



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 AM UTC

PDB ID : 1YW4 / pdb_00001yw4
Title : Crystal Structure of the Succinylglutamate Desuccinylase from *Chromobacterium violaceum*, Northeast Structural Genomics Target CvR22.
Authors : Forouhar, F.; Abashidze, M.; Conover, K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-02-17
Resolution : 2.00 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

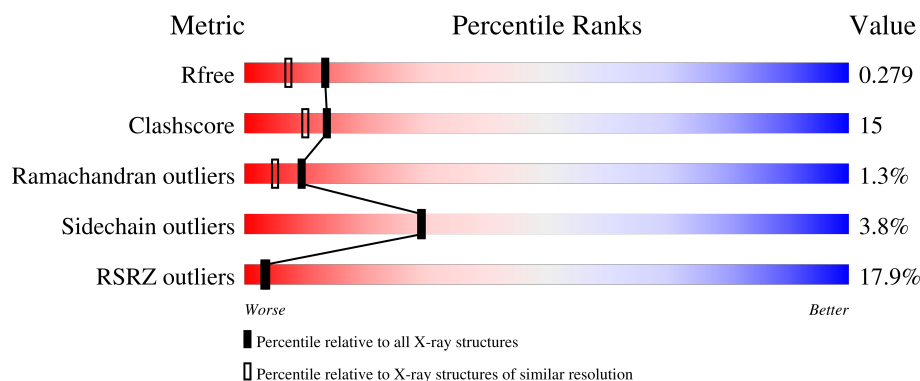
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	341	17% 66% 25% 6%
1	B	341	15% 63% 24% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5277 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 Succinylglutamate desuccinylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	Se	0	0	0
			2465	1563	442	451	5	4			
1	B	309	Total	C	N	O	S	Se	0	0	0
			2388	1511	426	442	5	4			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q7NU26
A	69	MSE	MET	modified residue	UNP Q7NU26
A	87	MSE	MET	modified residue	UNP Q7NU26
A	105	MSE	MET	modified residue	UNP Q7NU26
A	289	MSE	MET	modified residue	UNP Q7NU26
A	334	LEU	-	expression tag	UNP Q7NU26
A	335	GLU	-	expression tag	UNP Q7NU26
A	336	HIS	-	expression tag	UNP Q7NU26
A	337	HIS	-	expression tag	UNP Q7NU26
A	338	HIS	-	expression tag	UNP Q7NU26
A	339	HIS	-	expression tag	UNP Q7NU26
A	340	HIS	-	expression tag	UNP Q7NU26
A	341	HIS	-	expression tag	UNP Q7NU26
B	1	MSE	MET	modified residue	UNP Q7NU26
B	69	MSE	MET	modified residue	UNP Q7NU26
B	87	MSE	MET	modified residue	UNP Q7NU26
B	105	MSE	MET	modified residue	UNP Q7NU26
B	289	MSE	MET	modified residue	UNP Q7NU26
B	334	LEU	-	expression tag	UNP Q7NU26
B	335	GLU	-	expression tag	UNP Q7NU26
B	336	HIS	-	expression tag	UNP Q7NU26
B	337	HIS	-	expression tag	UNP Q7NU26
B	338	HIS	-	expression tag	UNP Q7NU26
B	339	HIS	-	expression tag	UNP Q7NU26
B	340	HIS	-	expression tag	UNP Q7NU26

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Chain	Residue	Modelled	Actual	Comment	Reference
B	341	HIS	-	expression tag	UNP Q7NU26

