



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:40 AM UTC

PDB ID : 1ZL6 / pdb_00001zl6
Title : Crystal structure of Tyr350Ala mutant of Clostridium botulinum neurotoxin E catalytic domain
Authors : Agarwal, R.; Binz, T.; Swaminathan, S.
Deposited on : 2005-05-05
Resolution : 2.40 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

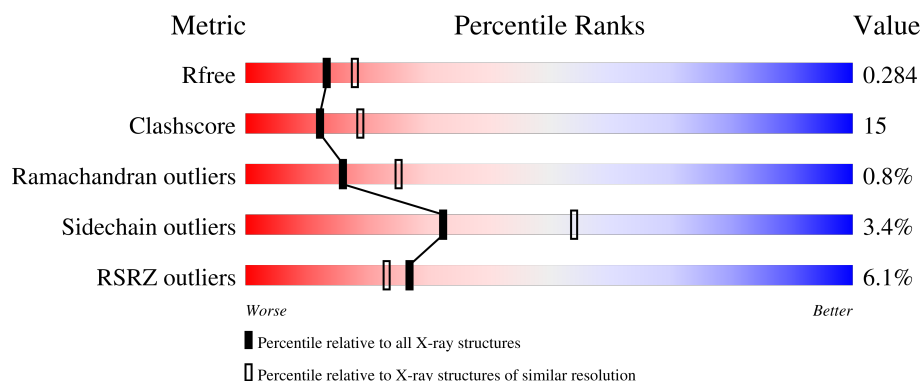
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 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	420	2% 66% 28% • 5%
1	B	420	9% 58% 31% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6517 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 botulinum neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3200	2046	533	613	8			
1	B	387	Total	C	N	O	S	0	0	0
			3103	1986	516	594	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	ALA	TYR	engineered mutation	UNP Q00496
B	350	ALA	TYR	engineered mutation	UNP Q00496

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

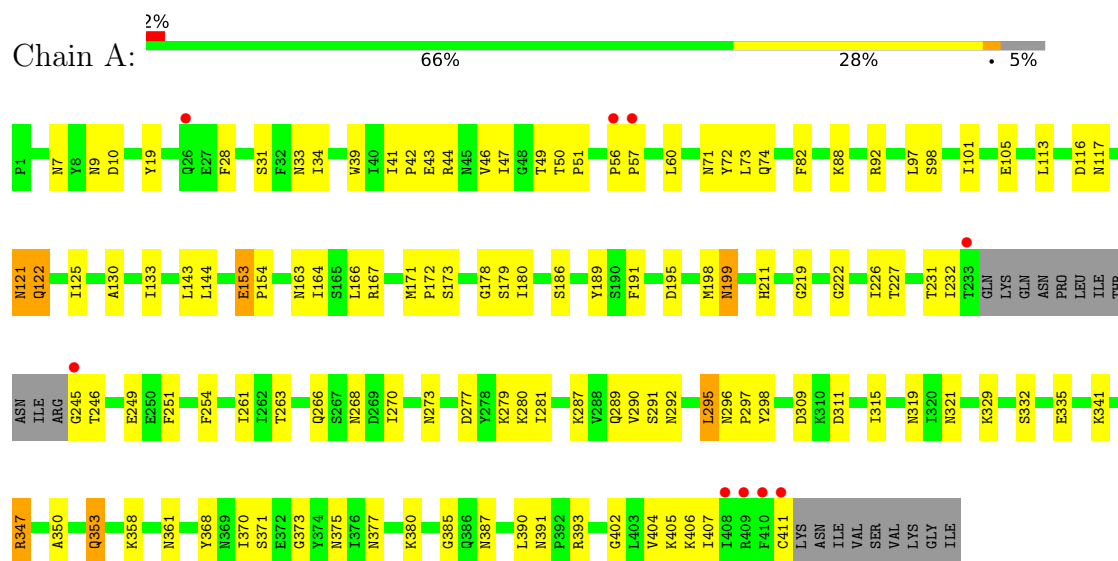
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	81	Total	O	0	0
			81	81		

