



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:59 AM UTC

PDB ID : 1FS2 / pdb_00001fs2
Title : INSIGHTS INTO SCF UBIQUITIN LIGASES FROM THE STRUCTURE OF THE SKP1-SKP2 COMPLEX
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Deposited on : 2000-09-08
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

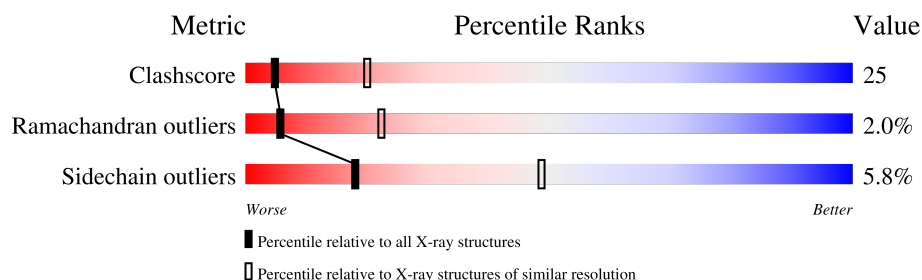
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	272	
1	C	272	
2	B	141	
2	D	141	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6035 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 SKP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2025	1289	340	384	12			
1	C	259	Total	C	N	O	S	0	0	0
			2012	1280	337	383	12			

- Molecule 2 is a protein called SKP1.

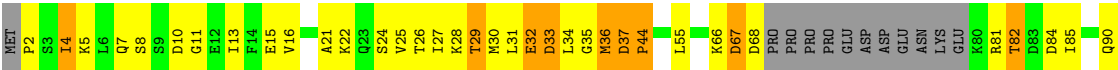
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			999	638	161	195	5			
2	D	128	Total	C	N	O	S	0	0	0
			999	638	161	195	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	GLU	deletion	UNP P63208
B	?	-	GLY	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
B	?	-	ASP	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208
D	?	-	GLU	deletion	UNP P63208
D	?	-	GLY	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208



● Molecule 2: SKP1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.67Å 87.02Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6035	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.71	1/2062 (0.0%)	1.26	19/2798 (0.7%)
1	C	0.65	1/2047 (0.0%)	1.21	20/2777 (0.7%)
2	B	0.61	0/1014	1.28	12/1371 (0.9%)
2	D	0.65	0/1014	1.27	9/1371 (0.7%)
All	All	0.66	2/6137 (0.0%)	1.25	60/8317 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	MET	SD-CE	8.93	2.01	1.79
1	A	198	MET	SD-CE	8.01	1.99	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	PHE	N-CA-C	11.79	128.47	109.85
2	B	67	ASP	N-CA-C	11.16	125.44	112.72
1	A	281	PHE	N-CA-C	11.12	127.42	109.85
1	A	106	GLY	N-CA-C	-11.10	93.29	111.38
2	D	67	ASP	N-CA-C	9.93	124.04	112.72
2	D	32	GLU	N-CA-C	9.92	122.17	111.36
2	B	32	GLU	N-CA-C	9.61	121.83	111.36
2	B	37	ASP	CA-C-N	-9.54	109.88	119.90
2	B	37	ASP	C-N-CA	-9.54	109.88	119.90
2	D	37	ASP	CA-C-N	-8.69	110.78	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	37	ASP	C-N-CA	-8.69	110.78	119.90
2	B	82	THR	N-CA-C	-8.63	92.41	110.80
1	C	106	GLY	N-CA-C	-8.61	96.07	110.80
2	D	82	THR	N-CA-C	-8.51	92.69	110.80
1	C	256	SER	N-CA-C	7.28	120.38	110.55
1	A	380	PHE	N-CA-C	7.12	120.81	110.28
