



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:24 AM UTC

PDB ID : 3E4Q / pdb_00003e4q
Title : Crystal structure of apo DctB
Authors : Zhou, Y.F.; Nan, J.; Nan, B.Y.; Liang, Y.H.; Panjekar, S.; Su, X.D.
Deposited on : 2008-08-12
Resolution : 2.75 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

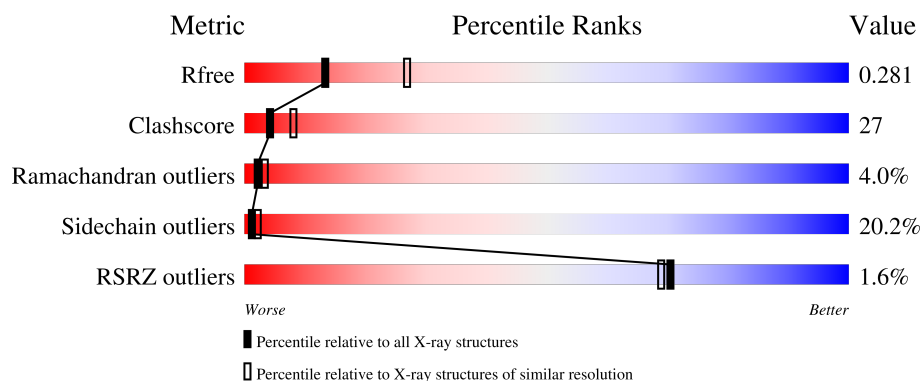
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	305	2% 39% 30% 12% 17%
1	B	305	% 38% 32% 11% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3902 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 C4-dicarboxylate transport sensor protein dctB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1945	1232	349	360	4			
1	B	254	Total	C	N	O	S	0	0	0
			1945	1232	349	360	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP P13633
A	9	GLY	-	expression tag	UNP P13633
A	10	SER	-	expression tag	UNP P13633
A	11	SER	-	expression tag	UNP P13633
A	12	HIS	-	expression tag	UNP P13633
A	13	HIS	-	expression tag	UNP P13633
A	14	HIS	-	expression tag	UNP P13633
A	15	HIS	-	expression tag	UNP P13633
A	16	HIS	-	expression tag	UNP P13633
A	17	HIS	-	expression tag	UNP P13633
A	18	SER	-	expression tag	UNP P13633
A	19	SER	-	expression tag	UNP P13633
A	20	GLY	-	expression tag	UNP P13633
A	21	LEU	-	expression tag	UNP P13633
A	22	VAL	-	expression tag	UNP P13633
A	23	PRO	-	expression tag	UNP P13633
A	24	ARG	-	expression tag	UNP P13633
A	25	GLY	-	expression tag	UNP P13633
A	26	SER	-	expression tag	UNP P13633
A	27	HIS	-	expression tag	UNP P13633
A	28	MET	-	expression tag	UNP P13633
A	29	ALA	-	expression tag	UNP P13633
A	30	SER	-	expression tag	UNP P13633
A	31	MET	-	expression tag	UNP P13633
A	32	THR	-	expression tag	UNP P13633

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP P13633
A	34	GLY	-	expression tag	UNP P13633
A	35	GLU	-	expression tag	UNP P13633
A	36	GLU	-	expression tag	UNP P13633
A	37	MET	-	expression tag	UNP P13633
A	38	GLY	-	expression tag	UNP P13633
A	39	ARG	-	expression tag	UNP P13633
A	40	GLY	-	expression tag	UNP P13633
A	41	SER	-	expression tag	UNP P13633
A	174	LYS	ASN	SEE REMARK 999	UNP P13633
A	309	ASN	LYS	SEE REMARK 999	UNP P13633
B	8	MET	-	expression tag	UNP P13633
B	9	GLY	-	expression tag	UNP P13633
B	10	SER	-	expression tag	UNP P13633
B	11	SER	-	expression tag	UNP P13633
B	12	HIS	-	expression tag	UNP P13633
B	13	HIS	-	expression tag	UNP P13633
B	14	HIS	-	expression tag	UNP P13633
B	15	HIS	-	expression tag	UNP P13633
B	16	HIS	-	expression tag	UNP P13633
B	17	HIS	-	expression tag	UNP P13633
B	18	SER	-	expression tag	UNP P13633
B	19	SER	-	expression tag	UNP P13633
B	20	GLY	-	expression tag	UNP P13633
B	21	LEU	-	expression tag	UNP P13633
B	22	VAL	-	expression tag	UNP P13633
B	23	PRO	-	expression tag	UNP P13633
B	24	ARG	-	expression tag	UNP P13633
B	25	GLY	-	expression tag	UNP P13633
B	26	SER	-	expression tag	UNP P13633
B	27	HIS	-	expression tag	UNP P13633
B	28	MET	-	expression tag	UNP P13633
B	29	ALA	-	expression tag	UNP P13633
B	30	SER	-	expression tag	UNP P13633
B	31	MET	-	expression tag	UNP P13633
B	32	THR	-	expression tag	UNP P13633
B	33	GLY	-	expression tag	UNP P13633
B	34	GLY	-	expression tag	UNP P13633
B	35	GLU	-	expression tag	UNP P13633
B	36	GLU	-	expression tag	UNP P13633
B	37	MET	-	expression tag	UNP P13633
B	38	GLY	-	expression tag	UNP P13633

