



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:22 AM UTC

PDB ID : 7D5P / pdb_00007d5p
Title : Structure of NorC transporter in an outward-open conformation in complex with a single-chain Indian camelid antibody
Authors : Kumar, S.; Athreya, A.; Penmatsa, A.
Deposited on : 2020-09-27
Resolution : 3.65 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

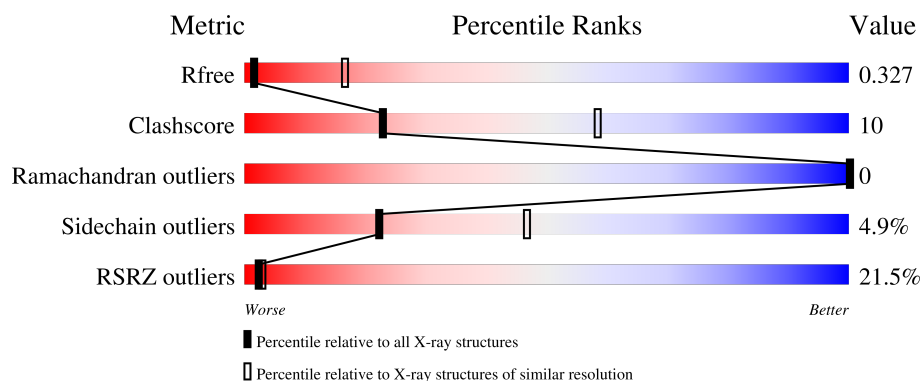
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	479	19% 67% 16% • 15%
1	B	479	21% 70% 15% •• 14%
2	C	131	15% 91% 8% •
2	D	131	10% 89% 9% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7575 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 Drug transporter, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	Se	0	0	0
			2818	1860	444	495	4	15			
1	B	413	Total	C	N	O	S	Se	0	0	0
			2851	1878	452	502	4	15			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	463	GLY	-	expression tag	UNP A0A0H2WZS4
A	464	THR	-	expression tag	UNP A0A0H2WZS4
A	465	LEU	-	expression tag	UNP A0A0H2WZS4
A	466	VAL	-	expression tag	UNP A0A0H2WZS4
A	467	PRO	-	expression tag	UNP A0A0H2WZS4
A	468	ARG	-	expression tag	UNP A0A0H2WZS4
A	469	GLY	-	expression tag	UNP A0A0H2WZS4
A	470	SER	-	expression tag	UNP A0A0H2WZS4
A	471	GLY	-	expression tag	UNP A0A0H2WZS4
A	472	HIS	-	expression tag	UNP A0A0H2WZS4
A	473	HIS	-	expression tag	UNP A0A0H2WZS4
A	474	HIS	-	expression tag	UNP A0A0H2WZS4
A	475	HIS	-	expression tag	UNP A0A0H2WZS4
A	476	HIS	-	expression tag	UNP A0A0H2WZS4
A	477	HIS	-	expression tag	UNP A0A0H2WZS4
A	478	HIS	-	expression tag	UNP A0A0H2WZS4
A	479	HIS	-	expression tag	UNP A0A0H2WZS4
B	463	GLY	-	expression tag	UNP A0A0H2WZS4
B	464	THR	-	expression tag	UNP A0A0H2WZS4
B	465	LEU	-	expression tag	UNP A0A0H2WZS4
B	466	VAL	-	expression tag	UNP A0A0H2WZS4
B	467	PRO	-	expression tag	UNP A0A0H2WZS4
B	468	ARG	-	expression tag	UNP A0A0H2WZS4
B	469	GLY	-	expression tag	UNP A0A0H2WZS4
B	470	SER	-	expression tag	UNP A0A0H2WZS4