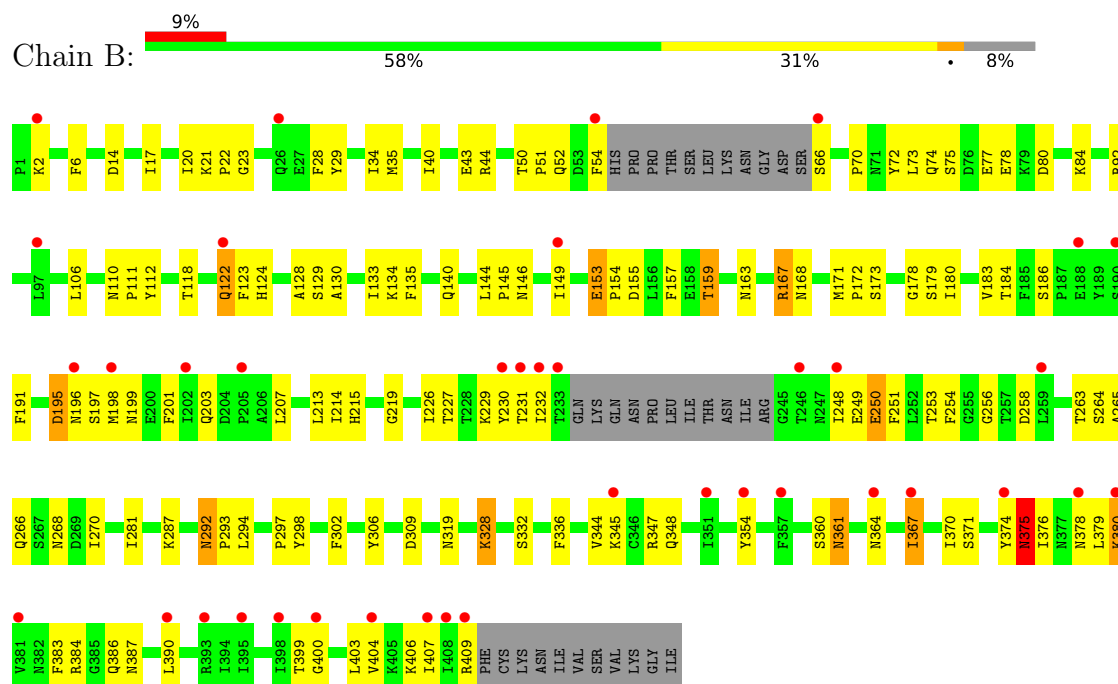
3 Residue-property plots [i](#)

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: botulinum neurotoxin type E



• Molecule 1: botulinum neurotoxin type E



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.80Å 144.96Å 83.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.40 46.54 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (46.54-2.40) 92.8 (46.54-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.284 0.235 , 0.284	Depositor DCC
R_{free} test set	1206 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6517	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: ZN, SO4

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	0.48	0/3271	0.98	15/4429 (0.3%)
1	B	0.41	0/3169	0.94	9/4288 (0.2%)
All	All	0.45	0/6440	0.96	24/8717 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	THR	N-CA-C	7.88	122.48	113.02
1	B	186	SER	CA-C-N	7.78	128.19	119.32
1	B	186	SER	C-N-CA	7.78	128.19	119.32
1	B	23	GLY	N-CA-C	-7.31	102.81	111.36
1	A	371	SER	N-CA-C	7.07	120.02	111.82
1	A	377	ASN	CB-CA-C	-6.88	108.63	116.54
1	A	56	PRO	N-CA-C	6.62	118.78	110.70
1	B	371	SER	N-CA-C	6.61	119.32	111.33
1	B	229	LYS	N-CA-C	-6.39	106.07	114.31
1	A	249	GLU	N-CA-C	-6.09	104.71	111.71
1	A	57	PRO	N-CA-C	-6.05	105.12	113.53
1	B	74	GLN	N-CA-C	-5.93	105.96	113.43
1	A	279	LYS	N-CA-C	-5.79	105.06	111.36
1	A	122	GLN	N-CA-C	5.76	117.28	108.42
1	A	199	ASN	N-CA-C	-5.76	101.96	110.48
1	A	7	ASN	N-CA-C	-5.74	100.35	109.59
1	A	273	ASN	N-CA-C	5.57	117.34	111.28
1	A	186	SER	CA-C-N	5.52	125.14	119.56
1	A	186	SER	C-N-CA	5.52	125.14	119.56
1	B	367	ILE	CB-CA-C	-5.49	107.04	111.71
1	A	164	ILE	N-CA-C	5.33	115.92	108.89
1	A	332	SER	N-CA-C	-5.32	106.74	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ALA	N-CA-C	5.15	117.08	108.99
1	A	34	ILE	N-CA-C	5.03	116.35	110.62

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	3200	0	3154	81	0
1	B	3103	0	3064	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	A	126	0	0	7	0
4	B	81	0	0	3	0
All	All	6517	0	6218	194	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 15.