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ARG	-	expression tag	UNP P13633
B	40	GLY	-	expression tag	UNP P13633
B	41	SER	-	expression tag	UNP P13633
B	174	LYS	ASN	SEE REMARK 999	UNP P13633
B	309	ASN	LYS	SEE REMARK 999	UNP P13633

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

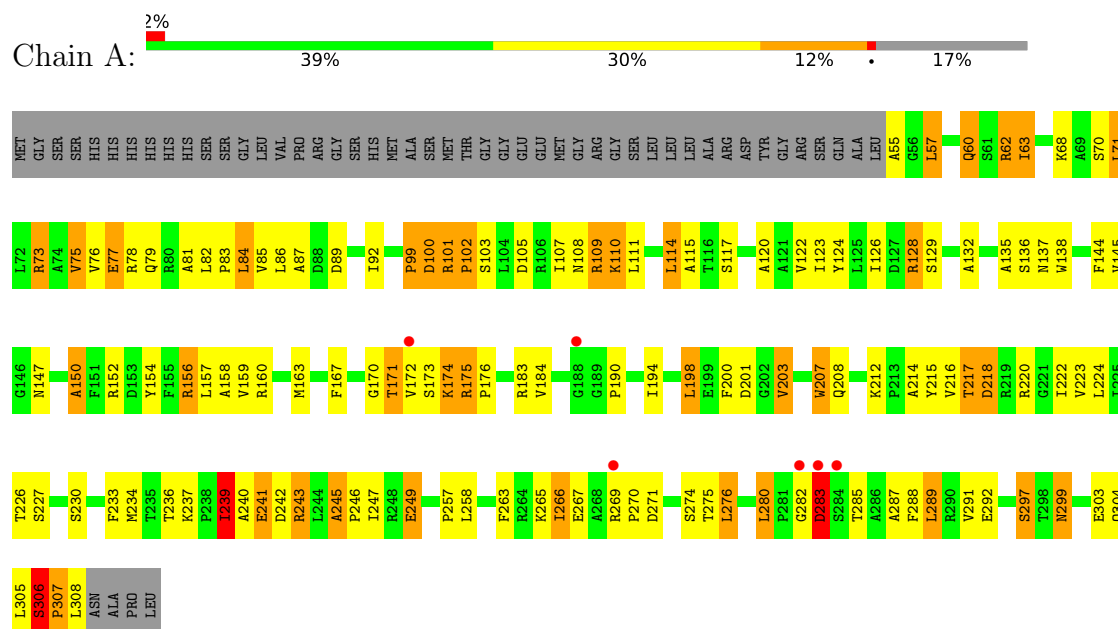
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	6	Total O 6 6	0	0

