



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:40 PM UTC

PDB ID : 2GGT / pdb_00002ggt
Title : Crystal structure of human SCO1 complexed with nickel.
Authors : Banci, L.; Bertini, I.; Calderone, V.; Ciofi-Baffoni, S.; Mangani, S.; Martinelli, M.; Palumaa, P.; Wang, S.
Deposited on : 2006-03-24
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

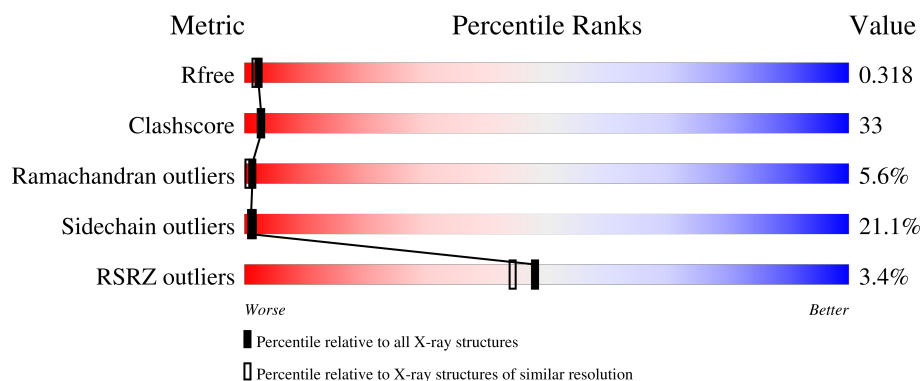
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	164	6% 44% 34% 18% •
1	B	164	6% 29% 41% 23% 7% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2691 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 SCO1 protein homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1321	846	212	258	5			
1	B	163	Total	C	N	O	S	0	0	0
			1309	840	208	256	5			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

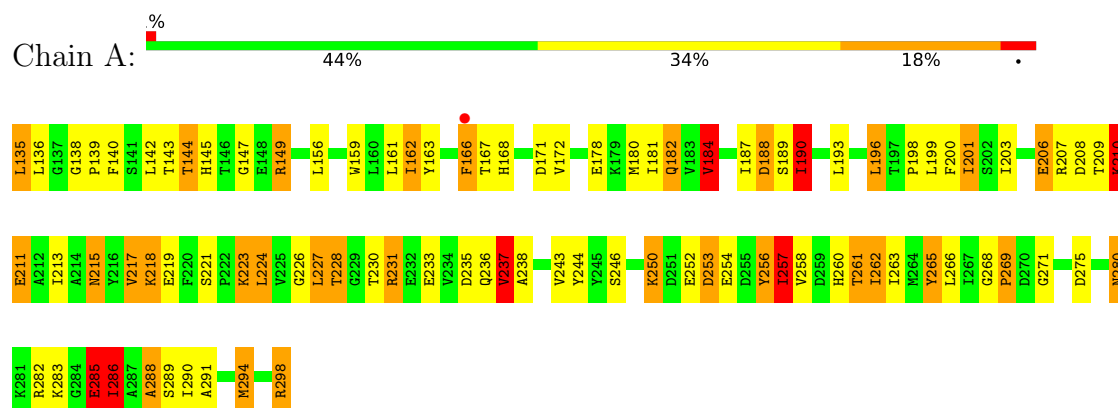
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	12	Total	O	0	0
			12	12		

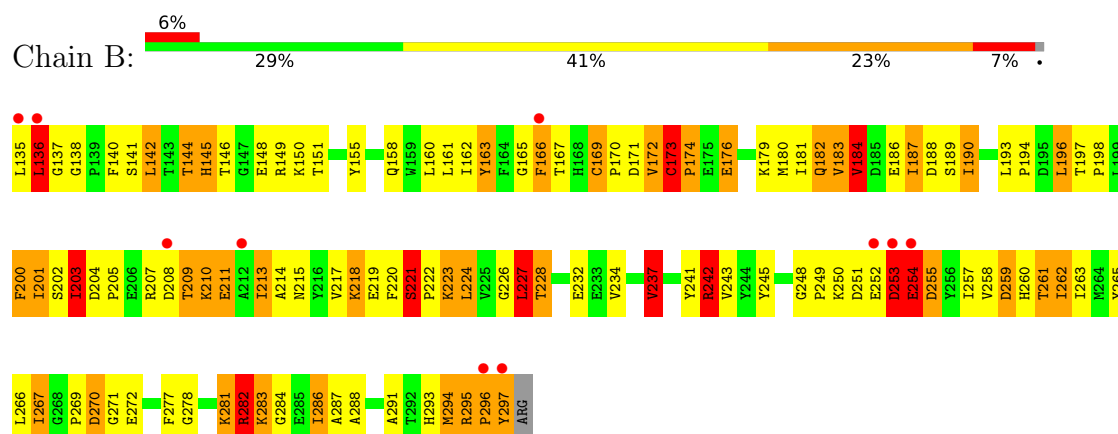
3 Residue-property plots [i](#)

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: SCO1 protein homolog, mitochondrial



- Molecule 1: SCO1 protein homolog, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.46Å 52.44Å 136.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.74 – 2.40 36.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.74-2.40) 97.1 (36.74-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.318 0.223 , 0.318	Depositor DCC
R_{free} test set	1253 reflections (8.53%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2691	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: CL, NI

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	2.06	32/1354 (2.4%)	1.81	31/1838 (1.7%)
1	B	2.08	40/1342 (3.0%)	1.86	37/1824 (2.0%)
All	All	2.07	72/2696 (2.7%)	1.83	68/3662 (1.9%)

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	0	3