All (194) 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:263:THR:H	1:B:266:GLN:HE21	1.08	1.02
1:B:75:SER:HB3	1:B:78:GLU:HG3	1.47	0.96
1:B:250:GLU:HA	1:B:250:GLU:OE1	1.72	0.89
1:A:292:ASN:O	1:A:295:LEU:HD22	1.82	0.80
1:B:292:ASN:C	1:B:292:ASN:HD22	1.94	0.75
1:B:263:THR:H	1:B:266:GLN:NE2	1.85	0.72
1:A:44:ARG:NH1	1:A:72:TYR:HB3	2.04	0.71
1:A:153:GLU:HB2	1:A:154:PRO:CD	2.20	0.70
1:B:309:ASP:OD2	1:B:319:ASN:HB2	1.91	0.70
1:B:292:ASN:HD22	1:B:293:PRO:N	1.89	0.70
1:B:375:ASN:HB3	1:B:380:LYS:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:PHE:HD2	1:B:258:ASP:HB3	1.55	0.70
1:A:289:GLN:HG3	1:A:291:SER:H	1.56	0.69
1:B:406:LYS:HE2	4:B:903:HOH:O	1.92	0.68
1:B:215:HIS:NE2	1:B:250:GLU:OE1	2.27	0.68
1:A:370:ILE:HG12	4:A:535:HOH:O	1.94	0.67
1:B:292:ASN:ND2	1:B:294:LEU:H	1.93	0.67
1:B:215:HIS:CE1	1:B:250:GLU:OE1	2.50	0.65
1:B:263:THR:OG1	1:B:266:GLN:HG3	1.97	0.65
1:B:400:GLY:O	1:B:404:VAL:HG23	1.97	0.65
1:B:153:GLU:HB2	1:B:154:PRO:CD	2.27	0.64
1:A:153:GLU:HB2	1:A:154:PRO:HD2	1.80	0.63
1:A:289:GLN:HE21	1:A:290:VAL:H	1.44	0.63
1:A:97:LEU:O	1:A:101:ILE:HG12	1.99	0.63
1:B:380:LYS:HD2	1:B:380:LYS:C	2.24	0.63
1:B:328:LYS:NZ	1:B:328:LYS:HB3	2.13	0.63
1:B:75:SER:HB3	1:B:78:GLU:CG	2.27	0.62
1:A:163:ASN:ND2	1:A:219:GLY:HA3	2.15	0.62
1:A:163:ASN:HD21	1:A:219:GLY:HA3	1.65	0.62
1:A:347:ARG:HG2	4:A:518:HOH:O	2.01	0.61
1:B:191:PHE:CE1	1:B:203:GLN:HB2	2.35	0.61
1:A:71:ASN:O	1:A:74:GLN:HG2	2.01	0.61
1:B:34:ILE:HD12	1:B:40:ILE:HD11	1.82	0.60
1:B:344:VAL:HG13	1:B:386:GLN:HE22	1.66	0.60
1:A:173:SER:HA	1:A:178:GLY:HA2	1.82	0.60
1:A:130:ALA:HB2	1:A:144:LEU:CD2	2.31	0.60
1:B:80:ASP:O	1:B:84:LYS:HD3	2.01	0.59
1:A:33:ASN:HB2	1:A:39:TRP:CH2	2.37	0.59
1:A:198:MET:HE2	1:A:198:MET:H	1.68	0.59
1:B:292:ASN:HD21	1:B:294:LEU:CD2	2.15	0.59
1:B:122:GLN:NE2	1:B:123:PHE:O	2.36	0.58
1:A:311:ASP:OD2	1:A:315:ILE:HB	2.02	0.58
1:B:375:ASN:HD22	1:B:375:ASN:N	2.00	0.58
1:A:195:ASP:OD1	1:A:199:ASN:HB2	2.02	0.58
1:B:149:ILE:HD13	1:B:183:VAL:HB	1.85	0.58
1:B:263:THR:N	1:B:266:GLN:HE21	1.90	0.58
1:B:292:ASN:HD21	1:B:294:LEU:HD23	1.69	0.57
1:B:153:GLU:HB2	1:B:154:PRO:HD2	1.87	0.57
1:B:215:HIS:CE1	1:B:250:GLU:CD	2.82	0.57