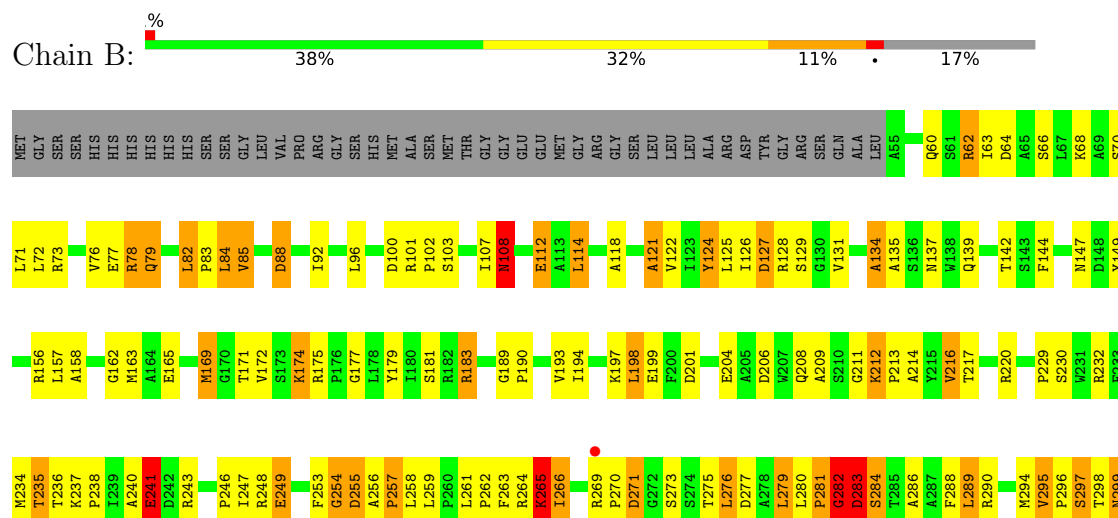
3 Residue-property plots

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: C4-dicarboxylate transport sensor protein dctB



- Molecule 1: C4-dicarboxylate transport sensor protein dctB



H300	R301	L302	E303	Q304	L305	S306	F307	L308	ASN	ALA	PRO	LEU
------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.99Å 38.73Å 111.17Å 90.00° 94.47° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.75) 95.8 (30.00-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.274 0.204 , 0.281	Depositor DCC
R_{free} test set	668 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	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	0.94	EDS
Total number of atoms	3902	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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: CA

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	7/1985 (0.4%)	1.40	18/2699 (0.7%)
1	B	1.27	5/1985 (0.3%)	1.46	22/2699 (0.8%)
All	All	1.24	12/3970 (0.3%)	1.43	40/5398 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	3
All	All	1	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	LYS	CE-NZ	11.17	1.82	1.49
1	A	263	PHE	CA-C	-6.23	1.45	1.52
1	A	159	VAL	CA-CB	6.13	1.61	1.54
1	A	115	ALA	CA-CB	-6.07	1.43	1.53
1	A	87	ALA	CA-CB	-6.02	1.42	1.53
1	B	108	ASN	CA-C	-5.91	1.45	1.52
1	B	134	ALA	CA-C	5.86	1.59	1.52
1	B	121	ALA	C-O	-5.57	1.17	1.24
1	B	193	VAL	C-O	-5.36	1.18	1.24
1	A	216	VAL	CA-CB	-5.30	1.48	1.54
1	A	247	ILE	CA-CB	-5.26	1.48	1.54
1	A	150	ALA	CA-CB	-5.18	1.44	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	SER	CA-C-N	10.84	133.38	119.84
1	A	306	SER	C-N-CA	10.84	133.38	119.84
1	B	175	ARG	CA-C-N	9.33	129.39	119.78
1	B	175	ARG	C-N-CA	9.33	129.39	119.78
1	B	108	ASN	N-CA-C	-8.32	102.29	111.36
1	B	162	GLY	N-CA-C	-7.89	105.14	113.58
1	A	175	ARG	CA-C-N	7.53	127.46	119.85
1	A	175	ARG	C-N-CA	7.53	127.46	119.85
1	B	112	GLU	N-CA-C	-7.38	102.19	112.45
1	A	242	ASP	N-CA-C	7.00	121.48	113.15
1	A	85	VAL	N-CA-C	6.73	116.86	110.53
1	A	137	ASN	N-CA-C	6.71	120.09	112.97
1	B	79	GLN	N-CA-C	6.65	118.18	111.07
1	A	76	VAL	N-CA-C	-6.57	104.36	110.53
1	B	82	LEU	CA-CB-CG	-6.45	93.71	116.30
1	B	235	THR	N-CA-C	6.39	119.91	109.24
1	A	207	TRP	N-CA-C	6.34	117.85	111.07
1	B	295	VAL	CA-C-N	-5.79	113.82	119.78
1	B	295	VAL	C-N-CA	-5.79	113.82	119.78
1	A	145	VAL	N-CA-C	5.67	116.73	109.30
1	B	114	LEU	N-CA-C	5.61	117.84	111.11
1	B	78	ARG	N-CA-C	-5.54	105.14	111.07
1	A	102	PRO	N-CA-C	-5.53	105.85	113.53
1	B	283	ASP	N-CA-C	-5.52	95.54	111.00
1	A	75	VAL	N-CA-C	-5.50	105.74	111.58
1	B	273	SER	N-CA-C	-5.44	101.25	109.85
1	A	266	ILE	N-CA-C	5.43	116.26	108.93
1	B	126	ILE	CA-C-N	-5.40	112.61	122.12
1	B	126	ILE	C-N-CA	-5.40	112.61	122.12
1	A	239	ILE	CA-C-N	-5.40	114.18	122.87
1	A	239	ILE	C-N-CA	-5.40	114.18	122.87
1	A	123	ILE	N-CA-C	-5.35	100.62	108.11
1	B	85	VAL	CB-CA-C	-5.13	105.36	112.24
1	B	183	ARG	N-CA-C	-5.11	103.65	110.55
1	B	212	LYS	CA-C-N	-5.08	114.71	119.85
1	B	212	LYS	C-N-CA	-5.08	114.71	119.85
1	A	129	SER	N-CA-C	-5.06	106.88	113.16
1	B	127	ASP	CA-C-N	5.02	127.52	120.28
1	B	127	ASP	C-N-CA	5.02	127.52	120.28
1	A	81	ALA	N-CA-C	5.01	118.49	112.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	174	LYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ASP	Peptide
1	B	211	GLY	Peptide
1	B	271	ASP	Peptide
1	B	282	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1945	0	1975	115	0
1	B	1945	0	1975	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	2	0
3	B	6	0	0	0	0
All	All	3902	0	3950	213	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 27.