2	D	44	PRO	N-CA-C	-6.78	100.56	110.80
2	B	2	PRO	N-CA-CB	6.53	110.18	103.00
1	A	371	ILE	N-CA-C	-6.51	101.64	107.56
2	D	2	PRO	N-CA-CB	6.50	110.14	103.00
1	A	256	SER	N-CA-C	6.45	119.94	110.59
1	A	371	ILE	CA-C-N	6.42	127.87	119.84
1	A	371	ILE	C-N-CA	6.42	127.87	119.84
1	C	320	ARG	N-CA-C	6.37	120.25	112.23
2	B	44	PRO	N-CA-C	-6.35	101.21	110.80
1	C	371	ILE	CA-C-N	6.30	127.72	119.84
1	C	371	ILE	C-N-CA	6.30	127.72	119.84
1	C	369	GLY	N-CA-C	-6.26	107.54	115.31
1	A	369	GLY	N-CA-C	-6.16	107.68	115.31
2	B	11	GLY	N-CA-C	6.00	121.84	114.69
1	A	292	HIS	N-CA-C	5.94	121.32	112.94
1	C	371	ILE	N-CA-C	-5.84	102.25	107.56
1	C	380	PHE	N-CA-C	5.77	118.82	110.28
1	A	321	CYS	CA-C-N	5.68	125.36	119.56
1	A	321	CYS	C-N-CA	5.68	125.36	119.56
1	C	221	GLN	N-CA-C	-5.61	107.07	114.31
1	A	280	ASP	CA-C-N	-5.60	113.41	122.81
1	A	280	ASP	C-N-CA	-5.60	113.41	122.81
2	B	23	GLN	N-CA-C	-5.52	106.50	113.18
1	A	357	CYS	N-CA-C	-5.47	101.41	109.62
1	C	257	GLU	N-CA-C	-5.46	105.43	111.71
1	C	137	LYS	N-CA-C	5.44	117.63	111.11
1	C	280	ASP	CA-C-N	-5.37	113.78	122.81
1	C	280	ASP	C-N-CA	-5.37	113.78	122.81
1	A	221	GLN	N-CA-C	-5.37	106.65	114.12
1	A	320	ARG	N-CA-C	5.34	118.96	112.23
1	A	282	THR	N-CA-C	5.33	118.31	109.94
1	C	297	ILE	N-CA-C	5.31	116.54	109.37
1	A	297	ILE	N-CA-C	5.25	116.46	109.37
2	B	123	VAL	N-CA-C	-5.24	105.43	110.72
1	C	321	CYS	CA-C-N	5.22	124.88	119.56
1	C	321	CYS	C-N-CA	5.22	124.88	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	VAL	N-CA-C	-5.14	105.39	111.00
2	B	84	ASP	CA-C-N	-5.12	119.12	122.60
2	B	84	ASP	C-N-CA	-5.12	119.12	122.60
1	A	225	LEU	N-CA-C	-5.12	105.34	112.30
2	D	11	GLY	N-CA-C	5.11	120.89	114.25
1	C	292	HIS	N-CA-C	5.08	120.59	113.02
1	C	282	THR	N-CA-C	5.04	117.85	109.94
1	C	358	TYR	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	281	PHE	Sidechain

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	2025	0	2032	126	0
1	C	2012	0	2013	108	0
2	B	999	0	1003	46	0
2	D	999	0	1003	48	0
All	All	6035	0	6051	307	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 25.

All (307) 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:C:198:MET:CE	1:C:198:MET:SD	2.01	1.47
1:A:197:HIS:O	1:A:198:MET:HG2	1.64	0.96
1:A:198:MET:O	1:A:200:LEU:N	1.98	0.96
1:C:220:LEU:H	1:C:241:ASN:HD22	1.12	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:HB2	1:A:285:HIS:ND1	1.86	0.90
1:A:220:LEU:H	1:A:241:ASN:HD22	1.22	0.87
2:B:25:VAL:O	2:B:29:THR:HG22	1.75	0.86