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

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

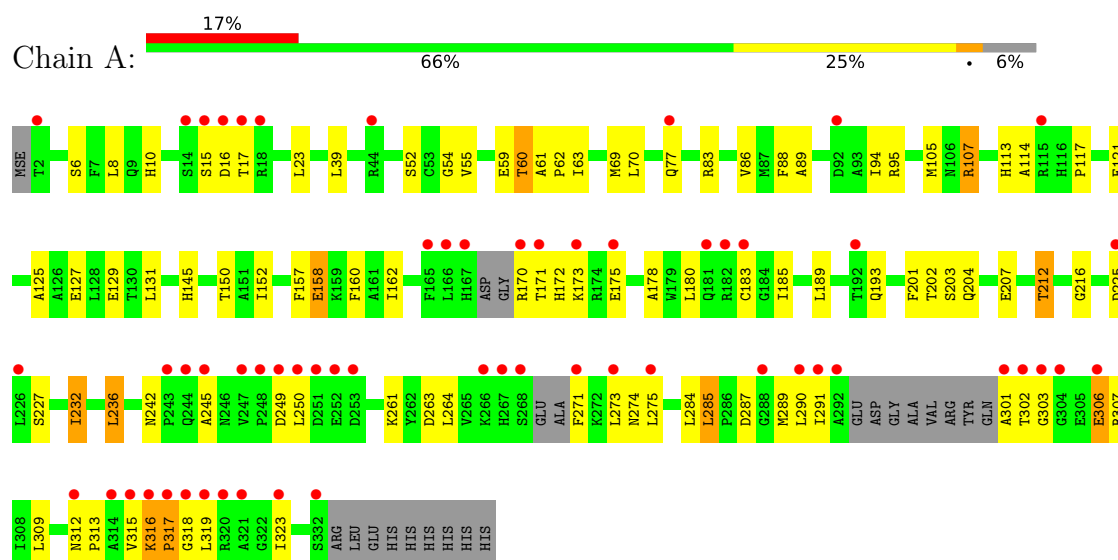
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total 241	O 241	0	0
3	B	181	Total 181	O 181	0	0

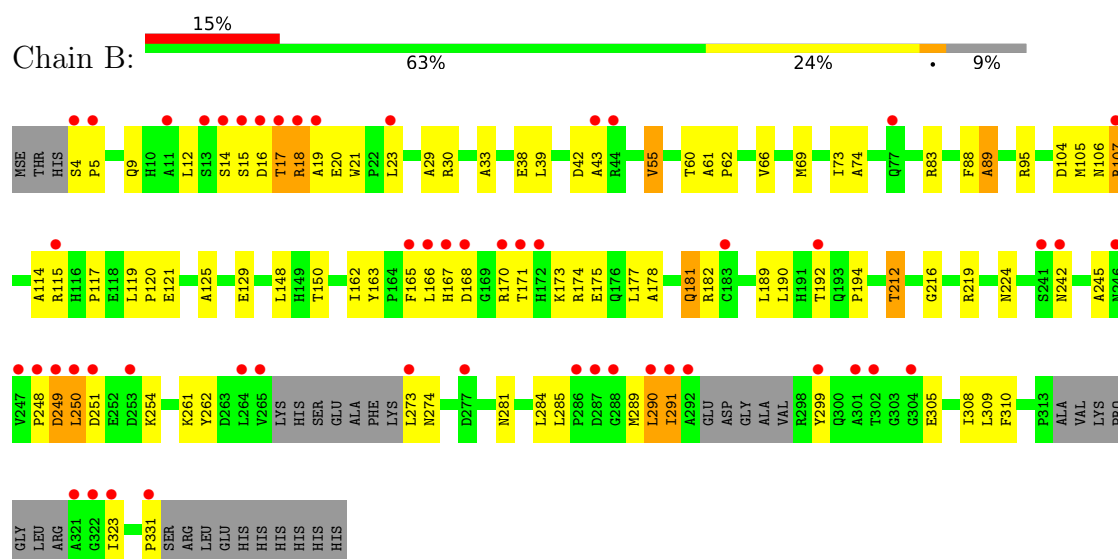
3 Residue-property plots

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: Succinylglutamate desuccinylase



