



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:51 AM UTC

PDB ID : 1F80 / pdb_00001f80
Title : HOLO-(ACYL CARRIER PROTEIN) SYNTHASE IN COMPLEX WITH
HOLO-(ACYL CARRIER PROTEIN)
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Deposited on : 2000-06-28
Resolution : 2.30 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)	:	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

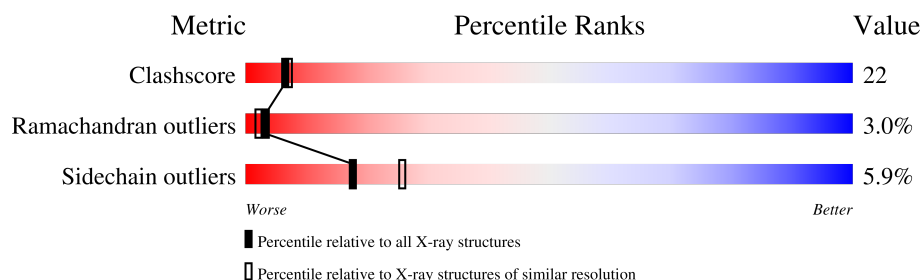
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	120	67% 28% . .
1	B	120	76% 20% . .
1	C	120	62% 29% 5% . .
2	D	81	41% 42% 7% . 9%
2	E	81	46% 40% . . 9%
2	F	81	47% 36% 7% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4543 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 HOLO-(ACYL CARRIER PROTEIN) SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			908	577	159	170	2			
1	B	118	Total	C	N	O	S	0	0	0
			892	565	156	169	2			
1	C	116	Total	C	N	O	S	0	0	0
			879	559	150	168	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	ILE	engineered mutation	UNP P96618
B	2	ALA	ILE	engineered mutation	UNP P96618
C	2	ALA	ILE	engineered mutation	UNP P96618

- Molecule 2 is a protein called ACYL CARRIER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	74	Total	C	N	O	P	S	0	0
			584	359	87	134	1	3		
2	E	74	Total	C	N	O	P	S	0	0
			590	362	88	136	1	3		
2	F	73	Total	C	N	O	P	S	0	0
			565	347	84	131	1	2		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	see remark 999	UNP P80643
D	-3	PRO	-	see remark 999	UNP P80643
D	-2	LEU	-	see remark 999	UNP P80643
D	-1	GLY	-	see remark 999	UNP P80643
D	0	SER	-	see remark 999	UNP P80643

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	see remark 999	UNP P80643
E	-3	PRO	-	see remark 999	UNP P80643
E	-2	LEU	-	see remark 999	UNP P80643
E	-1	GLY	-	see remark 999	UNP P80643
E	0	SER	-	see remark 999	UNP P80643
F	-4	GLY	-	see remark 999	UNP P80643
F	-3	PRO	-	see remark 999	UNP P80643
F	-2	LEU	-	see remark 999	UNP P80643
F	-1	GLY	-	see remark 999	UNP P80643
F	0	SER	-	see remark 999	UNP P80643

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	35	Total O 35 35	0	0
4	C	26	Total O 26 26	0	0
4	D	7	Total O 7 7	0	0
4	E	2	Total O 2 2	0	0
4	F	7	Total O 7 7	0	0

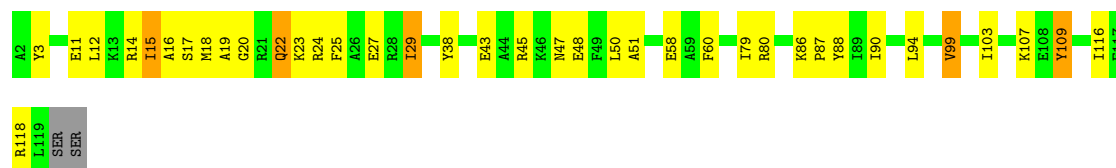
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain A: 



• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain B: 