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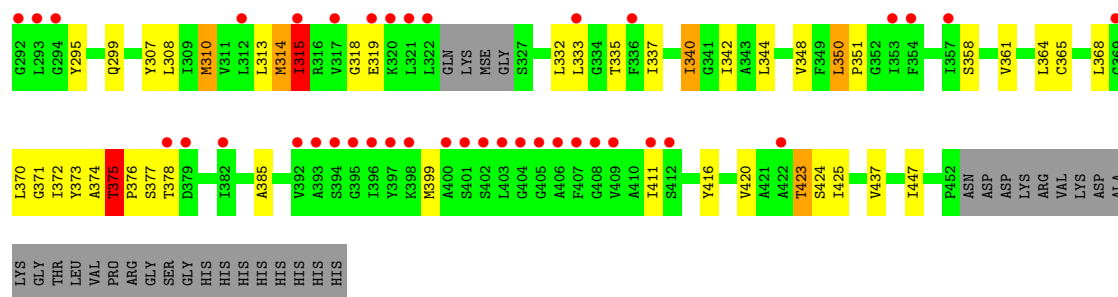
Chain	Residue	Modelled	Actual	Comment	Reference
B	471	GLY	-	expression tag	UNP A0A0H2WZS4
B	472	HIS	-	expression tag	UNP A0A0H2WZS4
B	473	HIS	-	expression tag	UNP A0A0H2WZS4
B	474	HIS	-	expression tag	UNP A0A0H2WZS4
B	475	HIS	-	expression tag	UNP A0A0H2WZS4
B	476	HIS	-	expression tag	UNP A0A0H2WZS4
B	477	HIS	-	expression tag	UNP A0A0H2WZS4
B	478	HIS	-	expression tag	UNP A0A0H2WZS4
B	479	HIS	-	expression tag	UNP A0A0H2WZS4

- Molecule 2 is a protein called ICab.

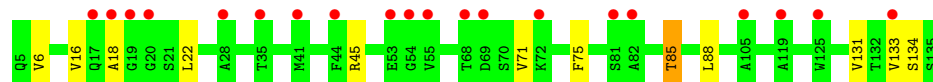
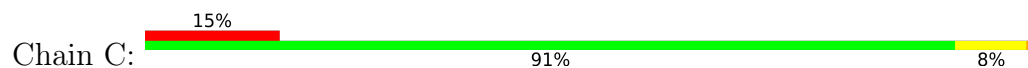
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	0	0
			952	596	160	190	6			
2	D	131	Total	C	N	O	S	0	0	0
			952	596	160	190	6			

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

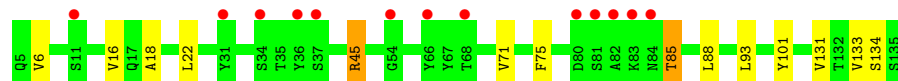
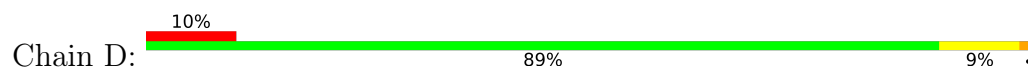
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		



- Molecule 2: ICab



- Molecule 2: ICab



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.21Å 139.88Å 118.03Å 90.00° 106.03° 90.00°	Depositor
Resolution (Å)	48.96 – 3.65 48.96 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.96-3.65) 99.1 (48.96-3.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.297 , 0.318 0.304 , 0.327	Depositor DCC
R_{free} test set	1153 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	148.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 115.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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	1.07	1/2847 (0.0%)	1.80	9/3865 (0.2%)
1	B	1.06	1/2880 (0.0%)	1.81	13/3907 (0.3%)
2	C	1.08	0/975	1.40	1/1326 (0.1%)
2	D	1.07	0/975	1.40	1/1326 (0.1%)
All	All	1.06	2/7677 (0.0%)	1.71	24/10424 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	THR	C-N	13.52	1.50	1.34
1	B	375	THR	C-N	12.19	1.50	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	THR	CA-C-N	15.38	135.62	118.85
1	A	375	THR	C-N-CA	15.38	135.62	118.85
1	B	375	THR	CA-C-N	14.97	135.66	119.05
1	B	375	THR	C-N-CA	14.97	135.66	119.05
1	B	315	ILE	N-CA-C	-9.38	101.72	110.82
1	B	423	THR	CB-CA-C	-7.69	104.78	114.40
2	D	85	THR	CA-CB-OG1	-7.11	98.94	109.60
1	A	375	THR	CA-CB-OG1	-6.42	99.97	109.60
1	B	310	MSE	CB-CG-SE	-6.35	93.66	112.70
1	B	60	MSE	CG-SE-CE	6.18	112.51	98.92
1	B	314	MSE	CB-CG-SE	-5.89	95.03	112.70
1	A	131	GLU	N-CA-C	-5.80	106.06	113.02
1	B	424	SER	N-CA-C	5.70	119.20	110.36
1	A	314	MSE	CG-SE-CE	5.66	111.38	98.92
1	A	310	MSE	CB-CG-SE	-5.63	95.81	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	MSE	CB-CG-SE	-5.61	95.86	112.70
2	C	85	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	423	THR	N-CA-C	-5.52	100.41	109.80
1	B	310	MSE	CG-SE-CE	5.25	110.48	98.92
1	B	423	THR	N-CA-C	-5.24	101.90	109.29
1	B	313	LEU	N-CA-C	-5.21	106.69	112.57
1	A	208	MSE	CG-SE-CE	5.10	110.14	98.92
1	A	424	SER	N-CA-C	5.09	118.25	110.36
1	B	424	SER	N-CA-CB	-5.08	102.72	110.49