• Molecule 1: Succinylglutamate desuccinylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.95Å 39.44Å 131.59Å 90.00° 94.74° 90.00°	Depositor
Resolution (Å)	29.95 – 2.00 29.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.95-2.00) 96.7 (29.95-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.262 0.236 , 0.279	Depositor DCC
R_{free} test set	8204 reflections (9.79%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5277	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

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	0.38	0/2517	0.82	8/3407 (0.2%)
1	B	0.39	0/2436	0.85	9/3298 (0.3%)
All	All	0.38	0/4953	0.84	17/6705 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ARG	N-CA-C	-9.45	94.74	109.76
1	A	55	VAL	N-CA-C	-8.12	102.33	110.62
1	B	88	PHE	N-CA-C	-6.68	96.23	107.99
1	B	55	VAL	N-CA-C	-6.54	102.88	111.05
1	A	88	PHE	N-CA-C	-6.50	95.76	107.98
1	B	331	PRO	N-CA-CB	6.39	110.03	103.00
1	B	150	THR	N-CA-C	-6.37	99.87	108.86
1	B	60	THR	N-CA-C	6.37	120.79	112.89
1	A	216	GLY	N-CA-C	5.95	117.90	110.29
1	A	107	ARG	N-CA-C	-5.62	105.02	113.89
1	A	212	THR	N-CA-C	-5.55	100.20	109.24
1	A	60	THR	N-CA-C	5.51	119.72	112.89
1	A	89	ALA	N-CA-C	5.50	122.51	110.80
1	A	83	ARG	N-CA-C	-5.47	100.88	109.25
1	B	148	LEU	N-CA-C	5.12	117.11	108.96
1	B	212	THR	N-CA-C	-5.07	100.97	109.24
1	B	216	GLY	N-CA-C	5.05	116.75	110.29