All	All	0	4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ASP	C-N	21.30	1.63	1.33
1	B	254	GLU	C-N	16.84	1.55	1.33
1	A	167	THR	CA-CB	9.68	1.68	1.53
1	A	258	VAL	CA-CB	8.55	1.62	1.53
1	B	172	VAL	CA-CB	8.33	1.64	1.54
1	B	184	VAL	CA-CB	7.77	1.65	1.54
1	B	138	GLY	N-CA	7.43	1.54	1.44
1	A	268	GLY	C-O	7.30	1.33	1.24
1	A	237	VAL	CA-CB	7.26	1.65	1.54
1	B	286	ILE	C-O	-7.21	1.17	1.24
1	A	200	PHE	C-O	-7.12	1.15	1.24
1	B	137	GLY	CA-C	6.99	1.61	1.51
1	A	139	PRO	C-O	-6.97	1.15	1.23
1	A	257	ILE	N-CA	-6.87	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	VAL	CA-C	-6.84	1.43	1.52
1	B	187	ILE	CA-CB	6.75	1.62	1.54
1	A	181	ILE	C-O	-6.73	1.16	1.24
1	A	298	ARG	CZ-NH1	6.54	1.42	1.32
1	B	188	ASP	C-O	6.54	1.31	1.24
1	B	136	LEU	CA-CB	6.50	1.64	1.53
1	B	137	GLY	N-CA	6.49	1.54	1.45
1	A	226	GLY	CA-C	-6.38	1.46	1.52
1	A	166	PHE	C-O	-6.33	1.16	1.23
1	B	197	THR	CA-CB	6.22	1.62	1.52
1	A	257	ILE	CB-CG2	6.15	1.72	1.52
1	B	136	LEU	CA-C	6.12	1.60	1.52
1	B	189	SER	C-O	-6.11	1.15	1.24
1	A	269	PRO	N-CA	-6.09	1.39	1.47
1	A	190	ILE	N-CA	6.02	1.53	1.46
1	B	243	VAL	CA-CB	-6.02	1.46	1.54
1	B	267	ILE	CG1-CD1	6.01	1.75	1.51
1	B	241	TYR	CA-C	-5.96	1.44	1.52
1	B	155	TYR	C-O	-5.93	1.16	1.24
1	B	162	ILE	CA-CB	5.90	1.61	1.54
1	A	201	ILE	N-CA	-5.88	1.39	1.46
1	B	270	ASP	CB-CG	5.75	1.66	1.52
1	B	207	ARG	CA-C	5.74	1.60	1.52
1	B	163	TYR	CA-C	5.70	1.59	1.52
1	A	135	LEU	CA-C	5.59	1.64	1.52
1	B	138	GLY	CA-C	5.48	1.59	1.51
1	B	136	LEU	N-CA	5.48	1.53	1.46
1	A	228	THR	C-O	-5.47	1.17	1.23
1	A	149	ARG	C-O	-5.46	1.17	1.23
1	B	243	VAL	CA-C	5.42	1.59	1.52
1	B	183	VAL	CA-C	5.39	1.59	1.52
1	B	282	ARG	CB-CG	5.36	1.68	1.52
1	B	293	HIS	CA-CB	5.34	1.61	1.53
1	A	138	GLY	C-O	5.31	1.31	1.24
1	B	201	ILE	C-O	5.28	1.30	1.24
1	A	162	ILE	CA-CB	-5.24	1.47	1.54
1	B	200	PHE	CA-C	-5.24	1.46	1.52
1	B	146	THR	CA-C	5.20	1.59	1.52
1	B	173	CYS	C-O	-5.20	1.19	1.24
1	B	224	LEU	C-O	5.20	1.30	1.23