1:A:253:SER:HB2	1:A:280:ASP:HB2	1.54	0.86
1:C:253:SER:HB2	1:C:280:ASP:HB2	1.57	0.86
1:A:138:ARG:CZ	1:C:138:ARG:NE	2.43	0.81
2:D:33:ASP:O	2:D:34:LEU:HD23	1.81	0.81
1:C:281:PHE:HB2	1:C:285:HIS:ND1	1.95	0.80
1:A:281:PHE:HB2	1:A:285:HIS:CG	2.16	0.79
1:A:152:LEU:HD22	1:A:192:GLU:O	1.83	0.79
1:A:289:ALA:O	1:A:293:VAL:HG23	1.82	0.79
1:C:195:VAL:HG23	1:C:225:LEU:HA	1.64	0.79
2:D:25:VAL:O	2:D:29:THR:HG22	1.83	0.79
1:A:138:ARG:NH1	1:C:138:ARG:HD2	1.99	0.77
2:B:33:ASP:O	2:B:34:LEU:HD23	1.83	0.77
1:A:138:ARG:NE	1:C:138:ARG:CZ	2.48	0.76
1:C:195:VAL:CG2	1:C:225:LEU:HA	2.16	0.76
1:C:110:ASP:OD1	2:D:141:ILE:HA	1.84	0.76
1:C:379:VAL:HG22	1:C:382:ILE:HD11	1.67	0.75
1:C:281:PHE:HB2	1:C:285:HIS:CG	2.21	0.75
1:C:289:ALA:O	1:C:293:VAL:HG23	1.87	0.75
2:D:22:LYS:HD2	2:D:28:LYS:HG3	1.69	0.75
2:B:7:GLN:HE22	1:C:236:ASN:HD22	1.35	0.74
1:A:195:VAL:HG23	1:A:225:LEU:HA	1.70	0.73
1:C:206:GLU:HB3	1:C:209:THR:HG23	1.71	0.73
1:A:138:ARG:HD2	1:C:138:ARG:NH1	2.04	0.73
1:C:293:VAL:HG12	1:C:297:ILE:HG13	1.71	0.73
2:B:130:LYS:HE3	2:B:138:THR:HG21	1.72	0.72
1:C:293:VAL:CG1	1:C:297:ILE:HG13	2.20	0.72
1:A:379:VAL:HG22	1:A:382:ILE:HD11	1.72	0.71
1:A:137:LYS:HG3	2:B:144:ASP:HB3	1.73	0.70
2:B:22:LYS:HD2	2:B:28:LYS:HG3	1.71	0.70
1:A:236:ASN:HD22	2:D:7:GLN:HE22	1.38	0.69
1:A:293:VAL:CG1	1:A:297:ILE:HG13	2.23	0.69
1:C:137:LYS:HG3	2:D:144:ASP:HB3	1.75	0.68
2:B:4:ILE:HD13	2:B:5:LYS:H	1.58	0.68
2:D:7:GLN:HG3	2:D:13:ILE:HG12	1.76	0.67
1:A:206:GLU:HB3	1:A:209:THR:HG23	1.77	0.66
1:A:220:LEU:H	1:A:241:ASN:ND2	1.93	0.66
2:D:130:LYS:HE3	2:D:138:THR:HG21	1.76	0.66
1:C:220:LEU:H	1:C:241:ASN:ND2	1.90	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:CD2	1:A:342:GLU:HB3	2.25	0.66
1:A:293:VAL:HG12	1:A:297:ILE:HG13	1.79	0.65
1:A:314:LEU:O	1:A:318:VAL:HG23	1.96	0.65
1:C:314:LEU:O	1:C:318:VAL:HG23	1.96	0.64
1:A:195:VAL:CG2	1:A:225:LEU:HA	2.27	0.64
2:B:34:LEU:O	2:B:36:MET:N	2.31	0.64
1:A:317:LEU:HD21	1:A:324:LEU:HD11	1.80	0.64
1:C:113:PRO:HD2	1:C:116:LEU:HD12	1.79	0.64
2:D:131:THR:O	2:D:135:ILE:HG13	1.97	0.63
2:D:16:VAL:HG23	2:D:21:ALA:HB2	1.79	0.63
2:B:22:LYS:NZ	2:B:32:GLU:OE2	2.23	0.63
1:C:317:LEU:HD21	1:C:324:LEU:HD11	1.80	0.62
2:B:16:VAL:CG2	2:B:21:ALA:HB2	2.29	0.62
1:C:231:SER:OG	1:C:234:ILE:HG22	1.98	0.62
2:D:4:ILE:HD13	2:D:5:LYS:H	1.64	0.62
2:D:22:LYS:NZ	2:D:32:GLU:OE2	2.27	0.62
1:C:116:LEU:HD13	2:D:104:ILE:CG2	2.30	0.62
2:B:16:VAL:HG23	2:B:21:ALA:HB2	1.81	0.61
1:C:130:LEU:HD12	1:C:198:MET:HE3	1.82	0.61