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	2818	0	2843	71	0
1	B	2851	0	2883	69	0
2	C	952	0	844	7	0
2	D	952	0	844	9	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	7575	0	7414	156	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 10.

All (156) 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:310:MSE:HE3	1:A:368:LEU:HB3	1.27	1.12
1:B:310:MSE:HE3	1:B:364:LEU:HD12	1.34	1.07
1:A:310:MSE:CE	1:A:368:LEU:HB3	1.96	0.95
1:A:310:MSE:HE3	1:A:368:LEU:CB	2.00	0.90
1:A:315:ILE:HG22	1:A:374:ALA:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PHE:HA	1:A:60:MSE:HE2	1.56	0.86
1:A:57:PHE:HA	1:A:60:MSE:CE	2.10	0.80
1:A:310:MSE:HE2	1:A:368:LEU:HD23	1.65	0.78
1:B:315:ILE:HG22	1:B:374:ALA:HB3	1.66	0.77
1:A:315:ILE:HG22	1:A:374:ALA:CB	2.15	0.76
1:B:375:THR:HG22	1:B:376:PRO:HD3	1.67	0.76
1:B:310:MSE:CE	1:B:364:LEU:HD12	2.15	0.73
1:B:149:ILE:HG22	1:B:149:ILE:O	1.89	0.71
1:B:315:ILE:HG22	1:B:374:ALA:CB	2.21	0.70
1:B:314:MSE:HB3	1:B:371:GLY:HA3	1.74	0.69
1:B:319:GLU:N	1:B:375:THR:HG21	2.09	0.68
1:B:344:LEU:HD13	1:B:361:VAL:HG23	1.79	0.65
1:A:332:LEU:HG	1:A:447:ILE:HG21	1.80	0.63
1:A:345:ILE:O	1:A:348:VAL:HG12	1.99	0.63
1:B:332:LEU:HG	1:B:447:ILE:HG21	1.80	0.63
1:A:60:MSE:HA	1:A:209:LEU:HD13	1.81	0.62
1:A:205:LEU:HD12	1:A:208:MSE:HE3	1.82	0.61
1:A:214:VAL:HG23	1:A:232:LEU:HD21	1.83	0.61
1:B:141:ILE:HG13	1:B:315:ILE:HD13	1.81	0.61
1:B:91:LEU:HD12	1:B:104:GLY:HA3	1.82	0.60
1:B:214:VAL:HG23	1:B:232:LEU:HD21	1.82	0.60
1:A:199:VAL:HG12	1:A:199:VAL:O	2.01	0.60
1:A:337:ILE:HD13	1:A:368:LEU:HD11	1.84	0.60
1:A:149:ILE:O	1:A:149:ILE:HG22	2.02	0.59
1:A:340:ILE:HG22	1:A:344:LEU:HD11	1.83	0.59
1:B:337:ILE:HD13	1:B:368:LEU:HD11	1.85	0.59
1:A:314:MSE:HG3	1:A:368:LEU:HA	1.84	0.58
1:A:310:MSE:CE	1:A:368:LEU:CD2	2.81	0.58
1:B:141:ILE:HG13	1:B:315:ILE:CD1	2.35	0.57
1:A:310:MSE:CE	1:A:368:LEU:HD23	2.34	0.57
1:B:275:LEU:O	1:B:278:VAL:HG22	2.05	0.56