1	B	227	LEU	N-CA	-5.19	1.40	1.46
1	A	243	VAL	CA-CB	5.17	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	THR	CA-CB	5.16	1.62	1.53
1	B	190	ILE	C-O	5.15	1.29	1.24
1	B	221	SER	C-O	-5.14	1.17	1.24
1	A	289	SER	C-O	5.14	1.30	1.24
1	A	227	LEU	CA-C	-5.14	1.46	1.52
1	B	173	CYS	CA-CB	5.12	1.60	1.53
1	A	215	ASN	N-CA	5.12	1.52	1.46
1	A	294	MET	SD-CE	-5.11	1.66	1.79
1	A	190	ILE	CA-C	-5.11	1.47	1.52
1	A	262	ILE	C-O	5.10	1.30	1.24
1	A	211	GLU	N-CA	5.09	1.52	1.46
1	B	258	VAL	CA-CB	5.08	1.59	1.53
1	B	295	ARG	CA-C	5.05	1.59	1.52
1	A	188	ASP	C-O	5.04	1.30	1.24
1	B	187	ILE	C-O	5.02	1.29	1.24
1	A	288	ALA	CA-C	-5.01	1.46	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	ASN	N-CA-C	11.68	123.57	111.07
1	B	253	ASP	O-C-N	10.09	136.01	122.59
1	B	294	MET	N-CA-C	9.58	124.22	112.54
1	B	237	VAL	CB-CA-C	-9.49	99.13	112.22
1	B	248	GLY	CA-C-N	8.80	130.85	119.84
1	B	248	GLY	C-N-CA	8.80	130.85	119.84
1	A	190	ILE	N-CA-CB	8.20	120.39	110.31
1	A	298	ARG	NE-CZ-NH2	-7.74	112.23	119.20
1	A	257	ILE	CB-CA-C	7.64	122.27	110.50
1	B	254	GLU	O-C-N	7.46	132.52	122.59
1	B	295	ARG	NE-CZ-NH2	7.41	125.87	119.20
1	B	158	GLN	N-CA-C	7.25	121.27	109.59
1	B	221	SER	CA-C-N	7.19	128.83	119.84
1	B	221	SER	C-N-CA	7.19	128.83	119.84
1	A	136	LEU	N-CA-C	7.18	121.11	110.48
1	A	210	LYS	N-CA-C	6.99	119.75	111.71
1	B	138	GLY	N-CA-C	6.95	126.52	112.34
1	A	166	PHE	CA-C-N	6.80	129.39	120.28
1	A	166	PHE	C-N-CA	6.80	129.39	120.28
1	A	289	SER	N-CA-C	6.78	118.75	111.36
1	B	197	THR	N-CA-CB	6.74	119.85	110.01
1	A	223	LYS	N-CA-C	6.67	121.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ILE	N-CA-C	6.67	116.82	110.42
1	A	171	ASP	N-CA-C	6.50	124.64	110.80
1	A	182	GLN	N-CA-C	6.45	120.36	112.23
1	A	238	ALA	N-CA-C	-6.30	105.24	113.12
1	B	261	THR	CB-CA-C	6.16	120.19	109.65
1	B	259	ASP	CB-CA-C	6.11	122.21	109.68
1	A	294	MET	CG-SD-CE	-6.09	87.51	100.90
1	A	138	GLY	CA-C-N	6.07	125.98	119.85