1:C:379:VAL:CG2	1:C:382:ILE:HD11	2.30	0.60
2:D:16:VAL:CG2	2:D:21:ALA:HB2	2.31	0.60
1:C:314:LEU:CD2	1:C:342:GLU:HB3	2.32	0.60
1:C:333:VAL:HG12	1:C:333:VAL:O	2.02	0.59
2:B:37:ASP:HB3	2:B:44:PRO:HD3	1.84	0.59
1:A:110:ASP:OD1	2:B:141:ILE:HA	2.03	0.58
2:B:131:THR:O	2:B:135:ILE:HG13	2.03	0.58
1:C:363:GLU:OE2	1:C:387:THR:HG21	2.03	0.58
1:A:140:TYR:HE2	1:A:209:THR:HG22	1.67	0.58
1:A:116:LEU:HD13	2:B:104:ILE:CG2	2.33	0.58
1:A:138:ARG:CZ	1:C:138:ARG:CZ	2.82	0.58
1:A:281:PHE:CB	1:A:285:HIS:CG	2.86	0.58
1:A:379:VAL:HG13	1:A:379:VAL:O	2.04	0.58
2:B:30:MET:O	2:B:34:LEU:O	2.22	0.57
1:A:140:TYR:CE2	1:A:209:THR:HG22	2.38	0.57
1:A:271:ASP:O	1:A:297:ILE:HD13	2.04	0.57
1:C:195:VAL:HG23	1:C:224:SER:O	2.04	0.57
1:C:111:SER:HA	1:C:138:ARG:HH12	1.70	0.57
1:C:137:LYS:H	2:D:144:ASP:HB2	1.70	0.57
1:C:231:SER:H	1:C:234:ILE:CG2	2.16	0.57
2:D:34:LEU:O	2:D:36:MET:N	2.34	0.57
1:A:333:VAL:O	1:A:333:VAL:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:HB	1:A:374:LEU:HB2	1.87	0.57
1:A:211:HIS:HE1	1:A:237:THR:OG1	1.89	0.56
1:A:257:GLU:OE1	1:A:284:LYS:HD2	2.06	0.56
2:D:37:ASP:HB3	2:D:44:PRO:HD3	1.87	0.56
1:A:138:ARG:NE	1:C:138:ARG:NH2	2.53	0.56
2:B:33:ASP:OD1	2:B:33:ASP:N	2.38	0.56
1:A:129:LEU:O	1:A:132:VAL:HG22	2.06	0.55
2:D:33:ASP:N	2:D:33:ASP:OD1	2.39	0.55
1:A:111:SER:HA	1:A:138:ARG:HH12	1.72	0.55
1:C:195:VAL:HG22	1:C:228:LEU:HD11	1.89	0.55
1:A:195:VAL:HG22	1:A:228:LEU:HD11	1.88	0.54
2:B:5:LYS:HG2	2:B:15:GLU:HG2	1.89	0.54
1:A:307:LYS:HE3	1:A:308:ASN:OD1	2.07	0.54
1:C:271:ASP:O	1:C:297:ILE:HD13	2.07	0.54
1:C:258:PHE:O	1:C:262:THR:HG22	2.08	0.54
1:C:371:ILE:HB	1:C:374:LEU:HB2	1.90	0.54
1:A:309:LEU:HD12	1:A:313:ASP:HB2	1.89	0.54
1:A:138:ARG:CD	1:C:138:ARG:CZ	2.86	0.54
1:A:113:PRO:HD2	1:A:116:LEU:HD12	1.90	0.53
1:C:146:GLU:HG2	1:C:150:GLN:NE2	2.24	0.53
1:A:331:ASP:OD2	1:A:356:ARG:NH1	2.41	0.53
1:A:281:PHE:CE1	1:A:305:TYR:CE2	2.97	0.53
2:B:5:LYS:HG2	2:B:15:GLU:CG	2.38	0.53
2:B:133:GLU:HA	2:B:136:ARG:HH11	1.72	0.53
2:D:30:MET:O	2:D:34:LEU:O	2.25	0.53
1:A:124:LEU:HD22	1:A:128:GLU:HG2	1.90	0.53
2:D:133:GLU:HA	2:D:133:GLU:OE2	2.07	0.53
2:D:24:SER:HB3	2:D:27:ILE:HB	1.90	0.53
2:D:126:MET:O	2:D:130:LYS:HE2	2.09	0.53
1:C:309:LEU:HD12	1:C:313:ASP:HB2	1.90	0.53
1:C:146:GLU:O	1:C:150:GLN:HB2	2.08	0.52
1:C:207:VAL:CG1	1:C:208:SER:N	2.72	0.52
1:A:138:ARG:NH2	1:C:138:ARG:NE	2.57	0.52
2:B:7:GLN:HG3	2:B:13:ILE:HG12	1.91	0.52
1:C:379:VAL:HG13	1:C:379:VAL:O	2.09	0.52