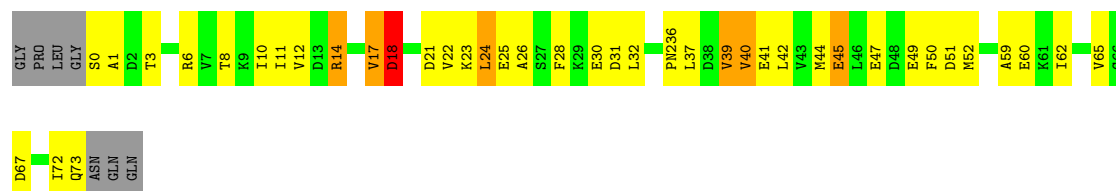
• Molecule 1: HOLO-(ACYL CARRIER PROTEIN) SYNTHASE

Chain C: 



• Molecule 2: ACYL CARRIER PROTEIN

Chain D: 



• Molecule 2: ACYL CARRIER PROTEIN

N74	GLN		GLY	SER	A1	R6	V7	T8	K9	I10	I11	V12	L15	G16	V17	D18	E19	A20	D21	V22	K23	L24	E25	F28	K29	E30	D31	L32	D35	PIN236	V39	V40	V43	M44	E45	E53	I54	D58	A59	E60	K61	I62	A63	T64	V65	G66	D67	N70	O72
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Chain F: 47% 36% 7% 10%

ASN	GLN	GLN	GLN
GLY			
PRO			
LEU			
GLY			
SER			
A1			
D2			
E5			
R6			
V7			
I10			
I11			
V12			
D13			
R14			
V17			
D18			
E19			
A20			
D21			
A26			
E30			
PV236			
L37			
D38			
V39			
V40			
E41			
L42			
V43			
M44			
E45			
L46			
E47			
D48			
E49			
F50			
D51			
M52			
E53			
I54			
E57			
E60			
R61			
I62			
A63			
I64			
A68			
I72			
F73			

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.46 Å 122.03 Å 136.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.4 (50.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.222 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PN2

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	1.03	1/921 (0.1%)	1.30	6/1238 (0.5%)
1	B	1.02	0/905	1.27	4/1222 (0.3%)
1	C	0.82	0/892	1.19	7/1202 (0.6%)
2	D	0.75	0/558	1.23	4/754 (0.5%)
2	E	0.72	0/564	1.13	4/762 (0.5%)
2	F	0.61	0/556	1.06	4/751 (0.5%)
All	All	0.87	1/4396 (0.0%)	1.21	29/5929 (0.5%)

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	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ILE	CA-CB	6.50	1.62	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	ASP	N-CA-C	-9.73	101.40	113.18
2	D	1	ALA	N-CA-C	-9.37	101.54	113.72
1	A	22	GLN	O-C-N	-9.10	111.57	122.22
2	D	14	ARG	N-CA-C	8.02	119.93	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	62	ILE	N-CA-C	7.42	116.99	106.53
1	B	89	ILE	N-CA-C	7.36	119.08	108.48
1	A	109	TYR	N-CA-C	7.13	120.58	109.52
1	B	111	ALA	O-C-N	-6.90	114.75	123.24
2	F	30	GLU	N-CA-C	6.61	119.82	111.69
1	A	29	ILE	N-CA-C	6.42	118.38	111.58
2	D	30	GLU	N-CA-C	6.31	118.04	111.03
1	A	15	ILE	CB-CA-C	-6.28	103.83	112.24
1	C	20	GLY	N-CA-C	-6.25	107.13	115.32
1	A	43	GLU	N-CA-C	5.83	117.64	111.28
2	E	19	GLU	N-CA-C	-5.45	99.19	110.80
2	E	30	GLU	N-CA-C	5.43	117.00	111.14
2	F	14	ARG	N-CA-C	-5.39	107.07	113.97
1	C	108	GLU	CA-C-N	-5.38	113.41	122.29
1	C	108	GLU	C-N-CA	-5.38	113.41	122.29
1	B	74	PHE	N-CA-C	-5.36	105.60	111.82
2	F	47	GLU	N-CA-C	-5.27	105.54	111.28
1	A	90	ILE	N-CA-C	-5.27	100.80	108.17
2	E	73	GLN	N-CA-C	5.25	119.44	113.19
2	D	31	ASP	N-CA-C	5.22	118.81	112.23
1	C	16	ALA	N-CA-C	-5.21	105.21	112.45
1	C	41	LEU	N-CA-C	5.16	118.14	110.14
1	C	30	LEU	N-CA-C	5.13	118.43	110.17
1	B	23	LYS	N-CA-C	5.03	118.52	112.38
1	C	31	THR	N-CA-C	-5.01	102.59	110.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TYR	Sidechain
1	B	111	ALA	Mainchain