1:B:266:GLN:O	1:B:270:ILE:HG12	2.04	0.57
1:A:163:ASN:HB3	1:A:179:SER:OG	2.05	0.57
1:B:251:PHE:CD2	1:B:258:ASP:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HD3	1:B:73:LEU:HB2	1.87	0.57
1:B:54:PHE:C	1:B:70:PRO:HG3	2.29	0.57
1:B:20:ILE:HG12	1:B:133:ILE:HG22	1.86	0.56
1:B:44:ARG:NH1	1:B:72:TYR:HB3	2.20	0.56
1:B:403:LEU:C	1:B:403:LEU:HD13	2.31	0.56
1:A:98:SER:OG	1:A:341:LYS:HD3	2.06	0.56
1:B:344:VAL:HG13	1:B:386:GLN:NE2	2.21	0.56
1:B:294:LEU:O	1:B:297:PRO:HD2	2.05	0.56
1:B:379:LEU:HD23	1:B:384:ARG:HD2	1.87	0.56
1:B:201:PHE:HE1	1:B:383:PHE:O	1.88	0.55
1:B:227:THR:HA	1:B:248:ILE:HD11	1.88	0.55
1:B:375:ASN:HD21	1:B:386:GLN:HG3	1.70	0.55
1:B:378:ASN:ND2	1:B:384:ARG:HH12	2.03	0.55
1:B:403:LEU:CD1	1:B:407:ILE:HD11	2.37	0.55
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.07	0.55
1:A:404:VAL:HG23	4:A:537:HOH:O	2.07	0.55
1:B:292:ASN:HD22	1:B:294:LEU:H	1.54	0.55
1:B:6:PHE:CD1	1:B:17:ILE:HD11	2.42	0.54
1:B:167:ARG:HB2	1:B:167:ARG:HH11	1.73	0.54
1:B:54:PHE:O	1:B:70:PRO:HG3	2.08	0.54
1:B:409:ARG:N	1:B:409:ARG:HD2	2.23	0.54
1:A:375:ASN:HD22	1:A:385:GLY:HA3	1.73	0.54
1:A:117:ASN:HD22	1:A:117:ASN:N	2.04	0.53
1:A:226:ILE:HB	1:A:270:ILE:HD13	1.89	0.53
1:B:168:ASN:HD22	1:B:168:ASN:N	2.06	0.53
1:B:360:SER:O	1:B:361:ASN:C	2.51	0.53
1:B:344:VAL:HG12	1:B:345:LYS:O	2.08	0.53
1:B:328:LYS:HB3	1:B:328:LYS:HZ3	1.73	0.53
1:A:171:MET:HE3	4:A:595:HOH:O	2.08	0.52
1:B:375:ASN:N	1:B:375:ASN:ND2	2.56	0.52
1:B:112:TYR:HA	1:B:302:PHE:CE1	2.44	0.52
1:B:292:ASN:C	1:B:292:ASN:ND2	2.67	0.52
1:B:256:GLY:HA3	1:B:336:PHE:CD1	2.45	0.52
1:B:163:ASN:HB3	1:B:179:SER:OG	2.09	0.52
1:B:287:LYS:HE3	4:B:839:HOH:O	2.10	0.52
1:B:364:ASN:HB3	1:B:367:ILE:HD12	1.91	0.52
1:B:328:LYS:O	1:B:332:SER:HB3	2.10	0.52
1:A:130:ALA:HB2	1:A:144:LEU:HD23	1.92	0.52
1:B:254:PHE:HD2	1:B:258:ASP:OD2	1.93	0.52
1:A:261:ILE:HD12	1:A:261:ILE:N	2.25	0.51
1:A:19:TYR:HB3	1:A:28:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:O	1:A:222:GLY:HA2	2.09	0.51
1:A:113:LEU:HD22	1:A:125:ILE:HG12	1.91	0.51
1:B:21:LYS:O	1:B:21:LYS:HE2	2.10	0.51
1:A:391:ASN:OD1	1:A:393:ARG:HG2	2.11	0.51
1:B:21:LYS:HB2	1:B:28:PHE:CD1	2.45	0.51
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.76	0.51