1:C:124:LEU:HD22	1:C:128:GLU:HG2	1.92	0.51
2:B:133:GLU:HA	2:B:133:GLU:OE2	2.09	0.51
1:C:129:LEU:HD23	1:C:149:TRP:CZ2	2.46	0.51
1:C:129:LEU:O	1:C:132:VAL:HG22	2.10	0.51
2:D:25:VAL:O	2:D:28:LYS:HB3	2.11	0.51
1:C:211:HIS:HE1	1:C:237:THR:OG1	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:SER:OG	1:A:233:PRO:HD2	2.10	0.51
1:A:231:SER:H	1:A:234:ILE:CG2	2.22	0.51
1:C:259:ALA:HA	1:C:262:THR:HG23	1.92	0.51
1:A:194:ARG:H	1:A:197:HIS:CE1	2.28	0.51
1:A:272:GLU:HB3	1:A:299:GLN:HB2	1.92	0.51
1:A:259:ALA:HA	1:A:262:THR:HG23	1.93	0.51
1:C:314:LEU:HD11	1:C:343:PHE:CZ	2.45	0.51
1:A:146:GLU:O	1:A:150:GLN:HB2	2.11	0.51
1:A:138:ARG:CZ	1:C:138:ARG:CD	2.88	0.50
1:C:220:LEU:HB2	1:C:241:ASN:ND2	2.27	0.50
2:D:5:LYS:HG2	2:D:15:GLU:CG	2.41	0.50
1:A:198:MET:C	1:A:200:LEU:H	2.13	0.50
1:C:257:GLU:OE1	1:C:284:LYS:HD2	2.12	0.50
1:A:253:SER:HB2	1:A:280:ASP:CB	2.35	0.50
1:A:274:ASN:C	1:A:274:ASN:HD22	2.19	0.50
1:A:314:LEU:HD11	1:A:343:PHE:CZ	2.47	0.50
1:A:307:LYS:HD2	1:A:307:LYS:C	2.37	0.50
1:C:269:ARG:HB2	1:C:269:ARG:HH11	1.76	0.50
1:C:281:PHE:CB	1:C:285:HIS:CG	2.92	0.49
1:C:137:LYS:H	2:D:144:ASP:CB	2.25	0.49
1:A:138:ARG:NH1	1:C:138:ARG:CD	2.73	0.49
2:B:24:SER:HB3	2:B:27:ILE:HB	1.94	0.49
2:D:91:GLU:O	2:D:94:LYS:HB2	2.12	0.49
1:C:353:SER:OG	1:C:378:GLN:HB2	2.13	0.49
1:A:129:LEU:HD23	1:A:149:TRP:CZ2	2.48	0.49
1:A:293:VAL:HG11	1:A:297:ILE:HG13	1.95	0.49
1:C:307:LYS:HE3	1:C:308:ASN:OD1	2.13	0.49
1:A:363:GLU:OE2	1:A:387:THR:HG21	2.13	0.48
1:A:365:LEU:O	1:A:366:LEU:C	2.56	0.48
2:B:97:GLN:O	2:B:98:GLY:C	2.57	0.48
1:C:365:LEU:O	1:C:366:LEU:C	2.56	0.48
1:A:362:PRO:HG3	1:A:382:ILE:O	2.13	0.48
1:A:283:GLU:HB3	1:A:287:GLN:HE21	1.79	0.48
2:B:91:GLU:O	2:B:94:LYS:HB2	2.14	0.48
1:C:281:PHE:CE1	1:C:305:TYR:CE2	3.02	0.48
2:D:24:SER:O	2:D:25:VAL:C	2.55	0.48
1:A:269:ARG:HH11	1:A:269:ARG:HB2	1.78	0.48
1:C:274:ASN:C	1:C:274:ASN:HD22	2.22	0.48
2:D:130:LYS:HB3	2:D:134:GLU:HB3	1.96	0.48
2:B:85:ILE:HG22	2:B:90:GLN:HG3	1.94	0.47
1:C:257:GLU:H	1:C:257:GLU:HG2	1.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HG2	1:A:128:GLU:H	1.79	0.47
1:A:279:PHE:CD1	1:A:280:ASP:N	2.83	0.47
1:A:317:LEU:CD2	1:A:324:LEU:HD11	2.44	0.47
1:A:395:LEU:HD12	1:A:398:LEU:HD12	1.96	0.47
1:C:317:LEU:CD2	1:C:324:LEU:HD11	2.43	0.47
1:C:140:TYR:CD1	1:C:140:TYR:C	2.93	0.47
1:A:231:SER:OG	1:A:234:ILE:HG22	2.15	0.47
2:B:102:GLU:OE2	2:B:102:GLU:HA	2.13	0.47
2:D:26:THR:O	2:D:29:THR:HG23	2.15	0.47
1:A:197:HIS:O	1:A:198:MET:CG	2.49	0.47