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	908	0	902	36	0
1	B	892	0	860	20	0
1	C	879	0	853	42	0
2	D	584	0	554	53	0
2	E	590	0	559	29	0
2	F	565	0	532	28	0
3	A	1	0	0	0	0
4	A	47	0	0	0	0
4	B	35	0	0	1	0
4	C	26	0	0	0	0
4	D	7	0	0	1	0
4	E	2	0	0	1	0
4	F	7	0	0	0	0
All	All	4543	0	4260	189	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 22.

All (189) 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:18:MET:HE1	2:D:37:LEU:HD22	1.26	1.09
2:E:62:ILE:HG22	2:E:67:ASP:HB3	1.45	0.98
1:C:106:THR:HG22	1:C:109:TYR:H	1.24	0.96
2:F:52:MET:HE1	2:F:72:ILE:HA	1.48	0.95
2:D:72:ILE:O	2:D:73:GLN:HG3	1.66	0.94
1:A:86:LYS:HD2	1:A:87:PRO:HD2	1.51	0.91
2:D:14:ARG:HD2	2:D:41:GLU:HG2	1.52	0.91
2:E:18:ASP:O	2:E:19:GLU:HB2	1.70	0.89
2:F:62:ILE:HG13	2:F:62:ILE:O	1.74	0.87
2:E:40:VAL:O	2:E:44:MET:HG3	1.76	0.86
1:A:94:LEU:HD21	1:A:99:VAL:HG22	1.58	0.85
2:D:14:ARG:CD	2:D:41:GLU:HG2	2.07	0.84
2:D:10:ILE:HG23	2:D:45:GLU:HG2	1.60	0.82
2:E:24:LEU:HD12	2:E:66:GLY:HA2	1.64	0.79
1:C:93:LYS:O	1:C:94:LEU:CB	2.30	0.78
1:A:15:ILE:O	1:A:18:MET:HG2	1.84	0.77
2:D:36:PN2:H72	2:D:60:GLU:HA	1.65	0.76
1:C:18:MET:O	1:C:22:GLN:HB2	1.85	0.76
1:B:18:MET:HE1	2:D:37:LEU:CD2	2.12	0.74
2:F:14:ARG:HD3	2:F:41:GLU:HG2	1.69	0.74
2:D:28:PHE:CD2	2:D:36:PN2:H31	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG13	1:A:116:ILE:HG12	1.70	0.74
2:D:50:PHE:CB	2:D:52:MET:HE3	2.17	0.74
1:B:18:MET:CE	2:D:37:LEU:HD22	2.13	0.74
1:C:106:THR:HG22	1:C:109:TYR:N	2.01	0.73
2:D:11:ILE:HG22	2:D:17:VAL:HG21	1.73	0.71
1:A:94:LEU:HD21	1:A:99:VAL:CG2	2.20	0.70
2:D:50:PHE:HB3	2:D:52:MET:HE3	1.73	0.70
1:C:25:PHE:N	2:F:44:MET:HE1	2.06	0.70
1:C:3:TYR:HD2	1:C:4:GLY:N	1.90	0.70
1:C:91:CYS:SG	1:C:93:LYS:HB2	2.32	0.69
2:D:8:THR:O	2:D:12:VAL:HG23	1.91	0.69
2:F:12:VAL:HG12	2:F:12:VAL:O	1.93	0.69
1:A:94:LEU:CD2	1:A:99:VAL:CG2	2.72	0.68
1:A:14:ARG:NH2	2:E:35:ASP:OD2	2.23	0.68
2:D:17:VAL:CG1	2:D:32:LEU:HB3	2.24	0.67
2:D:36:PN2:H472	2:D:62:ILE:HG13	1.79	0.65
2:D:0:SER:N	2:D:73:GLN:HE21	1.94	0.65
1:C:28:ARG:HH22	2:F:43:VAL:CG1	2.10	0.65
2:F:68:ALA:O	2:F:72:ILE:HG13	1.96	0.64
2:D:12:VAL:HG13	2:D:18:ASP:O	1.97	0.64
1:A:18:MET:HB2	1:A:22:GLN:HB2	1.79	0.64
1:B:28:ARG:HD2	2:D:44:MET:HE3	1.80	0.64