1:A:318:GLY:HA3	1:A:375:THR:HG22	1.88	0.56
1:B:91:LEU:C	1:B:91:LEU:HD13	2.31	0.56
1:A:375:THR:N	1:A:376:PRO:CD	2.69	0.56
1:B:333:LEU:HD22	1:B:372:ILE:HD13	1.89	0.55
1:A:275:LEU:O	1:A:278:VAL:HG22	2.06	0.55
1:B:420:VAL:HG23	1:B:425:ILE:HA	1.89	0.55
1:A:333:LEU:HD22	1:A:372:ILE:HD13	1.87	0.55
1:A:86:ILE:HG23	1:A:171:ILE:HG23	1.89	0.54
1:B:350:LEU:HG	1:B:351:PRO:HD2	1.90	0.54
1:A:57:PHE:CA	1:A:60:MSE:HE2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD23	1:B:56:LEU:HD23	1.90	0.54
1:A:342:ILE:HG21	1:A:437:VAL:HG23	1.90	0.53
1:B:319:GLU:N	1:B:375:THR:CG2	2.72	0.53
1:A:420:VAL:HG23	1:A:425:ILE:HA	1.90	0.53
1:B:33:VAL:N	1:B:34:PRO:CD	2.71	0.53
1:B:342:ILE:HG21	1:B:437:VAL:HG23	1.91	0.53
1:A:33:VAL:N	1:A:34:PRO:CD	2.72	0.52
2:D:18:ALA:N	2:D:134:SER:O	2.42	0.52
1:B:314:MSE:HG2	1:B:368:LEU:CA	2.40	0.52
1:A:344:LEU:HD22	1:A:361:VAL:HG23	1.92	0.52
1:B:371:GLY:O	1:B:374:ALA:HB3	2.10	0.51
2:C:18:ALA:N	2:C:134:SER:O	2.42	0.51
1:A:314:MSE:HE3	1:A:372:ILE:CG1	2.40	0.51
1:B:314:MSE:HG2	1:B:368:LEU:HA	1.93	0.51
1:B:149:ILE:O	1:B:149:ILE:CG2	2.58	0.51
1:A:57:PHE:CD1	1:A:60:MSE:HE3	2.46	0.51
1:B:60:MSE:HA	1:B:209:LEU:HD13	1.93	0.51
1:B:373:TYR:CE1	1:B:377:SER:CB	2.93	0.51
1:A:275:LEU:HD13	1:A:335:THR:HG22	1.93	0.50
2:C:71:VAL:HB	2:C:75:PHE:CG	2.47	0.50
1:A:319:GLU:N	1:A:375:THR:CG2	2.75	0.50
2:D:71:VAL:HB	2:D:75:PHE:CG	2.47	0.50
1:B:91:LEU:HD12	1:B:104:GLY:CA	2.42	0.49
1:B:375:THR:CG2	1:B:376:PRO:HD3	2.41	0.49
1:A:375:THR:HG22	1:A:376:PRO:HD3	1.94	0.49
1:B:310:MSE:C	1:B:310:MSE:SE	3.05	0.49
1:B:344:LEU:HD13	1:B:361:VAL:CG2	2.42	0.49
1:B:141:ILE:CG1	1:B:315:ILE:CD1	2.91	0.49
2:C:22:LEU:HD13	2:C:131:VAL:HG23	1.95	0.49
1:B:315:ILE:CG2	1:B:374:ALA:HB3	2.41	0.49
1:A:280:GLY:O	1:A:283:ILE:HG22	2.13	0.49
1:A:319:GLU:N	1:A:375:THR:HG21	2.28	0.49
1:B:24:LEU:HD12	1:B:146:GLY:HA2	1.95	0.49
1:A:375:THR:CG2	1:A:376:PRO:HD3	2.43	0.48