1:C:253:SER:HB2	1:C:280:ASP:CB	2.38	0.47
2:D:24:SER:HA	2:D:112:ILE:HG12	1.97	0.47
1:A:126:LEU:HD13	1:A:152:LEU:HD11	1.97	0.47
1:A:138:ARG:HD2	1:C:138:ARG:CZ	2.45	0.47
1:C:236:ASN:O	1:C:239:ALA:HB3	2.15	0.46
1:C:368:LEU:C	1:C:370:GLU:H	2.23	0.46
1:A:119:GLY:O	1:A:122:SER:OG	2.29	0.46
1:A:257:GLU:H	1:A:257:GLU:HG2	1.43	0.46
2:D:84:ASP:OD1	2:D:84:ASP:N	2.49	0.46
1:A:253:SER:CB	1:A:280:ASP:HB2	2.36	0.46
2:D:102:GLU:OE2	2:D:102:GLU:HA	2.16	0.46
1:C:194:ARG:O	1:C:195:VAL:C	2.58	0.46
1:C:362:PRO:HG3	1:C:382:ILE:O	2.16	0.46
1:A:136:CYS:SG	1:A:139:TRP:CD1	3.09	0.46
2:D:111:ASP:OD1	2:D:111:ASP:O	2.33	0.46
2:B:84:ASP:OD1	2:B:84:ASP:N	2.48	0.46
1:C:283:GLU:HB3	1:C:287:GLN:NE2	2.31	0.46
1:C:307:LYS:HD2	1:C:307:LYS:C	2.41	0.45
1:A:330:SER:O	1:A:331:ASP:HB2	2.15	0.45
2:B:4:ILE:CD1	2:B:5:LYS:H	2.27	0.45
1:A:230:LEU:HD22	1:A:234:ILE:HD13	1.98	0.45
2:D:5:LYS:HG2	2:D:15:GLU:HG2	1.99	0.45
2:B:126:MET:O	2:B:130:LYS:HE2	2.17	0.45
1:C:312:SER:O	1:C:315:SER:HB2	2.16	0.45
1:C:331:ASP:OD2	1:C:356:ARG:NH1	2.49	0.45
1:A:274:ASN:C	1:A:274:ASN:ND2	2.73	0.45
2:B:25:VAL:O	2:B:28:LYS:HB3	2.17	0.45
2:B:133:GLU:HA	2:B:136:ARG:NH1	2.31	0.45
1:C:140:TYR:CE2	1:C:209:THR:HG22	2.52	0.45
1:C:371:ILE:HA	1:C:372:PRO:HD2	1.75	0.45
1:A:353:SER:OG	1:A:378:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HB3	1:A:198:MET:HA	1.98	0.45
2:B:24:SER:O	2:B:25:VAL:C	2.60	0.45
2:D:133:GLU:HA	2:D:136:ARG:HH11	1.81	0.45
2:D:85:ILE:HG22	2:D:90:GLN:HG3	1.98	0.44
1:A:278:CYS:HB2	1:A:281:PHE:CE2	2.53	0.44
1:A:387:THR:HA	1:A:390:LEU:HD12	1.99	0.44
1:A:140:TYR:C	1:A:140:TYR:CD1	2.95	0.44
1:A:371:ILE:HA	1:A:372:PRO:HD2	1.72	0.44
1:A:197:HIS:C	1:A:198:MET:HG2	2.40	0.44
2:B:27:ILE:O	2:B:31:LEU:HG	2.18	0.44
1:C:207:VAL:HG13	1:C:208:SER:N	2.32	0.44
2:D:66:LYS:HE3	2:D:67:ASP:OD2	2.18	0.44
2:D:113:LYS:O	2:D:117:ASP:HB2	2.17	0.44
1:C:293:VAL:HG11	1:C:297:ILE:HG13	2.00	0.44
1:A:281:PHE:HB2	1:A:285:HIS:CE1	2.51	0.43
1:A:307:LYS:HE2	1:A:308:ASN:HD21	1.83	0.43
1:A:344:PHE:HE2	1:A:370:GLU:HB3	1.83	0.43
1:A:361:ILE:O	1:A:362:PRO:C	2.60	0.43
2:B:5:LYS:CG	2:B:15:GLU:HG2	2.48	0.43
2:B:111:ASP:OD1	2:B:111:ASP:O	2.36	0.43
2:B:4:ILE:HD13	2:B:5:LYS:N	2.30	0.43
1:C:152:LEU:HD22	1:C:192:GLU:O	2.18	0.43
1:A:116:LEU:O	1:A:120:ILE:HG13	2.18	0.43
2:B:65:HIS:O	2:B:68:ASP:OD1	2.36	0.43
2:B:26:THR:O	2:B:29:THR:HG23	2.19	0.43
2:B:130:LYS:HB3	2:B:134:GLU:HB3	1.99	0.43
1:A:232:ASP:N	1:A:233:PRO:CD	2.82	0.43
1:C:281:PHE:HB2	1:C:285:HIS:CE1	2.54	0.43