1:C:93:LYS:O	1:C:94:LEU:HB2	1.97	0.63
1:C:53:ARG:O	1:C:57:LYS:HG3	1.98	0.63
2:F:43:VAL:HG13	2:F:54:ILE:HD12	1.80	0.63
1:C:3:TYR:CD2	1:C:116:ILE:O	2.53	0.62
1:C:18:MET:HB2	1:C:22:GLN:HB2	1.81	0.62
1:A:22:GLN:NE2	1:A:47:ASN:OD1	2.32	0.62
1:A:24:ARG:HD3	4:E:80:HOH:O	1.99	0.61
2:F:57:GLU:O	2:F:60:GLU:HG2	1.99	0.61
1:A:94:LEU:CD2	1:A:99:VAL:HG21	2.31	0.61
1:C:36:ASP:O	1:C:40:GLU:HG2	2.01	0.61
2:D:12:VAL:HA	2:D:17:VAL:CG2	2.31	0.61
1:A:103:ILE:O	1:C:62:LYS:NZ	2.33	0.60
2:F:26:ALA:O	2:F:64:THR:HB	2.00	0.60
1:A:11:GLU:HG2	1:A:109:TYR:HE1	1.65	0.60
2:F:14:ARG:HD2	2:F:45:GLU:OE1	2.02	0.60
2:E:36:PN2:O	2:E:39:VAL:HG12	2.03	0.59
1:B:31:THR:O	1:B:35:LEU:HB2	2.01	0.59
1:C:38:TYR:CE2	1:C:46:LYS:HG2	2.36	0.59
2:E:24:LEU:HD12	2:E:66:GLY:CA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:TYR:CD2	1:C:3:TYR:C	2.80	0.58
1:B:79:ILE:HD12	1:B:79:ILE:N	2.18	0.58
1:A:12:LEU:HD12	1:A:107:LYS:O	2.03	0.58
1:B:118:ARG:O	1:B:119:LEU:HB3	2.02	0.58
2:D:6:ARG:HD2	2:D:49:GLU:OE2	2.03	0.57
2:D:26:ALA:O	2:D:65:VAL:HG23	2.05	0.57
1:C:91:CYS:O	1:C:93:LYS:N	2.35	0.57
1:B:22:GLN:HG3	4:B:150:HOH:O	2.05	0.57
1:C:54:PHE:CZ	2:F:37:LEU:HD23	2.39	0.57
2:D:62:ILE:HA	2:D:67:ASP:HB3	1.86	0.57
1:A:11:GLU:HG2	1:A:109:TYR:CE1	2.40	0.56
2:E:70:ASN:O	2:E:74:ASN:ND2	2.38	0.56
2:E:8:THR:HG23	2:E:22:VAL:HG21	1.85	0.56
1:C:93:LYS:O	1:C:94:LEU:HB3	2.05	0.56
1:A:3:TYR:OH	1:A:118:ARG:HA	2.05	0.55
2:E:28:PHE:HA	2:E:32:LEU:HD12	1.88	0.55
2:E:19:GLU:O	2:E:21:ASP:N	2.40	0.55
1:C:24:ARG:C	2:F:44:MET:HE1	2.33	0.54
1:C:106:THR:CG2	1:C:109:TYR:H	2.10	0.54
2:E:19:GLU:C	2:E:21:ASP:N	2.63	0.54
2:F:36:PN2:C	2:F:39:VAL:HG12	2.38	0.54
1:A:18:MET:O	1:A:20:GLY:N	2.40	0.54
1:C:3:TYR:HD2	1:C:3:TYR:C	2.15	0.54
2:F:50:PHE:CE2	2:F:72:ILE:HD13	2.42	0.54
2:F:36:PN2:O	2:F:39:VAL:HG12	2.07	0.54
1:C:3:TYR:HA	1:C:116:ILE:O	2.09	0.53
2:E:19:GLU:C	2:E:21:ASP:H	2.16	0.53
1:C:106:THR:HG23	1:C:107:LYS:N	2.23	0.52
1:A:3:TYR:CZ	1:A:118:ARG:HA	2.45	0.52
2:D:28:PHE:HD2	2:D:36:PN2:H31	1.73	0.52
1:A:18:MET:HB3	1:A:22:GLN:N	2.25	0.52
2:F:6:ARG:NH1	2:F:49:GLU:OE2	2.42	0.52
1:C:91:CYS:C	1:C:93:LYS:H	2.17	0.52
2:D:50:PHE:O	2:D:51:ASP:C	2.52	0.52
2:E:36:PN2:O39	2:E:60:GLU:HA	2.10	0.52