All (213) 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:265:LYS:CE	1:B:265:LYS:NZ	1.82	1.42
1:B:169:MET:SD	1:B:174:LYS:HB2	1.81	1.20
1:B:257:PRO:HB2	1:B:259:LEU:HD12	1.39	1.02
1:A:299:ASN:H	1:A:299:ASN:HD22	1.11	0.98
1:A:249:GLU:HA	1:A:249:GLU:OE1	1.67	0.92
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.30	0.91
1:B:263:PHE:CD2	1:B:276:LEU:HD21	2.05	0.91
1:A:62:ARG:HH21	1:A:62:ARG:HG3	1.43	0.84
1:B:212:LYS:HD2	1:B:306:SER:OG	1.76	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:CB	1:B:259:LEU:HD12	2.07	0.84
1:A:152:ARG:NH2	1:A:171:THR:HG21	1.95	0.81
1:B:62:ARG:HH21	1:B:62:ARG:HG3	1.46	0.81
1:A:100:ASP:HB2	1:A:103:SER:HB2	1.63	0.80
1:A:110:LYS:NZ	1:B:88:ASP:HB3	1.97	0.80
1:B:257:PRO:HB2	1:B:259:LEU:CD1	2.12	0.78
1:A:79:GLN:HG3	1:A:198:LEU:HG	1.64	0.77
1:A:243:ARG:NH2	1:A:243:ARG:HB2	2.01	0.75
1:A:243:ARG:HH21	1:A:243:ARG:CB	2.00	0.75
1:A:89:ASP:HB3	1:A:92:ILE:HG12	1.70	0.73
1:A:79:GLN:HE22	1:A:120:ALA:HB2	1.52	0.73
1:A:170:GLY:HA3	1:A:173:SER:OG	1.90	0.72
1:A:109:ARG:HH11	1:A:109:ARG:CG	2.03	0.72
1:A:276:LEU:C	1:A:276:LEU:HD12	2.15	0.72
1:A:198:LEU:HD13	1:A:200:PHE:CE1	2.24	0.71
1:A:100:ASP:CB	1:A:103:SER:HB2	2.19	0.71
1:B:282:GLY:HA3	1:B:283:ASP:CG	2.16	0.71
1:A:101:ARG:N	1:A:102:PRO:HD2	2.05	0.71
1:A:269:ARG:HG2	1:A:270:PRO:HD2	1.71	0.71
1:A:282:GLY:O	1:A:283:ASP:CG	2.33	0.71
1:A:243:ARG:HB2	1:A:243:ARG:HH21	1.58	0.69
1:A:198:LEU:HD13	1:A:200:PHE:CZ	2.27	0.69
1:A:282:GLY:O	1:A:283:ASP:CB	2.41	0.68
1:A:299:ASN:HD22	1:A:299:ASN:N	1.88	0.67
1:A:245:ALA:HB3	1:A:246:PRO:CD	2.24	0.67
1:B:92:ILE:HD12	1:B:125:LEU:HD22	1.78	0.66
1:B:204:GLU:CD	1:B:232:ARG:HH12	2.03	0.66
1:A:101:ARG:H	1:A:102:PRO:HD2	1.60	0.66
1:A:280:LEU:O	1:A:283:ASP:N	2.30	0.65
1:B:280:LEU:O	1:B:281:PRO:C	2.39	0.64
1:A:71:LEU:O	1:A:75:VAL:HG23	1.96	0.64
1:B:213:PRO:HG2	1:B:305:LEU:HB2	1.78	0.64
1:A:62:ARG:HH21	1:A:62:ARG:CG	2.10	0.64
1:B:213:PRO:HD2	1:B:305:LEU:O	1.97	0.64
1:A:110:LYS:HZ2	1:B:88:ASP:HB3	1.62	0.63
1:B:108:ASN:HD21	1:B:134:ALA:HA	1.63	0.62
1:B:169:MET:SD	1:B:174:LYS:CB	2.75	0.62
1:B:217:THR:HG21	1:B:236:THR:CG2	2.29	0.62
1:B:269:ARG:NH1	1:B:289:LEU:CD1	2.63	0.62
1:A:77:GLU:HG2	1:B:78:ARG:NH1	2.15	0.62
1:A:269:ARG:HD3	1:A:271:ASP:OD2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:SER:O	1:A:297:SER:OG	2.16	0.62
1:B:294:MET:HE3	1:B:300:TRP:O	2.00	0.61