1:B:149:ILE:HD11	1:B:308:LEU:HD13	1.94	0.48
1:B:222:LEU:HD22	1:B:222:LEU:N	2.29	0.48
1:A:24:LEU:HD12	1:A:146:GLY:HA2	1.96	0.48
1:B:275:LEU:HD23	1:B:335:THR:HG22	1.95	0.48
1:B:141:ILE:CG1	1:B:315:ILE:HD11	2.44	0.48
1:B:375:THR:N	1:B:376:PRO:CD	2.77	0.48
1:B:315:ILE:CG2	1:B:374:ALA:CB	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD22	1:A:222:LEU:N	2.28	0.47
1:A:263:LYS:HG3	1:A:265:TYR:HB3	1.96	0.47
2:D:22:LEU:HD13	2:D:131:VAL:HG23	1.96	0.47
1:B:116:MSE:HB2	1:B:117:PRO:HD3	1.97	0.47
1:A:178:MSE:O	1:A:181:ILE:HG22	2.15	0.46
1:A:91:LEU:HD23	1:A:104:GLY:HA2	1.97	0.46
1:A:314:MSE:O	1:A:318:GLY:N	2.47	0.46
1:A:116:MSE:HB2	1:A:117:PRO:HD3	1.97	0.46
1:A:314:MSE:HE3	1:A:372:ILE:HG13	1.96	0.46
1:A:373:TYR:CD1	1:A:373:TYR:O	2.69	0.46
1:B:373:TYR:CD1	1:B:373:TYR:O	2.68	0.46
1:A:57:PHE:CZ	1:A:106:VAL:HG13	2.51	0.45
1:A:337:ILE:O	1:A:365:CYS:SG	2.72	0.45
1:A:204:VAL:HG13	1:A:243:PHE:HB2	1.99	0.45
1:B:57:PHE:CZ	1:B:106:VAL:HG13	2.52	0.45
1:B:375:THR:O	1:B:378:THR:OG1	2.34	0.45
2:C:85:THR:O	2:C:85:THR:HG23	2.17	0.45
1:B:373:TYR:CE1	1:B:377:SER:HB3	2.52	0.44
1:A:370:LEU:O	1:A:374:ALA:HB2	2.17	0.44
2:D:16:VAL:O	2:D:133:VAL:HA	2.17	0.44
1:B:204:VAL:HG13	1:B:243:PHE:HB2	1.99	0.44
2:C:16:VAL:O	2:C:133:VAL:HA	2.17	0.44
1:A:123:MSE:SE	1:A:135:ALA:HB1	2.68	0.44
1:A:57:PHE:CD1	1:A:60:MSE:CE	3.01	0.44
1:B:340:ILE:HG22	1:B:365:CYS:SG	2.58	0.44
2:D:85:THR:O	2:D:85:THR:HG23	2.18	0.43
1:A:218:LYS:O	1:A:222:LEU:N	2.44	0.43
1:A:344:LEU:HD22	1:A:361:VAL:CG2	2.47	0.43
1:B:150:CYS:SG	1:B:151:SER:N	2.91	0.43
1:B:370:LEU:O	1:B:374:ALA:HB2	2.18	0.43
1:A:124:LYS:NZ	1:A:385:ALA:O	2.51	0.43
1:A:201:GLY:O	1:A:204:VAL:HG12	2.18	0.43
1:B:57:PHE:CE2	1:B:106:VAL:HG22	2.53	0.43
1:B:124:LYS:NZ	1:B:385:ALA:O	2.51	0.43
1:A:141:ILE:CG1	1:A:315:ILE:HD11	2.49	0.43
2:D:45:ARG:NH1	2:D:101:TYR:OH	2.52	0.43
1:A:28:SER:HA	1:A:150:CYS:O	2.19	0.43
1:B:123:MSE:SE	1:B:135:ALA:HB1	2.69	0.43