2:D:72:ILE:O	2:D:72:ILE:HG22	2.10	0.51
1:B:44:ALA:O	1:B:48:GLU:OE1	2.27	0.51
1:C:37:GLN:O	1:C:41:LEU:HG	2.11	0.51
1:B:76:ASP:HB3	1:B:92:THR:OG1	2.10	0.51
1:C:18:MET:HE1	1:C:25:PHE:CD1	2.45	0.51
2:D:24:LEU:HD12	2:D:24:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:VAL:O	2:D:44:MET:HG3	2.11	0.51
2:E:10:ILE:HG23	2:E:45:GLU:HG2	1.94	0.50
2:F:12:VAL:O	2:F:12:VAL:CG1	2.59	0.50
1:A:15:ILE:HG13	1:A:51:ALA:HB2	1.93	0.49
1:A:25:PHE:O	1:A:29:ILE:HG12	2.12	0.49
1:A:86:LYS:HD2	1:A:87:PRO:CD	2.35	0.49
1:A:107:LYS:HG2	1:C:11:GLU:OE2	2.12	0.49
2:D:50:PHE:HB2	2:D:52:MET:HE3	1.94	0.49
1:C:18:MET:O	1:C:19:ALA:O	2.31	0.49
1:C:28:ARG:HH22	2:F:43:VAL:HG11	1.77	0.49
2:E:18:ASP:O	2:E:19:GLU:CB	2.51	0.49
2:F:10:ILE:HG23	2:F:45:GLU:HG2	1.95	0.49
1:C:106:THR:HG23	1:C:108:GLU:H	1.78	0.48
2:F:19:GLU:C	2:F:21:ASP:N	2.70	0.48
2:F:36:PN2:O	2:F:40:VAL:HG13	2.14	0.48
2:D:14:ARG:HG3	2:D:45:GLU:OE2	2.14	0.48
2:E:58:ASP:O	2:E:62:ILE:HG12	2.14	0.48
2:D:14:ARG:CG	2:D:45:GLU:OE2	2.62	0.48
1:A:18:MET:CB	1:A:22:GLN:HB2	2.43	0.48
2:E:11:ILE:HG23	2:E:15:LEU:HD12	1.96	0.47
2:E:28:PHE:CD2	2:E:63:ALA:O	2.68	0.47
2:D:22:VAL:HG12	2:D:65:VAL:HG11	1.96	0.47
1:C:87:PRO:HG2	1:C:101:VAL:HG13	1.97	0.47
2:E:43:VAL:HG13	2:E:54:ILE:HD12	1.96	0.47
2:D:18:ASP:OD2	2:D:18:ASP:N	2.48	0.47
2:D:0:SER:N	2:D:73:GLN:NE2	2.62	0.46
1:A:45:ARG:NH1	1:A:48:GLU:OE1	2.49	0.46
1:B:24:ARG:NH2	2:D:47:GLU:OE1	2.46	0.46
1:C:28:ARG:NH2	2:F:43:VAL:HG12	2.30	0.46
2:D:36:PN2:C7	2:D:60:GLU:HA	2.40	0.46
2:D:36:PN2:HCB2	4:D:80:HOH:O	2.16	0.46
1:C:38:TYR:CD2	1:C:46:LYS:HG2	2.51	0.45
2:E:6:ARG:O	2:E:10:ILE:HG12	2.16	0.45
1:C:42:SER:OG	1:C:45:ARG:HG2	2.17	0.45
2:E:36:PN2:O39	2:E:36:PN2:H421	2.16	0.45
2:D:36:PN2:H472	2:D:62:ILE:O	2.17	0.45
2:E:17:VAL:O	2:E:19:GLU:N	2.49	0.45
2:E:19:GLU:OE1	2:E:20:ALA:N	2.35	0.45
1:B:31:THR:HA	1:B:75:GLN:HE22	1.82	0.45
2:F:14:ARG:HD3	2:F:41:GLU:CG	2.44	0.45
2:D:17:VAL:HG12	2:D:32:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:TYR:C	1:C:41:LEU:H	2.25	0.44
2:D:0:SER:HB2	2:D:3:THR:HG23	1.99	0.44
1:A:23:LYS:O	1:A:27:GLU:HG3	2.17	0.44
2:E:64:THR:O	2:E:67:ASP:HB2	2.18	0.44
1:B:80:ARG:NH1	1:B:90:ILE:HG13	2.33	0.44