1:A:116:ASP:C	1:A:117:ASN:HD22	2.19	0.51
1:A:117:ASN:N	1:A:117:ASN:ND2	2.58	0.51
1:A:133:ILE:HG21	1:A:143:LEU:HB2	1.93	0.50
1:A:33:ASN:HB2	1:A:39:TRP:CZ2	2.47	0.50
1:B:215:HIS:CE1	1:B:249:GLU:HG3	2.47	0.50
1:B:6:PHE:CE1	1:B:17:ILE:HD11	2.47	0.50
1:B:118:THR:HG21	1:B:124:HIS:CD2	2.46	0.50
1:B:173:SER:HA	1:B:178:GLY:HA2	1.94	0.50
1:A:198:MET:HE2	1:A:198:MET:N	2.26	0.50
1:B:203:GLN:NE2	1:B:207:LEU:HB3	2.28	0.49
1:A:231:THR:O	1:A:232:ILE:HD13	2.11	0.49
1:A:226:ILE:CG2	1:A:270:ILE:HD13	2.42	0.49
1:B:292:ASN:ND2	1:B:294:LEU:HD23	2.27	0.49
1:A:261:ILE:HD12	1:A:261:ILE:H	1.78	0.49
1:B:214:ILE:CG2	1:B:253:THR:HG23	2.44	0.48
1:A:105:GLU:CD	1:A:329:LYS:HD2	2.39	0.48
1:B:21:LYS:HB2	1:B:28:PHE:CE1	2.49	0.48
1:B:215:HIS:NE2	1:B:250:GLU:CD	2.72	0.48
1:A:60:LEU:HB2	4:A:509:HOH:O	2.14	0.47
1:A:153:GLU:CB	1:A:154:PRO:CD	2.89	0.47
1:A:121:ASN:ND2	1:A:121:ASN:C	2.72	0.47
1:B:215:HIS:CE1	1:B:250:GLU:OE2	2.68	0.47
1:B:354:TYR:HE2	4:B:849:HOH:O	1.96	0.47
1:B:34:ILE:HG23	1:B:35:MET:HG2	1.97	0.47
1:A:191:PHE:HE1	1:A:347:ARG:HD3	1.80	0.46
1:A:387:ASN:HB3	1:A:390:LEU:HB2	1.96	0.46
1:A:232:ILE:O	1:A:245:GLY:HA2	2.15	0.46
1:B:264:SER:O	1:B:265:ALA:C	2.59	0.46
1:A:277:ASP:O	1:A:281:ILE:HG13	2.16	0.46
1:B:92:ARG:HA	1:B:370:ILE:HG23	1.98	0.46
1:A:263:THR:H	1:A:266:GLN:NE2	2.13	0.46
1:A:289:GLN:HB3	4:A:526:HOH:O	2.16	0.45
1:A:166:LEU:HD22	1:A:167:ARG:HH12	1.81	0.45
1:A:31:SER:OG	1:A:41:ILE:HG12	2.17	0.45
1:A:42:PRO:C	1:A:43:GLU:HG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ALA:O	1:B:180:ILE:HG13	2.17	0.45
1:A:121:ASN:HA	1:A:287:LYS:O	2.17	0.45
1:B:111:PRO:HD3	1:B:146:ASN:OD1	2.17	0.45
1:B:134:LYS:CE	1:B:140:GLN:HE21	2.30	0.45
1:B:163:ASN:ND2	1:B:219:GLY:HA3	2.31	0.45
1:B:231:THR:O	1:B:232:ILE:HD13	2.17	0.45
1:A:254:PHE:CG	1:A:350:ALA:HB2	2.51	0.45
1:A:88:LYS:HG3	1:A:370:ILE:HD11	1.98	0.44
1:A:246:THR:HG22	1:A:251:PHE:HE1	1.82	0.44
1:B:21:LYS:HE3	1:B:22:PRO:O	2.17	0.44
1:A:179:SER:O	1:A:180:ILE:C	2.60	0.44
1:B:66:SER:HA	1:B:157:PHE:CD2	2.52	0.44
1:B:197:SER:O	1:B:199:ASN:N	2.51	0.44
1:A:9:ASN:O	1:A:10:ASP:C	2.60	0.44
1:B:374:TYR:O	1:B:376:ILE:HG13	2.16	0.44
1:A:251:PHE:N	1:A:251:PHE:CD1	2.86	0.44