1:A:60:GLN:HA	1:A:60:GLN:OE1	2.01	0.61
1:A:299:ASN:H	1:A:299:ASN:ND2	1.91	0.60
1:A:62:ARG:HH12	1:A:271:ASP:HB3	1.64	0.60
1:A:218:ASP:OD1	1:A:220:ARG:HB2	2.02	0.60
1:A:157:LEU:HD22	1:A:160:ARG:NH1	2.17	0.59
1:A:172:VAL:HB	3:A:505:HOH:O	2.02	0.59
1:B:92:ILE:HD13	1:B:107:ILE:HD12	1.86	0.58
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.02	0.58
1:B:101:ARG:HB3	1:B:102:PRO:HD3	1.86	0.57
1:B:79:GLN:HG2	1:B:198:LEU:HG	1.87	0.57
1:A:60:GLN:OE1	1:A:63:ILE:HD11	2.04	0.56
1:A:215:TYR:HB2	1:A:223:VAL:HG13	1.86	0.56
1:B:79:GLN:NE2	1:B:82:LEU:HD12	2.21	0.56
1:B:158:ALA:HB2	1:B:181:SER:OG	2.05	0.56
1:A:239:ILE:CG2	1:A:240:ALA:N	2.68	0.56
1:A:223:VAL:HG23	1:A:234:MET:O	2.04	0.56
1:A:239:ILE:HG23	1:A:243:ARG:HG3	1.86	0.56
1:A:68:LYS:HG2	1:A:207:TRP:NE1	2.21	0.56
1:B:269:ARG:NH1	1:B:289:LEU:HD13	2.22	0.55
1:B:165:GLU:HA	1:B:179:TYR:O	2.07	0.55
1:B:216:VAL:HG13	1:B:300:TRP:HB3	1.89	0.55
1:B:234:MET:HB3	1:B:259:LEU:O	2.07	0.55
1:B:127:ASP:OD1	1:B:129:SER:OG	2.24	0.54
1:B:253:PHE:C	1:B:255:ASP:N	2.64	0.54
1:B:269:ARG:O	1:B:271:ASP:N	2.41	0.54
1:A:239:ILE:HG22	1:A:240:ALA:N	2.23	0.54
1:B:66:SER:O	1:B:70:SER:HB2	2.08	0.54
1:A:86:LEU:O	1:A:92:ILE:HG13	2.07	0.54
1:B:246:PRO:O	1:B:249:GLU:HB3	2.07	0.54
1:A:173:SER:N	3:A:505:HOH:O	2.39	0.54
1:B:204:GLU:OE1	1:B:232:ARG:NH1	2.38	0.53
1:B:217:THR:HG21	1:B:236:THR:HG21	1.90	0.53
1:B:235:THR:O	1:B:261:LEU:HD12	2.08	0.53
1:B:169:MET:HG3	1:B:253:PHE:HB2	1.90	0.53
1:A:282:GLY:O	1:A:283:ASP:HB2	2.09	0.53
1:A:110:LYS:HZ1	1:B:88:ASP:HB3	1.73	0.53
1:B:248:ARG:HG2	1:B:254:GLY:HA2	1.91	0.53
1:B:216:VAL:HA	1:B:301:ARG:O	2.08	0.52
1:A:71:LEU:HD12	1:B:71:LEU:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:O	1:B:247:ILE:HG13	2.10	0.52
1:A:217:THR:HG22	1:A:222:ILE:C	2.35	0.52
1:A:288:PHE:CD1	1:A:305:LEU:HB3	2.46	0.51
1:B:158:ALA:O	1:B:183:ARG:HB2	2.10	0.51
1:B:82:LEU:HD11	1:B:118:ALA:CB	2.40	0.51
1:A:215:TYR:CE2	1:A:303:GLU:HB2	2.46	0.51
1:B:68:LYS:NZ	1:B:304:GLN:OE1	2.40	0.51
1:B:299:ASN:HD22	1:B:299:ASN:C	2.19	0.51
1:B:253:PHE:O	1:B:255:ASP:N	2.44	0.51
1:B:257:PRO:HG2	1:B:258:LEU:H	1.76	0.51
1:A:173:SER:O	1:A:174:LYS:HB2	2.10	0.51
1:B:82:LEU:HB2	1:B:83:PRO:HD3	1.93	0.50
1:A:243:ARG:NH2	1:A:243:ARG:CB	2.67	0.50
1:B:253:PHE:C	1:B:255:ASP:H	2.18	0.50
1:A:101:ARG:N	1:A:102:PRO:CD	2.75	0.50
1:B:206:ASP:O	1:B:209:ALA:HB3	2.11	0.50
1:A:233:PHE:HB2	1:A:257:PRO:HD2	1.92	0.50