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	2465	0	2427	67	0
1	B	2388	0	2331	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	241	0	0	6	0
3	B	181	0	0	7	0
All	All	5277	0	4758	140	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 (140) 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:309:LEU:HD23	1:B:323:ILE:HD11	1.60	0.84
1:A:178:ALA:HB2	1:A:250:LEU:HB2	1.58	0.83
1:B:18:ARG:HH12	1:B:33:ALA:HA	1.45	0.82
1:A:317:PRO:HG2	1:A:319:LEU:H	1.45	0.81
1:B:181:GLN:HG2	1:B:250:LEU:HD23	1.62	0.79
1:A:203:SER:O	1:A:207:GLU:HA	1.86	0.76
1:A:315:VAL:C	1:A:317:PRO:HD3	2.11	0.75
1:B:106:ASN:C	1:B:107:ARG:HD2	2.13	0.74
1:A:171:THR:HG22	1:A:172:HIS:H	1.57	0.68
1:A:61:ALA:HB3	1:A:62:PRO:HD3	1.76	0.68
1:A:317:PRO:HG2	1:A:318:GLY:H	1.59	0.67
1:B:242:ASN:ND2	1:B:245:ALA:HB2	2.10	0.67
1:A:127:GLU:O	1:A:131:LEU:HD13	1.96	0.66
1:B:273:LEU:HB3	1:B:291:ILE:HG21	1.79	0.65
1:A:16:ASP:HB2	3:A:619:HOH:O	1.97	0.65
1:A:290:LEU:HD13	1:A:302:THR:HB	1.80	0.64
1:A:274:ASN:C	1:A:275:LEU:HD22	2.24	0.62
1:A:23:LEU:HD21	1:A:39:LEU:HD23	1.82	0.61
1:B:107:ARG:HD2	1:B:107:ARG:N	2.16	0.61
1:B:182:ARG:HB3	3:B:597:HOH:O	1.99	0.61
1:B:281:ASN:ND2	1:B:310:PHE:H	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:SER:HB3	3:B:673:HOH:O	2.02	0.60
1:A:232:ILE:HD12	1:A:236:LEU:HD22	1.84	0.60
1:A:261:LYS:HZ1	1:A:301:ALA:N	1.99	0.59
1:A:160:PHE:HE1	1:A:162:ILE:HD11	1.66	0.59
1:A:6:SER:HA	3:A:633:HOH:O	2.03	0.58
1:A:309:LEU:HB3	1:A:323:ILE:HG13	1.86	0.58
1:A:145:HIS:HD2	1:A:202:THR:OG1	1.86	0.57
1:A:114:ALA:O	1:A:117:PRO:HD3	2.05	0.56
1:B:194:PRO:HG2	3:B:621:HOH:O	2.04	0.56
1:B:12:LEU:O	1:B:95:ARG:HD3	2.05	0.56
1:A:10:HIS:CE1	1:A:15:SER:HB2	2.40	0.56
1:A:180:LEU:O	1:A:183:CYS:HB3	2.06	0.56
1:B:290:LEU:HD12	1:B:291:ILE:HG12	1.87	0.56
1:A:16:ASP:O	1:A:17:THR:HG23	2.06	0.55
1:B:274:ASN:HD22	1:B:291:ILE:HB	1.71	0.55
1:B:17:THR:HG23	1:B:18:ARG:N	2.21	0.54
1:B:178:ALA:HB2	1:B:250:LEU:HB2	1.89	0.54
1:B:4:SER:N	1:B:5:PRO:HD2	2.23	0.54
1:B:106:ASN:HB3	1:B:107:ARG:NH1	2.23	0.54
1:B:167:HIS:O	1:B:170:ARG:HG3	2.08	0.54
1:A:59:GLU:HB3	1:A:150:THR:OG1	2.08	0.53
1:A:175:GLU:HB2	3:A:689:HOH:O	2.07	0.53
1:B:61:ALA:HB3	1:B:62:PRO:HD3	1.89	0.53