1:B:14:ASP:OD1	1:B:135:PHE:HB3	2.17	0.44
1:A:73:LEU:HD21	1:A:82:PHE:HB2	2.00	0.44
1:B:207:LEU:O	1:B:207:LEU:HG	2.18	0.44
1:A:404:VAL:HG23	1:A:405:LYS:H	1.82	0.44
1:B:168:ASN:N	1:B:168:ASN:ND2	2.65	0.43
1:A:296:ASN:N	1:A:297:PRO:CD	2.81	0.43
1:B:50:THR:O	1:B:51:PRO:C	2.61	0.43
1:B:226:ILE:CG2	1:B:270:ILE:HD13	2.48	0.43
1:B:155:ASP:OD1	1:B:155:ASP:C	2.61	0.43
1:A:266:GLN:O	1:A:270:ILE:HG12	2.18	0.43
1:B:144:LEU:HD12	1:B:144:LEU:N	2.33	0.43
1:B:195:ASP:CG	1:B:196:ASN:N	2.76	0.43
1:A:309:ASP:OD2	1:A:319:ASN:HB2	2.19	0.43
1:B:201:PHE:HD1	1:B:386:GLN:C	2.27	0.43
1:A:211:HIS:ND1	1:A:335:GLU:OE1	2.48	0.43
1:B:29:TYR:CG	1:B:43:GLU:HG3	2.54	0.43
1:B:29:TYR:CD1	1:B:43:GLU:HG3	2.53	0.43
1:A:227:THR:HG23	1:A:270:ILE:HD12	2.01	0.43
1:A:280:LYS:O	1:A:280:LYS:HD3	2.19	0.42
1:B:215:HIS:NE2	1:B:250:GLU:OE2	2.52	0.42
1:B:230:TYR:HB2	1:B:248:ILE:HD13	2.01	0.42
1:A:171:MET:HA	1:A:172:PRO:HD2	1.85	0.42
1:B:201:PHE:HA	1:B:386:GLN:O	2.20	0.42
1:B:347:ARG:HG3	1:B:347:ARG:HH11	1.85	0.42
1:A:375:ASN:HB3	1:A:380:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASN:HB3	1:B:390:LEU:HB2	2.02	0.42
1:A:189:TYR:CE1	1:A:358:LYS:HG3	2.54	0.42
1:A:295:LEU:C	1:A:295:LEU:HD23	2.45	0.41
1:A:321:ASN:ND2	4:A:529:HOH:O	2.53	0.41
1:B:153:GLU:O	1:B:154:PRO:C	2.63	0.41
1:A:46:VAL:O	1:A:47:ILE:C	2.63	0.41
1:A:368:TYR:HA	1:A:373:GLY:O	2.21	0.41
1:B:159:THR:HA	1:B:184:THR:O	2.20	0.41
1:B:129:SER:C	1:B:180:ILE:HD11	2.44	0.41
1:B:106:LEU:HD11	1:B:213:LEU:HB3	2.03	0.41
1:B:171:MET:HA	1:B:172:PRO:HD2	1.86	0.41
1:A:47:ILE:O	1:A:49:THR:HG23	2.21	0.40
1:A:402:GLY:O	1:A:406:LYS:HD3	2.20	0.40
1:B:110:ASN:HA	1:B:146:ASN:OD1	2.21	0.40
1:A:172:PRO:HG2	1:A:179:SER:HB3	2.03	0.40
1:A:353:GLN:HE21	1:A:353:GLN:HB2	1.60	0.40
1:A:50:THR:O	1:A:51:PRO:C	2.65	0.40
1:A:297:PRO:HB2	1:B:297:PRO:HB2	2.03	0.40
1:B:281:ILE:HD12	1:B:306:TYR:CE2	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	396/420 (94%)	368 (93%)	26 (7%)	2 (0%)	24	37
1	B	381/420 (91%)	350 (92%)	27 (7%)	4 (1%)	12	20
All	All	777/840 (92%)	718 (92%)	53 (7%)	6 (1%)	16	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	MET
1	A	361	ASN
1	B	375	ASN
1	B	361	ASN
1	A	153	GLU
1	B	153	GLU