1:C:231:SER:OG	1:C:233:PRO:HD2	2.18	0.43
2:D:130:LYS:HB3	2:D:134:GLU:CB	2.48	0.43
1:A:230:LEU:HB3	1:A:234:ILE:HG21	2.00	0.43
1:A:309:LEU:CD1	1:A:313:ASP:HB2	2.48	0.43
1:C:230:LEU:HB3	1:C:234:ILE:HG21	2.01	0.43
2:D:132:PRO:O	2:D:135:ILE:HB	2.18	0.43
1:A:198:MET:C	1:A:200:LEU:N	2.73	0.43
1:A:289:ALA:O	1:A:293:VAL:CG2	2.61	0.43
1:A:153:ASP:HA	1:A:220:LEU:HA	2.01	0.42
1:A:193:PHE:C	1:A:193:PHE:CD2	2.96	0.42
1:A:258:PHE:O	1:A:262:THR:HG22	2.19	0.42
1:C:272:GLU:HB3	1:C:299:GLN:HB2	2.00	0.42
1:C:232:ASP:N	1:C:233:PRO:CD	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PHE:CD1	1:A:279:PHE:C	2.98	0.42
2:D:5:LYS:HG2	2:D:15:GLU:HG3	2.01	0.42
1:A:130:LEU:HD21	1:A:213:ILE:HD12	2.02	0.42
1:A:283:GLU:HB3	1:A:287:GLN:NE2	2.34	0.42
1:A:368:LEU:C	1:A:370:GLU:H	2.27	0.42
1:A:356:ARG:HH11	1:A:356:ARG:HB2	1.84	0.42
1:A:196:GLN:H	1:A:196:GLN:HG3	1.55	0.42
1:A:271:ASP:C	1:A:297:ILE:HD13	2.45	0.42
1:C:269:ARG:NH1	1:C:269:ARG:CB	2.83	0.42
1:A:231:SER:HA	1:A:254:GLY:O	2.20	0.42
1:C:232:ASP:O	1:C:233:PRO:C	2.61	0.42
2:D:114:GLY:O	2:D:117:ASP:HB3	2.19	0.42
1:C:279:PHE:CD1	1:C:280:ASP:N	2.88	0.42
1:C:286:VAL:CG1	1:C:309:LEU:HD13	2.50	0.42
1:A:395:LEU:CD1	1:A:398:LEU:HD12	2.50	0.41
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.87	0.41
1:C:220:LEU:N	1:C:241:ASN:HD22	1.96	0.41
1:A:332:SER:HB2	1:A:335:LEU:HD12	2.02	0.41
2:D:133:GLU:O	2:D:137:LYS:HG3	2.20	0.41
1:C:383:VAL:HA	1:C:384:PRO:HD3	1.87	0.41
2:D:27:ILE:O	2:D:31:LEU:HG	2.20	0.41
1:A:146:GLU:HG2	1:A:150:GLN:NE2	2.36	0.41
1:A:383:VAL:HG12	1:A:388:LEU:HB2	2.02	0.41
2:D:104:ILE:HG13	2:D:119:THR:HB	2.02	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.83	0.41
1:A:131:LYS:HE3	1:A:131:LYS:HB2	1.83	0.41
2:B:66:LYS:HE3	2:B:67:ASP:OD2	2.21	0.41
1:C:223:LEU:HD11	1:C:225:LEU:HD21	2.02	0.41
1:C:274:ASN:C	1:C:274:ASN:ND2	2.76	0.41
1:C:361:ILE:O	1:C:362:PRO:C	2.63	0.41
1:C:116:LEU:O	1:C:120:ILE:HG13	2.21	0.41
1:C:195:VAL:O	1:C:196:GLN:C	2.62	0.41
1:C:109:TRP:C	1:C:111:SER:H	2.29	0.41
1:A:109:TRP:C	1:A:111:SER:H	2.29	0.41
2:B:31:LEU:HD21	2:B:45:VAL:HG21	2.03	0.41
2:B:132:PRO:O	2:B:135:ILE:HB	2.20	0.41
1:C:126:LEU:HD13	1:C:152:LEU:HD11	2.02	0.41
2:D:133:GLU:OE2	2:D:136:ARG:NH1	2.53	0.41
1:A:130:LEU:CD2	1:A:213:ILE:HD12	2.51	0.41
2:B:55:LEU:O	2:B:59:ILE:HG13	2.21	0.41
1:C:198:MET:C	1:C:200:LEU:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:VAL:O	1:C:333:VAL:CG1	2.69	0.41