1:B:199:VAL:O	1:B:199:VAL:HG13	2.19	0.43
1:A:57:PHE:CE2	1:A:106:VAL:HG22	2.54	0.42
1:B:141:ILE:HG12	1:B:315:ILE:HD11	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ILE:O	1:B:365:CYS:SG	2.73	0.42
1:B:310:MSE:SE	1:B:310:MSE:O	2.87	0.42
1:B:318:GLY:C	1:B:375:THR:HG22	2.45	0.42
2:C:75:PHE:HB3	2:C:88:LEU:HD11	2.01	0.42
1:B:315:ILE:HG22	1:B:374:ALA:HB1	2.00	0.42
1:B:314:MSE:HG3	1:B:372:ILE:HG13	2.02	0.42
1:A:344:LEU:HB3	1:A:358:SER:O	2.19	0.41
2:D:75:PHE:HB3	2:D:88:LEU:HD11	2.01	0.41
1:B:420:VAL:O	1:B:423:THR:O	2.38	0.41
1:B:344:LEU:HB3	1:B:358:SER:O	2.21	0.41
2:D:93:LEU:HB3	2:D:133:VAL:HG11	2.02	0.41
1:A:205:LEU:HD12	1:A:208:MSE:CE	2.49	0.41
2:C:22:LEU:CD1	2:C:131:VAL:HG23	2.51	0.41
1:B:315:ILE:O	1:B:318:GLY:N	2.53	0.41
1:A:314:MSE:HB2	1:A:371:GLY:HA3	2.03	0.41
1:B:314:MSE:HG2	1:B:368:LEU:HB2	2.02	0.41
2:D:22:LEU:CD1	2:D:131:VAL:HG23	2.51	0.41
1:A:373:TYR:CE1	1:A:377:SER:HB2	2.56	0.41
1:B:344:LEU:CD1	1:B:361:VAL:HG23	2.49	0.41
1:A:202:LEU:C	1:A:202:LEU:HD13	2.46	0.41
1:A:375:THR:O	1:A:375:THR:OG1	2.32	0.41
1:B:416:TYR:O	1:B:420:VAL:HG12	2.21	0.41
1:A:295:TYR:CD2	1:A:299:GLN:HG2	2.56	0.40
1:A:373:TYR:CE1	1:A:377:SER:CB	3.04	0.40
1:A:416:TYR:O	1:A:420:VAL:HG12	2.21	0.40
1:B:295:TYR:CD2	1:B:299:GLN:HG2	2.57	0.40
1:A:420:VAL:O	1:A:423:THR:O	2.38	0.40
1:A:433:LEU:HD13	1:A:433:LEU:HA	1.97	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	398/479 (83%)	364 (92%)	34 (8%)	0	100	100
1	B	403/479 (84%)	372 (92%)	31 (8%)	0	100	100
2	C	129/131 (98%)	115 (89%)	14 (11%)	0	100	100
2	D	129/131 (98%)	115 (89%)	14 (11%)	0	100	100
All	All	1059/1220 (87%)	966 (91%)	93 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	270/363 (74%)	254 (94%)	16 (6%)	18	43
1	B	274/363 (76%)	258 (94%)	16 (6%)	18	43
2	C	93/105 (89%)	91 (98%)	2 (2%)	45	61
2	D	93/105 (89%)	91 (98%)	2 (2%)	45	61
All	All	730/936 (78%)	694 (95%)	36 (5%)	22	47