1:B:23:LEU:HD13	1:B:74:ALA:HA	1.91	0.53
1:B:261:LYS:HG3	1:B:262:TYR:CD1	2.43	0.52
1:A:225:ASP:OD1	1:A:227:SER:HB3	2.09	0.52
1:A:242:ASN:ND2	1:A:245:ALA:HB2	2.25	0.51
1:A:274:ASN:O	1:A:275:LEU:HD13	2.11	0.51
1:B:20:GLU:HG3	1:B:30:ARG:HG2	1.93	0.51
1:A:70:LEU:HD21	1:A:86:VAL:HG21	1.92	0.51
1:B:115:ARG:HH11	1:B:115:ARG:HG3	1.74	0.51
1:A:95:ARG:HD3	3:A:597:HOH:O	2.10	0.51
1:B:18:ARG:HH12	1:B:33:ALA:CA	2.20	0.50
1:B:42:ASP:HB2	3:B:554:HOH:O	2.11	0.50
1:B:178:ALA:HB1	1:B:249:ASP:O	2.11	0.50
1:A:285:LEU:HG	1:A:289:MSE:HE2	1.94	0.50
1:B:285:LEU:HD12	1:B:289:MSE:SE	2.62	0.50
1:B:290:LEU:CD1	1:B:291:ILE:HG12	2.42	0.50
1:B:16:ASP:OD2	1:B:19:ALA:N	2.44	0.49
1:B:175:GLU:HG3	3:B:636:HOH:O	2.11	0.49
1:A:204:GLN:HG3	3:A:590:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LEU:HD11	1:B:305:GLU:HA	1.95	0.49
1:A:54:GLY:HA3	1:A:94:ILE:HD11	1.95	0.49
1:A:113:HIS:HD2	3:A:653:HOH:O	1.96	0.49
1:A:315:VAL:HG23	1:A:316:LYS:N	2.28	0.48
1:B:21:TRP:HB2	1:B:29:ALA:HB3	1.94	0.48
1:A:317:PRO:HG2	1:A:318:GLY:N	2.28	0.48
1:B:171:THR:O	1:B:173:LYS:HD2	2.13	0.48
1:B:104:ASP:OD1	1:B:107:ARG:HD3	2.13	0.48
1:B:219:ARG:HB2	1:B:224:ASN:ND2	2.28	0.48
1:A:113:HIS:HE1	1:A:129:GLU:OE1	1.96	0.48
1:B:66:VAL:HA	1:B:69:MSE:HE3	1.96	0.48
1:B:178:ALA:CB	1:B:250:LEU:HB2	2.44	0.48
1:B:125:ALA:O	1:B:129:GLU:HG3	2.14	0.47
1:B:273:LEU:HD23	1:B:291:ILE:HG21	1.97	0.47
1:B:23:LEU:CD1	1:B:74:ALA:HA	2.45	0.47
1:B:17:THR:CG2	1:B:18:ARG:N	2.77	0.47
1:B:16:ASP:CG	1:B:17:THR:H	2.19	0.47
1:B:18:ARG:NH1	1:B:33:ALA:HA	2.23	0.47
1:B:9:GLN:NE2	3:B:579:HOH:O	2.48	0.46
1:A:273:LEU:CD1	1:A:275:LEU:HB2	2.46	0.46
1:A:170:ARG:HH12	1:A:173:LYS:HD2	1.78	0.46
1:A:287:ASP:HA	1:A:302:THR:OG1	2.16	0.46
1:B:16:ASP:CG	1:B:19:ALA:HB2	2.41	0.45
1:B:178:ALA:O	1:B:181:GLN:HG3	2.16	0.45
1:A:316:LYS:N	1:A:317:PRO:HD3	2.31	0.45
1:A:316:LYS:HB2	1:A:316:LYS:NZ	2.31	0.45
1:B:181:GLN:NE2	1:B:251:ASP:OD2	2.49	0.45
1:B:250:LEU:HD13	1:B:250:LEU:O	2.16	0.45
1:A:309:LEU:O	1:A:323:ILE:HG12	2.17	0.44
1:B:114:ALA:O	1:B:117:PRO:HD3	2.17	0.44
1:A:105:MSE:C	1:A:107:ARG:H	2.26	0.44
1:B:16:ASP:CG	1:B:17:THR:N	2.75	0.44
1:A:152:ILE:HD12	1:A:152:ILE:N	2.33	0.44
1:B:189:LEU:HD22	1:B:309:LEU:CD2	2.47	0.44