2:D:36:PN2:C14	2:D:39:VAL:HG22	2.47	0.44
1:A:24:ARG:C	2:E:44:MET:HE1	2.42	0.44
1:C:94:LEU:C	1:C:94:LEU:CD1	2.91	0.44
2:D:36:PN2:H2	2:D:39:VAL:CG2	2.48	0.44
2:D:50:PHE:CE2	2:D:72:ILE:HD13	2.53	0.44
2:E:8:THR:O	2:E:12:VAL:HG23	2.18	0.44
1:A:15:ILE:HG21	1:A:50:LEU:HB3	2.00	0.43
1:A:94:LEU:HD23	1:A:99:VAL:HG21	2.00	0.43
2:D:6:ARG:O	2:D:10:ILE:HG13	2.19	0.43
2:D:36:PN2:H72	2:D:59:ALA:O	2.18	0.43
1:C:28:ARG:HH22	2:F:43:VAL:HG12	1.84	0.43
2:F:50:PHE:CD2	2:F:72:ILE:HD13	2.54	0.42
2:D:0:SER:H3	2:D:73:GLN:HE21	1.67	0.42
2:D:12:VAL:HA	2:D:17:VAL:HG23	2.00	0.42
2:D:14:ARG:HD3	2:D:41:GLU:HG2	1.99	0.42
1:B:79:ILE:N	1:B:79:ILE:CD1	2.82	0.42
1:C:91:CYS:C	1:C:93:LYS:N	2.77	0.42
2:D:52:MET:HE1	2:D:72:ILE:HG23	2.01	0.42
1:B:44:ALA:O	1:B:46:LYS:N	2.52	0.42
1:A:16:ALA:C	1:A:18:MET:H	2.26	0.42
1:B:18:MET:HG2	2:D:41:GLU:OE1	2.19	0.42
2:D:10:ILE:HD11	2:D:49:GLU:HG2	2.02	0.42
1:B:100:HIS:O	1:B:114:VAL:HA	2.20	0.42
2:D:23:LYS:O	2:D:25:GLU:N	2.53	0.41
2:F:52:MET:HE3	2:F:72:ILE:HG23	2.01	0.41
1:A:22:GLN:HG2	1:A:38:TYR:OH	2.20	0.41
1:C:15:ILE:CD1	1:C:51:ALA:HA	2.50	0.41
1:A:80:ARG:O	1:A:87:PRO:HA	2.20	0.41
1:A:107:LYS:HA	1:A:107:LYS:HD3	1.77	0.41
1:B:58:GLU:OE2	2:D:36:PN2:O7	2.39	0.41
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.88	0.41
2:D:24:LEU:H	2:D:24:LEU:CD1	2.34	0.41
1:B:44:ALA:C	1:B:46:LYS:N	2.79	0.41
1:A:60:PHE:CE1	1:A:116:ILE:HD11	2.56	0.41
1:C:39:TYR:O	1:C:41:LEU:N	2.53	0.41
1:A:58:GLU:OE2	2:E:36:PN2:O7	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:NH2	1:C:79:ILE:O	2.53	0.41
2:F:47:GLU:O	2:F:51:ASP:HA	2.21	0.41
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.59	0.40
2:E:61:LYS:O	2:E:61:LYS:HG2	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	116/120 (97%)	113 (97%)	1 (1%)	2 (2%)	7	7
1	B	116/120 (97%)	109 (94%)	6 (5%)	1 (1%)	14	17
1	C	114/120 (95%)	106 (93%)	3 (3%)	5 (4%)	2	1
2	D	71/81 (88%)	58 (82%)	10 (14%)	3 (4%)	2	1
2	E	71/81 (88%)	60 (84%)	8 (11%)	3 (4%)	2	1
2	F	70/81 (86%)	61 (87%)	6 (9%)	3 (4%)	2	1
All	All	558/603 (92%)	507 (91%)	34 (6%)	17 (3%)	3	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	19	ALA
1	C	95	SER
2	D	17	VAL
2	E	19	GLU
2	F	17	VAL
1	B	45	ARG
1	C	40	GLU
1	C	94	LEU

