LEU	3.4
1	A	77	VAL	3.3
1	A	53	GLY	3.3
1	A	171	GLY	3.3
1	A	195	ILE	3.3
1	A	47	GLY	3.3
1	A	376	GLU	3.2
1	A	176	LEU	3.2
1	A	169	PRO	3.2
1	A	393	ILE	3.2
2	B	59	GLU	3.2
1	A	231	ILE	3.2
1	A	326	GLY	3.2
1	A	368	LEU	3.2
2	B	38	ARG	3.1
1	A	177	VAL	3.1
1	A	126	ILE	3.1
1	A	268	GLU	3.1
1	A	336	VAL	3.1
1	A	141	LYS	3.0
1	A	359	THR	3.0
1	A	32	ALA	3.0
1	A	8	THR	3.0
1	A	122	VAL	3.0
1	A	76	LYS	2.9
2	B	73	ASP	2.9
1	A	15	GLY	2.9
2	B	125	HIS	2.9
1	A	207	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	364	ALA	2.8
2	B	124	SER	2.8
1	A	158	LEU	2.8
1	A	244	LEU	2.8
1	A	408	LYS	2.8
1	A	84	PHE	2.8
2	B	12	VAL	2.8
1	A	187	LEU	2.8
2	B	130	HIS	2.8
1	A	223	LYS	2.8
2	B	58	THR	2.8
1	A	219	LYS	2.7
1	A	361	THR	2.7
1	A	241	ILE	2.7
1	A	25	LYS	2.7
1	A	313	PHE	2.6
1	A	233	MET	2.6
1	A	29	VAL	2.6
1	A	348	ASP	2.6
2	B	110	ASP	2.6
1	A	392	ILE	2.6
2	B	55	GLY	2.6
1	A	172	GLY	2.6
1	A	266	LEU	2.6
1	A	402	THR	2.6
1	A	236	TYR	2.5
1	A	403	LEU	2.5
2	B	43	GLU	2.5
2	B	131	GLU	2.5
1	A	46	ALA	2.5
1	A	104	ILE	2.5
1	A	387	ILE	2.4
2	B	16	GLY	2.4
1	A	360	LEU	2.4
2	B	11	VAL	2.4
1	A	166	LEU	2.4
1	A	323	PRO	2.3
1	A	362	PHE	2.3
2	B	14	ALA	2.3
1	A	410	ALA	2.3
1	A	429	LYS	2.3
2	B	127	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	27	ARG	2.3
1	A	396	LEU	2.2
1	A	380	ARG	2.2
1	A	350	ILE	2.2
1	A	320	THR	2.2
1	A	378	PRO	2.2
2	B	54	SER	2.2
1	A	343	PHE	2.2
1	A	146	ILE	2.2
1	A	31	GLY	2.2
1	A	139	GLY	2.2
1	A	5	SER	2.2
1	A	167	LEU	2.2
1	A	347	THR	2.1
1	A	182	GLU	2.1
2	B	114	TRP	2.1
1	A	315	ARG	2.1
2	B	80	TYR	2.1
1	A	54	GLY	2.1
1	A	33	ALA	2.1
1	A	107	ALA	2.1
2	B	25	SER	2.1
1	A	159	VAL	2.1
1	A	321	ASN	2.0
1	A	311	ASP	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 oligosaccharides 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. 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
3	ZN	B	201	1/1	0.98	0.10	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.