1:A:60:THR:HA	1:A:63:ILE:HD12	2.00	0.44
1:B:181:GLN:HG3	1:B:182:ARG:N	2.33	0.43
1:A:271:PHE:HZ	1:A:313:PRO:HB2	1.82	0.43
1:B:14:SER:O	1:B:15:SER:C	2.62	0.43
1:A:264:LEU:HD22	1:A:291:ILE:HD12	2.00	0.43
1:B:309:LEU:HB3	1:B:323:ILE:HG13	2.00	0.43
1:A:69:MSE:SE	1:A:236:LEU:HB3	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HD12	1:A:189:LEU:HD23	2.01	0.43
1:B:181:GLN:CG	1:B:250:LEU:HD23	2.41	0.43
1:A:312:ASN:O	1:A:315:VAL:HG22	2.19	0.43
1:B:163:TYR:HB3	1:B:190:LEU:HD23	2.00	0.43
1:B:248:PRO:O	1:B:249:ASP:O	2.37	0.43
1:A:289:MSE:O	1:A:289:MSE:HG3	2.18	0.42
1:B:289:MSE:HE2	1:B:291:ILE:O	2.19	0.42
1:A:162:ILE:HB	1:A:212:THR:HB	2.00	0.42
1:B:162:ILE:HB	1:B:212:THR:HB	2.01	0.42
1:B:55:VAL:HA	1:B:89:ALA:HB3	2.01	0.42
1:A:125:ALA:O	1:A:129:GLU:HG3	2.20	0.42
1:B:105:MSE:HE2	1:B:121:GLU:O	2.20	0.42
1:B:165:PHE:O	1:B:192:THR:HA	2.20	0.42
1:B:224:ASN:ND2	3:B:504:HOH:O	2.50	0.41
1:A:160:PHE:HA	1:A:185:ILE:HG23	2.02	0.41
1:B:285:LEU:HD21	1:B:308:ILE:N	2.35	0.41
1:B:38:GLU:C	1:B:39:LEU:HD12	2.45	0.41
1:B:66:VAL:HA	1:B:69:MSE:CE	2.50	0.41
1:A:290:LEU:HD21	1:A:301:ALA:O	2.20	0.41
1:A:263:ASP:OD1	1:A:323:ILE:HG22	2.20	0.41
1:A:302:THR:HA	1:A:306:GLU:OE2	2.20	0.41
1:A:315:VAL:HB	1:A:317:PRO:HD3	2.03	0.41
1:B:23:LEU:HD12	1:B:73:ILE:HG22	2.02	0.41
1:A:105:MSE:HE3	1:A:121:GLU:HG2	2.02	0.41
1:A:129:GLU:HB3	1:A:201:PHE:CZ	2.56	0.41
1:A:178:ALA:CB	1:A:250:LEU:HB2	2.40	0.41
1:A:250:LEU:O	1:A:250:LEU:HD13	2.21	0.41
1:B:105:MSE:C	1:B:107:ARG:H	2.28	0.41
1:B:163:TYR:CD2	1:B:163:TYR:C	2.99	0.41
1:B:119:LEU:HA	1:B:120:PRO:HD3	1.96	0.41
1:B:18:ARG:NH1	1:B:18:ARG:HG3	2.36	0.40
1:A:284:LEU:HA	1:A:307:ARG:HG2	2.03	0.40
1:A:317:PRO:CG	1:A:318:GLY:H	2.24	0.40
1:A:52:SER:OG	1:A:145:HIS:HE1	2.04	0.40
1:A:157:PHE:O	1:A:158:GLU:C	2.64	0.40
1:A:232:ILE:CD1	1:A:236:LEU:HD22	2.49	0.40
1:B:165:PHE:O	1:B:166:LEU:HD23	2.21	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	311/341 (91%)	286 (92%)	22 (7%)	3 (1%)	12	8
1	B	301/341 (88%)	279 (93%)	17 (6%)	5 (2%)	7	3
All	All	612/682 (90%)	565 (92%)	39 (6%)	8 (1%)	9	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	PRO
1	B	249	ASP
1	B	17	THR
1	B	89	ALA
1	A	249	ASP
1	B	43	ALA
1	A	303	GLY
1	B	291	ILE