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	360/379 (95%)	351 (98%)	9 (2%)	42	64
1	B	348/379 (92%)	333 (96%)	15 (4%)	26	44
All	All	708/758 (93%)	684 (97%)	24 (3%)	32	54

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

Mol	Chain	Res	Type
1	A	121	ASN
1	A	122	GLN
1	A	268	ASN
1	A	295	LEU
1	A	298	TYR
1	A	347	ARG
1	A	353	GLN
1	A	407	ILE
1	A	411	CYS
1	B	2	LYS
1	B	52	GLN
1	B	122	GLN
1	B	145	PRO
1	B	159	THR
1	B	167	ARG
1	B	195	ASP
1	B	250	GLU
1	B	268	ASN

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Mol	Chain	Res	Type
1	B	292	ASN
1	B	298	TYR
1	B	328	LYS
1	B	348	GLN
1	B	375	ASN
1	B	380	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	117	ASN
1	A	121	ASN
1	A	124	HIS
1	A	163	ASN
1	A	174	ASN
1	A	194	ASN
1	A	266	GLN
1	A	289	GLN
1	A	296	ASN
1	A	348	GLN
1	A	353	GLN
1	A	375	ASN
1	A	378	ASN
1	A	389	ASN
1	B	71	ASN
1	B	95	ASN
1	B	122	GLN
1	B	124	HIS
1	B	140	GLN
1	B	163	ASN
1	B	168	ASN
1	B	175	HIS
1	B	199	ASN
1	B	203	GLN
1	B	266	GLN
1	B	292	ASN
1	B	296	ASN
1	B	375	ASN
1	B	377	ASN
1	B	378	ASN
1	B	387	ASN

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Mol	Chain	Res	Type
1	B	389	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	SO4	A	500	2	4,4,4	0.52	0	6,6,6	0.15	0

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

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

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	400/420 (95%)	0.07	9 (2%) 61 57	18, 42, 61, 86	0
1	B	387/420 (92%)	0.69	39 (10%) 12 9	25, 54, 81, 97	0
All	All	787/840 (93%)	0.38	48 (6%) 27 23	18, 47, 78, 97	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	THR	5.4
1	B	232	ILE	5.1
1	A	233	THR	3.8
1	A	408	ILE	3.7
1	B	390	LEU	3.6
1	B	54	PHE	3.5
1	B	351	ILE	3.4
1	B	246	THR	3.3
1	A	410	PHE	3.2
1	B	395	ILE	3.2
1	A	411	CYS	3.1
1	B	393	ARG	3.0
1	B	407	ILE	2.9
1	B	230	TYR	2.9
1	B	231	THR	2.8
1	A	409	ARG	2.8
1	B	202	ILE	2.7
1	B	374	TYR	2.7
1	B	409	ARG	2.7
1	B	248	ILE	2.6
1	B	188	GLU	2.6
1	B	26	GLN	2.6
1	B	190	SER	2.6
1	B	357	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	2.6
1	B	66	SER	2.5
1	B	408	ILE	2.5
1	A	245	GLY	2.5
1	B	364	ASN	2.5
1	B	367	ILE	2.5
1	B	122	GLN	2.4
1	B	198	MET	2.4
1	B	345	LYS	2.4
1	B	97	LEU	2.3
1	B	149	ILE	2.3
1	B	2	LYS	2.3
1	B	404	VAL	2.3
1	A	57	PRO	2.3
1	B	354	TYR	2.3
1	B	398	ILE	2.2
1	B	378	ASN	2.2
1	B	196	ASN	2.2
1	B	380	LYS	2.2
1	B	381	VAL	2.1
1	B	400	GLY	2.1
1	B	205	PRO	2.0
1	A	26	GLN	2.0
1	A	56	PRO	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
3	SO4	A	500	5/5	0.80	0.15	57,58,61,62	0
2	ZN	B	822	1/1	0.97	0.06	67,67,67,67	0
2	ZN	A	422	1/1	0.99	0.02	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.