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MSE
1	A	60	MSE
1	A	123	MSE
1	A	133	GLN
1	A	161	MSE
1	A	167	PHE
1	A	208	MSE
1	A	215	VAL
1	A	265	TYR
1	A	274	LEU
1	A	307	TYR
1	A	344	LEU
1	A	347	LEU

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Mol	Chain	Res	Type
1	A	348	VAL
1	A	399	MSE
1	A	411	ILE
1	B	44	MSE
1	B	60	MSE
1	B	123	MSE
1	B	161	MSE
1	B	167	PHE
1	B	215	VAL
1	B	261	GLU
1	B	263	LYS
1	B	272	ASN
1	B	307	TYR
1	B	315	ILE
1	B	340	ILE
1	B	348	VAL
1	B	350	LEU
1	B	375	THR
1	B	411	ILE
2	C	6	VAL
2	C	45	ARG
2	D	6	VAL
2	D	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	290	GLN
1	A	291	GLN
1	A	436	ASN
1	B	133	GLN
1	B	272	ASN
1	B	276	ASN
1	B	291	GLN
1	B	436	ASN
2	C	46	GLN
2	C	130	GLN
2	D	46	GLN
2	D	130	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](#)

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.

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	393/479 (82%)	1.40	93 (23%) 2 2	99, 162, 210, 236	0
1	B	398/479 (83%)	1.43	100 (25%) 1 2	109, 186, 227, 243	0
2	C	131/131 (100%)	0.75	20 (15%) 5 5	98, 125, 155, 194	0
2	D	131/131 (100%)	0.48	13 (9%) 13 11	95, 126, 161, 184	0
All	All	1053/1220 (86%)	1.22	226 (21%) 2 3	95, 161, 218, 243	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	LYS	14.2
1	B	402	SER	13.9
1	A	27	GLN	13.4
1	A	68	LEU	11.0
1	A	198	ASP	10.9
1	A	406	ALA	9.9
1	B	400	ALA	9.8
1	A	72	ILE	9.4
1	A	30	VAL	9.2
1	B	405	GLY	9.0
1	B	120	LEU	8.9
1	B	396	ILE	8.6
1	B	406	ALA	8.5
1	B	401	SER	8.2
1	B	398	LYS	8.2
1	B	320	LYS	8.1
1	B	38	GLN	7.5
1	B	14	GLY	7.5
2	D	82	ALA	7.5
1	A	64	GLY	7.4
2	C	82	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	29	LEU	7.2
1	B	122	ILE	7.2
1	A	26	ALA	7.0
1	B	27	GLN	6.8
1	A	75	VAL	6.8
1	A	70	ASP	6.7
1	B	172	ILE	6.7
1	A	388	ASP	6.6
1	A	23	TRP	6.4
1	B	21	THR	6.3
1	A	407	PHE	6.3
1	A	402	SER	6.1
1	B	404	GLY	6.1
1	A	295	TYR	6.0
1	B	397	TYR	5.9
1	B	407	PHE	5.9
1	B	279	ALA	5.8
1	A	292	GLY	5.7
1	B	168	ILE	5.5
1	A	405	GLY	5.5
1	B	87	ILE	5.5
1	B	175	VAL	5.5
1	B	394	SER	5.5
1	B	403	LEU	5.5
1	A	122	ILE	5.5
1	B	23	TRP	5.5
1	A	32	VAL	5.4
2	C	19	GLY	5.4
1	B	409	VAL	5.2
1	B	39	SER	5.1
1	B	382	ILE	5.0
1	B	160	THR	4.9
1	A	259	LEU	4.8
1	B	30	VAL	4.8
1	B	292	GLY	4.7
1	A	294	GLY	4.7
2	D	83	LYS	4.7
2	C	18	ALA	4.7
1	A	67	GLY	4.7
1	A	28	SER	4.6
1	B	336	PHE	4.5
1	A	74	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	125	THR	4.3
1	A	258	LYS	4.2
1	A	401	SER	4.2
1	A	25	PHE	4.2
1	A	279	ALA	4.1
1	A	293	LEU	4.1
1	B	293	LEU	4.1
1	A	403	LEU	4.1
1	B	121	ALA	4.1
1	B	408	GLY	4.0
1	B	207	VAL	4.0
2	D	66	TYR	4.0
1	A	410	ALA	4.0
1	A	48	SER	3.9
1	A	126	TYR	3.9
1	A	221	ALA	3.8
1	A	31	ASN	3.8
2	D	36	TYR	3.8
1	A	273	PHE	3.7