1:A:245:ALA:CB	1:A:246:PRO:CD	2.90	0.50
1:A:287:ALA:CB	1:A:308:LEU:HD12	2.41	0.50
1:B:240:ALA:O	1:B:241:GLU:C	2.55	0.50
1:A:167:PHE:CE2	1:A:224:LEU:HB3	2.47	0.50
1:A:124:TYR:OH	1:A:154:TYR:CZ	2.65	0.49
1:A:245:ALA:HB3	1:A:246:PRO:HD2	1.92	0.49
1:A:57:LEU:HD12	1:A:306:SER:HB2	1.93	0.49
1:A:103:SER:O	1:A:107:ILE:HG12	2.13	0.49
1:B:269:ARG:O	1:B:270:PRO:C	2.55	0.49
1:B:257:PRO:CB	1:B:259:LEU:CD1	2.82	0.48
1:A:83:PRO:O	1:A:84:LEU:C	2.55	0.48
1:A:126:ILE:HA	1:A:132:ALA:HA	1.95	0.48
1:A:174:LYS:N	1:A:174:LYS:HD3	2.28	0.48
1:A:77:GLU:HG2	1:B:78:ARG:CZ	2.44	0.48
1:B:122:VAL:HG12	1:B:124:TYR:CD1	2.49	0.47
1:A:62:ARG:NH1	1:A:271:ASP:OD1	2.47	0.47
1:B:214:ALA:HA	1:B:303:GLU:O	2.14	0.47
1:B:217:THR:HG21	1:B:236:THR:HG23	1.97	0.47
1:A:89:ASP:HB3	1:A:92:ILE:CG1	2.43	0.47
1:A:269:ARG:CG	1:A:270:PRO:HD2	2.40	0.47
1:A:243:ARG:HH21	1:A:243:ARG:HB3	1.77	0.47
1:A:100:ASP:HB2	1:A:103:SER:CB	2.38	0.47
1:B:62:ARG:HG3	1:B:62:ARG:NH2	2.22	0.47
1:B:108:ASN:ND2	1:B:135:ALA:H	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:NE2	1:A:120:ALA:HB2	2.23	0.47
1:A:99:PRO:O	1:A:100:ASP:O	2.33	0.47
1:A:240:ALA:O	1:A:241:GLU:C	2.58	0.47
1:B:124:TYR:CD1	1:B:124:TYR:N	2.82	0.46
1:A:152:ARG:HH21	1:A:171:THR:HG21	1.77	0.46
1:B:248:ARG:O	1:B:249:GLU:C	2.57	0.46
1:A:144:PHE:O	1:A:147:ASN:HB2	2.16	0.46
1:A:150:ALA:O	1:A:156:ARG:HD3	2.15	0.46
1:B:266:ILE:H	1:B:266:ILE:HG13	1.49	0.46
1:B:100:ASP:OD1	1:B:102:PRO:HD2	2.16	0.46
1:A:124:TYR:OH	1:A:154:TYR:OH	2.32	0.46
1:B:286:ALA:O	1:B:288:PHE:HD2	1.99	0.46
1:A:158:ALA:O	1:A:183:ARG:HB2	2.16	0.45
1:A:175:ARG:HA	1:A:176:PRO:HD2	1.84	0.45
1:B:296:PRO:O	1:B:297:SER:HB2	2.16	0.45
1:A:135:ALA:O	1:A:136:SER:C	2.57	0.45
1:B:269:ARG:NH1	1:B:289:LEU:HD11	2.31	0.45
1:A:167:PHE:HE1	1:A:200:PHE:CE2	2.34	0.45
1:A:128:ARG:HH11	1:A:190:PRO:HD2	1.81	0.45
1:B:79:GLN:HE22	1:B:82:LEU:HD12	1.82	0.44
1:A:266:ILE:HA	1:A:275:THR:O	2.18	0.44
1:B:217:THR:OG1	1:B:301:ARG:NH1	2.50	0.44
1:B:264:ARG:O	1:B:277:ASP:HB2	2.16	0.44
1:A:107:ILE:O	1:A:111:LEU:HG	2.18	0.44
1:A:212:LYS:HE3	1:A:306:SER:HB3	1.98	0.44
1:A:291:VAL:O	1:A:303:GLU:HA	2.18	0.44
1:B:156:ARG:HE	1:B:156:ARG:HB2	1.58	0.44
1:B:236:THR:OG1	1:B:237:LYS:N	2.50	0.44
1:A:71:LEU:CD2	1:A:203:VAL:HG13	2.47	0.44
1:B:108:ASN:ND2	1:B:134:ALA:HB1	2.33	0.44
1:B:137:ASN:ND2	1:B:142:THR:O	2.51	0.43