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	255/268 (95%)	246 (96%)	9 (4%)	32	32
1	B	245/268 (91%)	235 (96%)	10 (4%)	27	26
All	All	500/536 (93%)	481 (96%)	19 (4%)	29	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	77	GLN
1	A	158	GLU
1	A	193	GLN
1	A	232	ILE
1	A	236	LEU
1	A	285	LEU
1	A	306	GLU
1	A	316	LYS
1	B	18	ARG
1	B	107	ARG
1	B	168	ASP
1	B	174	ARG
1	B	177	LEU
1	B	181	GLN
1	B	250	LEU
1	B	254	LYS
1	B	290	LEU
1	B	299	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	77	GLN
1	A	102	ASN
1	A	113	HIS
1	A	116	HIS
1	A	145	HIS
1	A	176	GLN
1	A	181	GLN
1	A	193	GLN
1	A	204	GLN
1	A	242	ASN
1	A	274	ASN
1	B	110	ASN
1	B	191	HIS
1	B	193	GLN
1	B	196	ASN
1	B	224	ASN
1	B	246	ASN
1	B	274	ASN
1	B	281	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 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	315/341 (92%)	0.83	59 (18%) 3 3	10, 24, 51, 58	0
1	B	305/341 (89%)	0.81	52 (17%) 4 4	9, 23, 47, 56	0
All	All	620/682 (90%)	0.82	111 (17%) 3 3	9, 24, 50, 58	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	THR	8.5
1	B	292	ALA	7.7
1	A	15	SER	7.6
1	A	332	SER	7.2
1	B	18	ARG	6.9
1	B	291	ILE	6.4
1	A	290	LEU	6.1
1	B	19	ALA	6.1
1	A	301	ALA	5.8
1	A	316	LYS	5.8
1	A	271	PHE	5.6
1	B	248	PRO	5.5
1	B	264	LEU	5.4
1	B	265	VAL	5.3
1	B	290	LEU	5.0
1	B	247	VAL	4.9
1	B	253	ASP	4.6
1	B	14	SER	4.6
1	A	17	THR	4.5
1	A	247	VAL	4.4
1	B	249	ASP	4.4
1	A	268	SER	4.2
1	A	317	PRO	4.1
1	B	16	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	315	VAL	4.0
1	B	192	THR	4.0
1	A	250	LEU	3.7
1	A	245	ALA	3.7
1	B	5	PRO	3.6
1	B	171	THR	3.6
1	A	291	ILE	3.5
1	B	273	LEU	3.4
1	B	165	PHE	3.3
1	B	23	LEU	3.3
1	A	253	ASP	3.3
1	A	167	HIS	3.2
1	A	2	THR	3.2
1	B	13	SER	3.2
1	A	288	GLY	3.2
1	A	16	ASP	3.2
1	B	250	LEU	3.2
1	B	302	THR	3.2
1	B	183	CYS	3.2
1	A	249	ASP	3.1
1	B	44	ARG	3.1
1	A	275	LEU	3.1
1	B	166	LEU	3.1
1	A	303	GLY	2.9
1	B	168	ASP	2.9
1	A	252	GLU	2.9
1	A	266	LYS	2.9
1	B	251	ASP	2.9
1	B	15	SER	2.9
1	A	321	ALA	2.9
1	A	323	ILE	2.8
1	B	323	ILE	2.8
1	B	331	PRO	2.8
1	A	318	GLY	2.8
1	B	286	PRO	2.8
1	A	165	PHE	2.8
1	B	170	ARG	2.7
1	A	251	ASP	2.7
1	A	226	LEU	2.7
1	A	292	ALA	2.7
1	B	43	ALA	2.7
1	B	246	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	287	ASP	2.6
1	A	170	ARG	2.6
1	A	171	THR	2.6
1	A	319	LEU	2.6
1	B	299	TYR	2.6
1	B	321	ALA	2.6
1	B	4	SER	2.6
1	A	175	GLU	2.5
1	A	312	ASN	2.5
1	B	107	ARG	2.5
1	B	301	ALA	2.5
1	A	273	LEU	2.5
1	A	173	LYS	2.5
1	A	267	HIS	2.5
1	A	44	ARG	2.5
1	B	277	ASP	2.4
1	A	302	THR	2.4
1	A	166	LEU	2.4
1	A	306	GLU	2.4
1	B	242	ASN	2.4
1	A	244	GLN	2.3
1	A	192	THR	2.3
1	A	243	PRO	2.3
1	A	182	ARG	2.3
1	B	172	HIS	2.3
1	A	314	ALA	2.3
1	B	115	ARG	2.3
1	A	225	ASP	2.3
1	B	11	ALA	2.3
1	B	241	SER	2.2
1	A	248	PRO	2.2
1	A	77	GLN	2.2
1	A	18	ARG	2.2
1	B	77	GLN	2.1
1	B	304	GLY	2.1
1	A	183	CYS	2.1
1	A	181	GLN	2.1
1	A	320	ARG	2.1
1	B	167	HIS	2.1
1	B	322	GLY	2.1
1	A	92	ASP	2.0
1	B	288	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	14	SER	2.0
1	A	115	ARG	2.0
1	A	304	GLY	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(Å ²)	Q<0.9
2	ZN	B	502	1/1	0.98	0.12	40,40,40,40	0
2	ZN	A	501	1/1	0.99	0.06	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.