1	A	378	THR	3.6
1	B	16	VAL	3.6
1	A	387	LEU	3.6
1	B	20	ILE	3.6
1	A	216	ILE	3.6
1	B	125	THR	3.6
1	A	320	LYS	3.6
1	A	21	THR	3.6
2	C	81	SER	3.6
2	C	28	ALA	3.6
1	B	19	VAL	3.6
1	B	31	ASN	3.6
2	D	80	ASP	3.6
1	A	105	ARG	3.5
1	A	409	VAL	3.5
1	A	369	GLY	3.5
1	A	220	ALA	3.5
1	B	321	LEU	3.5
1	A	20	ILE	3.4
2	C	68	THR	3.4
1	B	378	THR	3.4
1	B	322	LEU	3.4
1	B	156	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	159	THR	3.3
1	B	357	ILE	3.3
1	B	395	GLY	3.3
1	B	422	ALA	3.3
1	B	200	ALA	3.3
1	B	333	LEU	3.3
2	D	11	SER	3.2
2	C	17	GLN	3.2
1	A	65	ALA	3.2
1	A	112	ALA	3.2
1	B	276	ASN	3.2
1	B	236	VAL	3.2
1	B	239	ALA	3.2
2	C	35	THR	3.1
1	A	270	ILE	3.1
2	C	20	GLY	3.1
1	A	199	VAL	3.1
1	B	15	ILE	3.0
1	B	228	TRP	3.0
1	A	372	ILE	3.0
1	B	13	LEU	3.0
1	B	17	LEU	3.0
2	C	72	LYS	2.9
1	A	448	LEU	2.9
1	B	354	PHE	2.9
1	A	283	ILE	2.9
1	A	35	ASN	2.9
1	B	280	GLY	2.9
1	B	12	ILE	2.9
1	A	289	VAL	2.9
1	A	334	GLY	2.9
1	A	52	SER	2.8
1	A	315	ILE	2.8
1	A	282	LEU	2.8
1	B	37	GLN	2.8
1	B	55	ALA	2.8
1	B	210	LEU	2.8
1	B	412	SER	2.8
2	D	34	SER	2.8
2	D	84	ASN	2.8
1	B	317	VAL	2.8
1	A	452	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	44	PHE	2.7
1	B	283	ILE	2.7
1	B	319	GLU	2.7
1	B	94	ILE	2.7
1	B	141	ILE	2.6
1	A	147	SER	2.6
1	B	59	GLY	2.6
2	C	69	ASP	2.6
1	B	235	ILE	2.6
1	A	389	LYS	2.5
1	A	114	CYS	2.5
1	A	98	PRO	2.5
1	A	376	PRO	2.5
1	A	235	ILE	2.5
1	A	367	GLY	2.5
2	D	81	SER	2.5
1	A	400	ALA	2.4
2	C	119	ALA	2.4
1	B	222	LEU	2.4
1	A	374	ALA	2.4
1	A	449	PHE	2.4
1	B	315	ILE	2.4
2	C	53	GLU	2.4
1	A	207	VAL	2.4
1	A	236	VAL	2.4
1	A	338	VAL	2.4
1	A	118	SER	2.4
1	B	206	VAL	2.4
1	B	217	THR	2.4
1	B	144	TRP	2.4
1	B	171	ILE	2.3
2	C	125	TRP	2.3
1	B	18	GLY	2.3
1	B	124	LYS	2.3
1	B	273	PHE	2.3
1	B	126	TYR	2.3
1	B	277	GLY	2.3
1	B	233	ILE	2.3
1	B	411	ILE	2.3
2	C	105	ALA	2.3
1	B	353	ILE	2.3
1	B	294	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	393	ALA	2.2
1	A	337	ILE	2.2
1	B	379	ASP	2.2
2	C	41	MET	2.2
1	A	73	GLY	2.2
2	C	54	GLY	2.2
2	D	68	THR	2.2
2	D	31	TYR	2.2
1	A	392	VAL	2.2
2	C	55	VAL	2.2
1	B	107	ILE	2.2
1	A	398	LYS	2.2
2	C	133	VAL	2.1
1	A	232	LEU	2.1
1	B	312	LEU	2.1
1	B	245	ASN	2.1
1	A	363	TYR	2.1
1	B	229	PHE	2.1
1	A	368	LEU	2.1
1	A	370	LEU	2.1
2	D	37	SER	2.1
1	A	63	VAL	2.1
1	B	176	LEU	2.1
1	B	133	GLN	2.1
1	A	212	LEU	2.1
1	A	404	GLY	2.1
1	A	437	VAL	2.1
1	B	67	GLY	2.1
1	A	87	ILE	2.1
1	A	203	ILE	2.0
1	A	66	GLY	2.0
1	B	369	GLY	2.0
1	B	232	LEU	2.0
1	B	392	VAL	2.0
2	D	54	GLY	2.0
1	B	184	THR	2.0
1	A	55	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 [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
3	ZN	C	201	1/1	1.00	0.02	112,112,112,112	0
3	ZN	D	201	1/1	1.00	0.06	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.