1	A	138	GLY	C-N-CA	6.07	125.98	119.85
1	A	147	GLY	N-CA-C	6.03	123.05	115.21
1	B	271	GLY	CA-C-N	6.00	129.28	120.82
1	B	271	GLY	C-N-CA	6.00	129.28	120.82
1	A	265	TYR	N-CA-C	5.96	118.12	108.41
1	A	187	ILE	CA-C-N	5.96	128.54	120.38
1	A	187	ILE	C-N-CA	5.96	128.54	120.38
1	A	256	TYR	CA-C-N	-5.91	114.72	122.94
1	A	256	TYR	C-N-CA	-5.91	114.72	122.94
1	A	280	ASN	N-CA-C	5.81	119.84	112.87
1	B	203	ILE	CA-C-N	-5.78	116.17	122.59
1	B	203	ILE	C-N-CA	-5.78	116.17	122.59
1	B	208	ASP	CB-CA-C	5.76	121.02	112.03
1	B	155	TYR	N-CA-C	-5.70	105.06	113.61
1	B	269	PRO	CA-C-N	5.63	131.56	121.66
1	B	269	PRO	C-N-CA	5.63	131.56	121.66
1	A	187	ILE	N-CA-C	5.62	115.86	110.74
1	B	260	HIS	N-CA-C	5.57	116.92	108.07
1	B	136	LEU	CB-CG-CD1	5.52	127.27	110.70
1	A	266	LEU	CA-C-N	5.43	129.78	122.93
1	A	266	LEU	C-N-CA	5.43	129.78	122.93
1	B	136	LEU	CB-CA-C	5.39	121.15	110.42
1	A	182	GLN	CA-C-N	5.38	127.54	120.60
1	A	182	GLN	C-N-CA	5.38	127.54	120.60
1	B	174	PRO	N-CA-C	5.37	120.64	114.03
1	A	228	THR	CB-CA-C	-5.34	99.24	111.95
1	B	197	THR	CB-CA-C	5.32	115.91	109.85
1	B	254	GLU	CB-CA-C	5.32	121.00	110.42
1	A	271	GLY	CA-C-N	5.28	129.63	122.19
1	A	271	GLY	C-N-CA	5.28	129.63	122.19
1	B	182	GLN	CA-C-N	5.26	127.38	120.60
1	B	182	GLN	C-N-CA	5.26	127.38	120.60
1	B	242	ARG	CA-CB-CG	-5.25	103.61	114.10
1	B	172	VAL	CB-CA-C	5.19	118.84	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ASP	N-CA-C	-5.14	106.86	113.23
1	B	255	ASP	N-CA-C	5.05	116.63	108.34
1	B	179	LYS	CA-C-N	5.03	126.98	120.44
1	B	179	LYS	C-N-CA	5.03	126.98	120.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ILE	Peptide
1	B	136	LEU	Peptide
1	B	227	LEU	Peptide
1	B	277	PHE	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	1321	0	1281	65	0
1	B	1309	0	1268	110	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	45	0	0	5	0
4	B	12	0	0	2	0
All	All	2691	0	2549	172	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 33.