1:B:122:VAL:HG11	1:B:144:PHE:CE2	2.53	0.43
1:A:57:LEU:HB3	1:A:289:LEU:HD22	2.00	0.43
1:B:201:ASP:OD2	1:B:201:ASP:N	2.52	0.43
1:B:177:GLY:HA3	1:B:197:LYS:CE	2.48	0.43
1:A:214:ALA:HB2	1:A:304:GLN:HG3	2.00	0.43
1:B:82:LEU:CB	1:B:83:PRO:HD3	2.49	0.43
1:A:245:ALA:HB3	1:A:246:PRO:HD3	1.98	0.43
1:A:73:ARG:NH2	1:A:77:GLU:OE2	2.52	0.43
1:B:82:LEU:HD11	1:B:118:ALA:HB1	2.00	0.43
1:B:82:LEU:CD1	1:B:118:ALA:CB	2.97	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:NH2	1:B:247:ILE:HG23	2.34	0.42
1:B:121:ALA:HB2	1:B:199:GLU:HG3	2.00	0.42
1:A:55:ALA:N	1:A:269:ARG:HH12	2.17	0.42
1:B:72:LEU:O	1:B:76:VAL:HG23	2.19	0.42
1:B:269:ARG:HB3	1:B:270:PRO:HD2	2.00	0.42
1:A:114:LEU:HD12	1:B:84:LEU:HD22	2.02	0.42
1:A:71:LEU:HD23	1:A:203:VAL:HG13	2.01	0.42
1:B:100:ASP:OD2	1:B:103:SER:CB	2.67	0.42
1:A:175:ARG:NH2	1:A:201:ASP:OD1	2.47	0.42
1:A:100:ASP:HB3	1:A:103:SER:HB2	1.99	0.42
1:A:108:ASN:HB3	1:A:138:TRP:CD1	2.55	0.42
1:A:82:LEU:O	1:A:86:LEU:HG	2.20	0.42
1:A:233:PHE:O	1:A:258:LEU:HA	2.20	0.42
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.11	0.41
1:B:290:ARG:HH21	1:B:290:ARG:HD3	1.72	0.41
1:A:62:ARG:HG3	1:A:62:ARG:NH2	2.22	0.41
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.70	0.41
1:A:217:THR:HG21	1:A:236:THR:HG23	2.02	0.41
1:B:295:VAL:HB	1:B:298:THR:OG1	2.20	0.41
1:A:276:LEU:C	1:A:276:LEU:CD1	2.88	0.41
1:B:177:GLY:HA3	1:B:197:LYS:HE3	2.01	0.41
1:B:82:LEU:CD1	1:B:118:ALA:HB1	2.50	0.41
1:B:294:MET:CE	1:B:300:TRP:O	2.68	0.41
1:B:96:LEU:HD11	1:B:125:LEU:HD11	2.02	0.41
1:B:279:LEU:HB2	1:B:284:SER:O	2.21	0.41
1:B:169:MET:HE3	1:B:253:PHE:CD1	2.56	0.41
1:B:147:ASN:HB2	1:B:149:TYR:CE2	2.56	0.41
1:B:257:PRO:CG	1:B:258:LEU:H	2.33	0.41
1:A:78:ARG:CZ	1:B:77:GLU:HB3	2.51	0.41
1:B:68:LYS:NZ	1:B:212:LYS:HB2	2.35	0.40
1:A:108:ASN:HB3	1:A:138:TRP:CE2	2.56	0.40
1:B:68:LYS:HZ2	1:B:212:LYS:HB2	1.85	0.40
1:B:100:ASP:OD2	1:B:103:SER:HB2	2.20	0.40
1:A:60:GLN:O	1:A:63:ILE:HG12	2.21	0.40
1:A:99:PRO:C	1:A:100:ASP:O	2.65	0.40
1:B:189:GLY:O	1:B:190:PRO:C	2.63	0.40
1:A:89:ASP:O	1:A:92:ILE:N	2.54	0.40
1:A:167:PHE:CD2	1:A:224:LEU:HD22	2.57	0.40
1:B:82:LEU:HD11	1:B:118:ALA:HB2	2.03	0.40
1:A:236:THR:OG1	1:A:237:LYS:N	2.55	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	252/305 (83%)	226 (90%)	19 (8%)	7 (3%)	4	6
1	B	252/305 (83%)	218 (86%)	21 (8%)	13 (5%)	1	2
All	All	504/610 (83%)	444 (88%)	40 (8%)	20 (4%)	2	3