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Mol	Chain	Res	Type
2	D	24	LEU
2	E	18	ASP
1	A	17	SER
1	A	19	ALA
1	C	92	THR
2	E	20	ALA
2	F	18	ASP
2	D	18	ASP
2	F	62	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	89/97 (92%)	88 (99%)	1 (1%)	65	81
1	B	85/97 (88%)	82 (96%)	3 (4%)	32	48
1	C	85/97 (88%)	81 (95%)	4 (5%)	23	35
2	D	61/68 (90%)	55 (90%)	6 (10%)	7	10
2	E	62/68 (91%)	57 (92%)	5 (8%)	11	14
2	F	61/68 (90%)	54 (88%)	7 (12%)	5	6
All	All	443/495 (90%)	417 (94%)	26 (6%)	18	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	B	35	LEU
1	B	84	ASN
1	B	96	GLN
1	C	28	ARG
1	C	33	SER
1	C	94	LEU
1	C	106	THR
2	D	18	ASP

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Mol	Chain	Res	Type
2	D	21	ASP
2	D	39	VAL
2	D	40	VAL
2	D	42	LEU
2	D	45	GLU
2	E	19	GLU
2	E	25	GLU
2	E	45	GLU
2	E	53	GLU
2	E	62	ILE
2	F	5	GLU
2	F	7	VAL
2	F	37	LEU
2	F	40	VAL
2	F	42	LEU
2	F	45	GLU
2	F	48	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	84	ASN
1	A	96	GLN
1	A	113	GLN
1	B	22	GLN
1	B	47	ASN
1	B	75	GLN
1	B	96	GLN
1	B	113	GLN
1	C	47	ASN
1	C	84	ASN
1	C	100	HIS
1	C	113	GLN
2	D	70	ASN
2	D	73	GLN
2	E	73	GLN
2	E	74	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 1 ligands modelled in this entry, 1 is 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

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.