1:C:369:GLY:HA3	1:C:395:LEU:HD13	2.03	0.41
1:A:307:LYS:HD2	1:A:308:ASN:CG	2.46	0.40
1:A:379:VAL:CG2	1:A:382:ILE:HD11	2.44	0.40
1:A:269:ARG:NH1	1:A:269:ARG:CB	2.83	0.40
1:A:310:GLN:O	1:A:311:LYS:C	2.64	0.40
1:A:320:ARG:O	1:A:322:PRO:HD2	2.21	0.40
1:A:368:LEU:C	1:A:370:GLU:N	2.79	0.40
1:C:258:PHE:O	1:C:262:THR:CG2	2.70	0.40
1:C:368:LEU:C	1:C:370:GLU:N	2.77	0.40
2:D:8:SER:OG	2:D:10:ASP:OD2	2.25	0.40
2:D:93:LEU:HD23	2:D:93:LEU:HA	1.90	0.40
2:B:24:SER:HA	2:B:112:ILE:HG12	2.04	0.40
2:B:57:LYS:O	2:B:58:VAL:C	2.64	0.40
1:C:309:LEU:HD12	1:C:313:ASP:CB	2.51	0.40
1:A:195:VAL:O	1:A:196:GLN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	257/272 (94%)	230 (90%)	24 (9%)	3 (1%)	10	34
1	C	257/272 (94%)	230 (90%)	21 (8%)	6 (2%)	5	19
2	B	124/141 (88%)	113 (91%)	8 (6%)	3 (2%)	4	18
2	D	124/141 (88%)	112 (90%)	9 (7%)	3 (2%)	4	18
All	All	762/826 (92%)	685 (90%)	62 (8%)	15 (2%)	6	22

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	ASP
2	B	82	THR
2	D	82	THR
2	B	35	GLY
1	C	241	ASN
1	C	358	TYR
2	D	35	GLY
1	A	150	GLN
1	A	241	ASN
2	B	81	ARG
1	C	150	GLN
2	D	81	ARG
1	C	199	ASP
1	C	200	LEU
1	C	195	VAL

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	236/254 (93%)	227 (96%)	9 (4%)	29	64
1	C	233/254 (92%)	220 (94%)	13 (6%)	19	50
2	B	113/130 (87%)	104 (92%)	9 (8%)	11	34
2	D	113/130 (87%)	104 (92%)	9 (8%)	11	34
All	All	695/768 (90%)	655 (94%)	40 (6%)	18	49

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ILE
1	A	262	THR
1	A	268	SER
1	A	296	THR
1	A	297	ILE
1	A	307	LYS
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	342	GLU
1	A	362	PRO
2	B	4	ILE
2	B	29	THR
2	B	33	ASP
2	B	36	MET
2	B	55	LEU
2	B	68	ASP
2	B	104	ILE
2	B	134	GLU
2	B	144	ASP
1	C	110	ASP
1	C	151	THR
1	C	205	ILE
1	C	256	SER
1	C	262	THR
1	C	268	SER
1	C	296	THR
1	C	297	ILE
1	C	307	LYS
1	C	311	LYS
1	C	342	GLU
1	C	362	PRO
1	C	373	THR
2	D	4	ILE
2	D	29	THR
2	D	33	ASP
2	D	36	MET
2	D	55	LEU
2	D	68	ASP
2	D	104	ILE
2	D	134	GLU
2	D	144	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	197	HIS
1	A	211	HIS
1	A	236	ASN
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	243	ASN
1	A	261	GLN
1	A	274	ASN
1	A	287	GLN
1	A	401	ASN
2	B	7	GLN
2	B	64	HIS
2	B	65	HIS
2	B	125	ASN
1	C	150	GLN
1	C	211	HIS
1	C	216	GLN
1	C	236	ASN
1	C	241	ASN
1	C	243	ASN
1	C	261	GLN
1	C	274	ASN
1	C	287	GLN
1	C	401	ASN
2	D	7	GLN
2	D	64	HIS

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](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.