All (172) 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:267:ILE:CG1	1:B:267:ILE:CD1	1.75	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:HD22	1:B:294:MET:HE3	1.26	1.08
1:B:202:SER:HB3	1:B:228:THR:HG23	1.33	1.07
1:B:242:ARG:HH11	1:B:242:ARG:HG2	1.20	0.99
1:B:217:VAL:HG13	1:B:224:LEU:HB3	1.43	0.99
1:A:193:LEU:HD22	1:A:294:MET:HE3	1.46	0.98
1:B:242:ARG:HG2	1:B:242:ARG:NH1	1.77	0.97
1:B:250:LYS:HD3	1:B:254:GLU:HG3	1.48	0.95
1:A:180:MET:HE2	1:A:198:PRO:HB2	1.52	0.92
1:B:220:PHE:HB2	1:B:224:LEU:HD12	1.49	0.92
1:B:193:LEU:HD13	1:B:294:MET:CE	1.99	0.91
1:A:217:VAL:HG22	1:A:224:LEU:HD13	1.52	0.89
1:B:282:ARG:HG2	1:B:283:LYS:H	1.36	0.88
1:B:145:HIS:CB	1:B:213:ILE:HG22	2.06	0.85
1:B:282:ARG:NH2	1:B:284:GLY:H	1.76	0.83
1:B:193:LEU:CD2	1:B:294:MET:HE3	2.09	0.83
1:B:140:PHE:CB	1:B:237:VAL:HG13	2.11	0.81
1:B:202:SER:HB3	1:B:228:THR:CG2	2.10	0.81
1:B:140:PHE:HB2	1:B:237:VAL:HG13	1.62	0.81
1:B:242:ARG:HH11	1:B:242:ARG:CG	1.95	0.80
1:A:140:PHE:HB3	1:A:237:VAL:HG13	1.64	0.79
1:B:145:HIS:HB3	1:B:213:ILE:CG2	2.11	0.79
1:B:172:VAL:HG11	1:B:262:ILE:HG12	1.65	0.79
1:B:145:HIS:HB3	1:B:213:ILE:HG22	1.61	0.79
1:A:180:MET:HE2	1:A:198:PRO:CB	2.14	0.78
1:B:254:GLU:O	4:B:65:HOH:O	2.01	0.76
1:B:282:ARG:HH22	1:B:284:GLY:H	1.33	0.76
1:A:223:LYS:HE3	4:A:63:HOH:O	1.85	0.75
1:A:168:HIS:CG	1:A:207:ARG:NH1	2.56	0.74
1:B:221:SER:C	1:B:223:LYS:H	1.97	0.72
1:A:193:LEU:HD22	1:A:294:MET:CE	2.17	0.72
1:B:174:PRO:HB3	1:B:220:PHE:HZ	1.53	0.72
1:B:218:LYS:C	1:B:220:PHE:H	1.96	0.71
1:A:180:MET:CE	1:A:198:PRO:CB	2.69	0.71
1:B:144:THR:CG2	1:B:150:LYS:HG3	2.23	0.69
1:A:256:TYR:O	1:A:257:ILE:CG2	2.41	0.69
1:B:205:PRO:HG3	1:B:234:VAL:HG21	1.73	0.69
1:B:182:GLN:HB3	1:B:283:LYS:HD3	1.75	0.68
1:A:162:ILE:HG22	1:A:163:TYR:N	2.08	0.67
1:A:188:ASP:HA	4:A:62:HOH:O	1.93	0.67
1:B:145:HIS:HB2	1:B:213:ILE:HG22	1.73	0.67
1:B:282:ARG:HH22	1:B:284:GLY:N	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:O	1:B:210:LYS:C	2.37	0.66
1:B:165:GLY:O	1:B:203:ILE:HG13	1.95	0.66
1:B:220:PHE:CB	1:B:224:LEU:HD12	2.25	0.66
1:A:193:LEU:HD13	1:A:294:MET:HE1	1.78	0.65
1:B:282:ARG:NH2	1:B:284:GLY:N	2.46	0.64
1:A:145:HIS:HB3	1:A:213:ILE:HG22	1.81	0.63
1:A:180:MET:CE	1:A:198:PRO:HB2	2.27	0.63
1:A:218:LYS:HD3	1:A:218:LYS:H	1.64	0.63
1:B:165:GLY:O	1:B:166:PHE:HB3	1.99	0.63
1:A:206:GLU:HG2	1:A:256:TYR:OH	1.99	0.62
1:B:140:PHE:HB3	1:B:237:VAL:HG13	1.82	0.62
1:B:218:LYS:HD2	1:B:219:GLU:OE2	2.00	0.61
1:B:283:LYS:HG3	1:B:284:GLY:N	2.14	0.61
1:B:282:ARG:HG2	1:B:283:LYS:N	2.12	0.61