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	283	ASP
1	A	307	PRO
1	B	283	ASP
1	B	282	GLY
1	B	284	SER
1	A	99	PRO
1	A	241	GLU
1	B	241	GLU
1	B	249	GLU
1	B	254	GLY
1	B	256	ALA
1	B	265	LYS
1	B	281	PRO
1	A	218	ASP
1	B	257	PRO
1	B	262	PRO
1	B	229	PRO
1	B	238	PRO
1	A	245	ALA

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	203/242 (84%)	158 (78%)	45 (22%)	1	1
1	B	203/242 (84%)	166 (82%)	37 (18%)	2	3
All	All	406/484 (84%)	324 (80%)	82 (20%)	1	2

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	60	GLN
1	A	62	ARG
1	A	63	ILE
1	A	70	SER
1	A	71	LEU
1	A	73	ARG
1	A	77	GLU
1	A	84	LEU
1	A	101	ARG
1	A	105	ASP
1	A	109	ARG
1	A	110	LYS
1	A	114	LEU
1	A	117	SER
1	A	122	VAL
1	A	128	ARG
1	A	156	ARG
1	A	163	MET
1	A	171	THR
1	A	174	LYS
1	A	184	VAL
1	A	194	ILE
1	A	198	LEU
1	A	203	VAL
1	A	208	GLN
1	A	217	THR
1	A	226	THR
1	A	227	SER
1	A	230	SER
1	A	239	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	ARG
1	A	249	GLU
1	A	265	LYS
1	A	267	GLU
1	A	274	SER
1	A	276	LEU
1	A	280	LEU
1	A	285	THR
1	A	289	LEU
1	A	292	GLU
1	A	297	SER
1	A	299	ASN
1	A	306	SER
1	A	307	PRO
1	B	60	GLN
1	B	62	ARG
1	B	63	ILE
1	B	64	ASP
1	B	73	ARG
1	B	84	LEU
1	B	85	VAL
1	B	88	ASP
1	B	108	ASN
1	B	112	GLU
1	B	114	LEU
1	B	124	TYR
1	B	128	ARG
1	B	131	VAL
1	B	139	GLN
1	B	157	LEU
1	B	163	MET
1	B	169	MET
1	B	171	THR
1	B	172	VAL
1	B	174	LYS
1	B	194	ILE
1	B	198	LEU
1	B	208	GLN
1	B	216	VAL
1	B	230	SER
1	B	241	GLU
1	B	255	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	ILE
1	B	275	THR
1	B	276	LEU
1	B	279	LEU
1	B	289	LEU
1	B	297	SER
1	B	299	ASN
1	B	304	GLN
1	B	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	108	ASN
1	A	139	GLN
1	A	299	ASN
1	B	79	GLN
1	B	108	ASN
1	B	299	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	254/305 (83%)	-0.21	6 (2%) 59 57	20, 51, 62, 70	1 (0%)
1	B	254/305 (83%)	-0.10	2 (0%) 82 82	24, 52, 64, 69	1 (0%)
All	All	508/610 (83%)	-0.16	8 (1%) 70 69	20, 51, 63, 70	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	5.7
1	A	284	SER	4.6
1	A	269	ARG	3.5
1	B	269	ARG	3.4
1	A	172	VAL	2.6
1	B	308	LEU	2.3
1	A	188	GLY	2.1
1	A	282	GLY	2.1

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
2	CA	A	501	1/1	0.96	0.06	49,49,49,49	1
2	CA	B	601	1/1	0.96	0.05	45,45,45,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.