1:B:193:LEU:HD13	1:B:294:MET:HE1	1.81	0.61
1:B:251:ASP:OD2	1:B:255:ASP:HB2	2.01	0.61
1:B:287:ALA:O	1:B:288:ALA:C	2.42	0.60
1:A:244:TYR:O	1:A:260:HIS:HA	2.01	0.60
1:B:220:PHE:O	1:B:221:SER:HB3	1.99	0.60
1:A:149:ARG:HH22	1:A:233:GLU:CD	2.10	0.60
1:A:211:GLU:N	1:A:211:GLU:OE2	2.35	0.60
1:B:193:LEU:HD22	1:B:294:MET:CE	2.17	0.60
1:B:215:ASN:O	1:B:218:LYS:HE2	2.02	0.59
1:A:140:PHE:CD1	1:A:142:LEU:HD12	2.37	0.59
1:B:176:GLU:HA	1:B:176:GLU:OE2	2.03	0.58
1:B:149:ARG:HH11	1:B:149:ARG:HG3	1.69	0.58
1:B:210:LYS:HD2	1:B:211:GLU:OE1	2.05	0.57
1:B:163:TYR:HE2	1:B:173:CYS:HB3	1.68	0.57
1:A:168:HIS:CG	1:A:207:ARG:HH11	2.23	0.56
1:A:256:TYR:O	1:A:257:ILE:HG23	2.05	0.56
1:A:178:GLU:O	1:A:182:GLN:HG3	2.05	0.56
1:B:172:VAL:CG1	1:B:262:ILE:HG12	2.35	0.55
1:B:252:GLU:O	1:B:253:ASP:OD1	2.24	0.55
1:B:161:LEU:HA	1:B:265:TYR:O	2.07	0.55
1:A:282:ARG:O	1:A:286:ILE:HG13	2.06	0.55
1:B:181:ILE:HD11	1:B:224:LEU:HG	1.87	0.55
1:A:172:VAL:HG11	1:A:262:ILE:HD13	1.89	0.54
1:A:201:ILE:HG12	1:A:227:LEU:HD12	1.89	0.54
1:A:168:HIS:CB	1:A:207:ARG:HH12	2.21	0.54
1:B:213:ILE:C	1:B:215:ASN:H	2.15	0.53
1:A:215:ASN:HA	1:A:218:LYS:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:HG3	1:B:149:ARG:NH1	2.23	0.52
1:A:159:TRP:CE2	1:A:269:PRO:HD3	2.45	0.52
1:A:166:PHE:HZ	1:A:257:ILE:HB	1.75	0.52
1:A:215:ASN:HD22	1:A:218:LYS:HE2	1.75	0.51
1:A:253:ASP:O	1:A:254:GLU:HB2	2.10	0.51
1:B:183:VAL:HG11	1:B:286:ILE:HG22	1.91	0.51
1:B:171:ASP:O	1:B:174:PRO:HD2	2.11	0.51
1:B:220:PHE:HB2	1:B:224:LEU:CD1	2.32	0.51
1:A:235:ASP:OD2	1:B:281:LYS:NZ	2.35	0.51
1:B:282:ARG:HH22	1:B:284:GLY:CA	2.24	0.51
1:A:166:PHE:CZ	1:A:257:ILE:HB	2.46	0.51
1:B:270:ASP:OD1	1:B:272:GLU:N	2.44	0.51
1:A:162:ILE:CG2	1:A:163:TYR:N	2.74	0.50
1:A:286:ILE:O	1:A:290:ILE:HG13	2.12	0.50
1:B:204:ASP:O	1:B:204:ASP:CG	2.52	0.50
1:B:218:LYS:C	1:B:220:PHE:N	2.59	0.50
1:B:220:PHE:O	1:B:221:SER:CB	2.59	0.50
1:A:261:THR:HB	1:A:263:ILE:HD12	1.93	0.50
1:B:184:VAL:HG12	1:B:196:LEU:HD13	1.94	0.49
1:B:176:GLU:OE2	1:B:176:GLU:CA	2.60	0.49
1:A:231:ARG:HG3	4:A:19:HOH:O	2.11	0.49
1:A:291:ALA:HA	1:A:294:MET:HE2	1.95	0.49
1:B:221:SER:C	1:B:223:LYS:N	2.70	0.49
1:B:144:THR:HG23	1:B:148:GLU:O	2.12	0.49
1:B:145:HIS:HB3	1:B:213:ILE:HG21	1.95	0.48
1:B:270:ASP:OD2	1:B:272:GLU:HB2	2.13	0.48
1:B:193:LEU:HD22	1:B:294:MET:HB2	1.95	0.48
1:B:263:ILE:HG22	1:B:265:TYR:CZ	2.48	0.48
1:B:270:ASP:CG	1:B:272:GLU:HB2	2.38	0.48
1:B:145:HIS:CD2	1:B:214:ALA:HA	2.49	0.48
1:B:282:ARG:HH22	1:B:284:GLY:HA3	1.78	0.48
1:A:210:LYS:HE3	1:A:210:LYS:HB3	1.41	0.47
1:B:141:SER:HA	1:B:151:THR:HG22	1.97	0.47
1:B:140:PHE:CD1	1:B:142:LEU:HD12	2.50	0.47
1:A:263:ILE:O	4:A:4:HOH:O	2.21	0.47
1:B:291:ALA:HA	1:B:294:MET:HE2	1.96	0.47
1:B:174:PRO:HB3	1:B:220:PHE:CZ	2.42	0.47
1:A:250:LYS:HZ1	1:A:250:LYS:H	1.63	0.46
1:A:161:LEU:HD22	1:A:196:LEU:HD11	1.96	0.46
1:A:168:HIS:CB	1:A:207:ARG:NH1	2.77	0.46
1:B:184:VAL:HG11	1:B:198:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TRP:CD2	1:A:269:PRO:HD3	2.51	0.46
1:A:213:ILE:O	1:A:217:VAL:HB	2.16	0.45
1:B:204:ASP:C	1:B:204:ASP:OD1	2.59	0.45
1:B:201:ILE:HA	1:B:227:LEU:O	2.17	0.45
1:A:143:THR:HG22	1:A:144:THR:N	2.31	0.45
1:B:180:MET:HE3	1:B:198:PRO:HA	1.99	0.45
1:A:265:TYR:CD1	1:A:265:TYR:N	2.85	0.44
1:B:296:PRO:HB2	1:B:297:TYR:H	1.46	0.44
1:B:148:GLU:OE1	1:B:150:LYS:NZ	2.47	0.44
1:B:161:LEU:HD12	1:B:265:TYR:O	2.17	0.44
1:B:144:THR:HG22	1:B:150:LYS:HG3	1.96	0.44
1:B:201:ILE:HG12	1:B:227:LEU:HD12	1.98	0.44
1:B:270:ASP:OD1	1:B:272:GLU:HB2	2.17	0.44
1:B:193:LEU:HD13	1:B:294:MET:HE2	1.92	0.43
1:B:295:ARG:O	1:B:296:PRO:O	2.35	0.43
1:A:145:HIS:O	1:A:210:LYS:HG3	2.18	0.43
1:B:218:LYS:O	1:B:220:PHE:N	2.51	0.43
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.87	0.43
1:B:145:HIS:HD2	1:B:214:ALA:HA	1.84	0.43
1:A:217:VAL:HG13	4:A:26:HOH:O	2.19	0.43
1:B:221:SER:O	1:B:223:LYS:N	2.47	0.43
1:B:140:PHE:CB	1:B:237:VAL:CG1	2.92	0.42
1:A:207:ARG:NH2	1:A:256:TYR:O	2.51	0.42
1:A:198:PRO:HB2	1:A:224:LEU:HD23	2.02	0.42
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.19	0.42
1:A:235:ASP:CG	1:B:281:LYS:HZ1	2.23	0.42
1:B:252:GLU:O	1:B:252:GLU:HG2	2.19	0.42
1:A:246:SER:OG	1:B:263:ILE:HD13	2.20	0.42
1:B:254:GLU:HB3	4:B:65:HOH:O	2.20	0.42
1:B:193:LEU:CD1	1:B:294:MET:CE	2.86	0.42
1:B:252:GLU:O	1:B:253:ASP:CG	2.63	0.42
1:B:148:GLU:OE1	1:B:150:LYS:CE	2.68	0.41
1:B:166:PHE:O	1:B:169:CYS:HB2	2.20	0.41
1:B:190:ILE:HD12	1:B:193:LEU:HD12	2.01	0.41
1:B:203:ILE:HD13	1:B:245:TYR:HB3	2.01	0.41
1:A:145:HIS:CB	1:A:213:ILE:HG22	2.47	0.41
1:A:180:MET:HE1	1:A:199:LEU:N	2.35	0.41
1:A:285:GLU:O	1:A:288:ALA:HB3	2.19	0.41
1:A:208:ASP:HB3	1:A:213:ILE:HG13	2.02	0.41
1:A:215:ASN:O	1:A:218:LYS:HE3	2.19	0.41
1:B:193:LEU:HB3	1:B:294:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:C	1:A:209:THR:O	2.62	0.41
1:A:294:MET:HE3	1:A:294:MET:HB3	1.85	0.41
1:B:200:PHE:O	1:B:226:GLY:HA2	2.20	0.41
1:B:296:PRO:O	1:B:297:TYR:C	2.64	0.41
1:A:180:MET:O	1:A:184:VAL:HG13	2.20	0.41
1:B:193:LEU:CG	1:B:294:MET:HE3	2.51	0.40
1:B:144:THR:HG21	1:B:150:LYS:HG3	2.03	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	162/164 (99%)	144 (89%)	13 (8%)	5 (3%)	3	3
1	B	161/164 (98%)	128 (80%)	20 (12%)	13 (8%)	1	0
All	All	323/328 (98%)	272 (84%)	33 (10%)	18 (6%)	1	1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLU
1	B	166	PHE
1	B	210	LYS
1	B	253	ASP
1	B	254	GLU
1	B	278	GLY
1	B	296	PRO
1	B	221	SER
1	B	170	PRO
1	B	249	PRO
1	A	285	GLU

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Mol	Chain	Res	Type
1	B	167	THR
1	B	194	PRO
1	B	222	PRO
1	A	236	GLN
1	A	189	SER
1	B	203	ILE
1	A	286	ILE

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	145/145 (100%)	118 (81%)	27 (19%)	1	2
1	B	144/145 (99%)	110 (76%)	34 (24%)	1	1
All	All	289/290 (100%)	228 (79%)	61 (21%)	1	1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	144	THR
1	A	156	LEU
1	A	184	VAL
1	A	190	ILE
1	A	196	LEU
1	A	203	ILE
1	A	206	GLU
1	A	210	LYS
1	A	217	VAL
1	A	218	LYS
1	A	221	SER
1	A	224	LEU
1	A	228	THR
1	A	230	THR
1	A	231	ARG

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Mol	Chain	Res	Type
1	A	237	VAL
1	A	250	LYS
1	A	253	ASP
1	A	257	ILE
1	A	261	THR
1	A	275	ASP
1	A	280	ASN
1	A	283	LYS
1	A	285	GLU
1	A	286	ILE
1	A	298	ARG
1	B	135	LEU
1	B	136	LEU
1	B	142	LEU
1	B	144	THR
1	B	145	HIS
1	B	160	LEU
1	B	169	CYS
1	B	173	CYS
1	B	176	GLU
1	B	184	VAL
1	B	186	GLU
1	B	187	ILE
1	B	196	LEU
1	B	203	ILE
1	B	209	THR
1	B	211	GLU
1	B	213	ILE
1	B	218	LYS
1	B	223	LYS
1	B	227	LEU
1	B	228	THR
1	B	232	GLU
1	B	237	VAL
1	B	242	ARG
1	B	254	GLU
1	B	257	ILE
1	B	259	ASP
1	B	261	THR
1	B	262	ILE
1	B	266	LEU
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	282	ARG
1	B	283	LYS
1	B	297	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	215	ASN
1	A	293	HIS
1	B	158	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 4 ligands modelled in this entry, 4 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	253:ASP	C	254:GLU	N	1.63

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	164/164 (100%)	-0.03	1 (0%) 85 83	15, 30, 50, 63	0
1	B	163/164 (99%)	0.49	10 (6%) 27 23	19, 39, 63, 78	0
All	All	327/328 (99%)	0.23	11 (3%) 48 44	15, 34, 59, 78	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	TYR	6.4
1	B	208	ASP	5.1
1	B	254	GLU	3.6
1	B	296	PRO	2.8
1	B	136	LEU	2.5
1	B	252	GLU	2.4
1	B	253	ASP	2.4
1	B	135	LEU	2.3
1	A	166	PHE	2.0
1	B	166	PHE	2.0
1	B	212	ALA	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
3	CL	A	300	1/1	0.88	0.09	46,46,46,46	0
3	CL	B	301	1/1	0.92	0.08	40,40,40,40	0
2	NI	B	299	1/1	0.97	0.06	39,39,39,39	0
2	NI	A	299	1/1	0.99	0.03	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.