



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 AM UTC

PDB ID : 1XES / pdb_00001xes
Title : Crystal structure of stilbene synthase from *Pinus sylvestris*
Authors : Ng, S.H.; Chirgadze, D.; Spiteller, D.; Li, T.L.; Spencer, J.B.; Blundell, T.L.
Deposited on : 2004-09-12
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

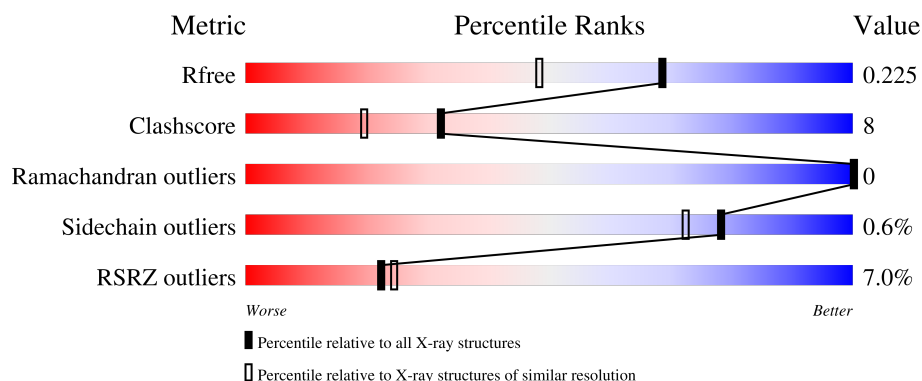
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	413	0% 77% 16% 6%
1	B	413	3% 81% 13% 6%
1	C	413	8% 74% 17% 8%
1	D	413	14% 73% 19% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12492 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 Dihydropinosylvin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2900	1847	497	539	17			
1	B	387	Total	C	N	O	S	0	0	0
			2896	1843	503	533	17			
1	C	378	Total	C	N	O	S	0	0	0
			2788	1779	478	514	17			
1	D	382	Total	C	N	O	S	0	0	0
			2771	1766	476	512	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q02323
A	-18	GLY	-	cloning artifact	UNP Q02323
A	-17	SER	-	cloning artifact	UNP Q02323
A	-16	SER	-	cloning artifact	UNP Q02323
A	-15	HIS	-	cloning artifact	UNP Q02323
A	-14	HIS	-	cloning artifact	UNP Q02323
A	-13	HIS	-	cloning artifact	UNP Q02323
A	-12	HIS	-	cloning artifact	UNP Q02323
A	-11	HIS	-	cloning artifact	UNP Q02323
A	-10	HIS	-	cloning artifact	UNP Q02323
A	-9	SER	-	cloning artifact	UNP Q02323
A	-8	SER	-	cloning artifact	UNP Q02323
A	-7	GLY	-	cloning artifact	UNP Q02323
A	-6	LEU	-	cloning artifact	UNP Q02323
A	-5	VAL	-	cloning artifact	UNP Q02323
A	-4	PRO	-	cloning artifact	UNP Q02323
A	-3	ARG	-	cloning artifact	UNP Q02323
A	-2	GLY	-	cloning artifact	UNP Q02323
A	-1	SER	-	cloning artifact	UNP Q02323
A	0	HIS	-	cloning artifact	UNP Q02323
B	-19	MET	-	cloning artifact	UNP Q02323

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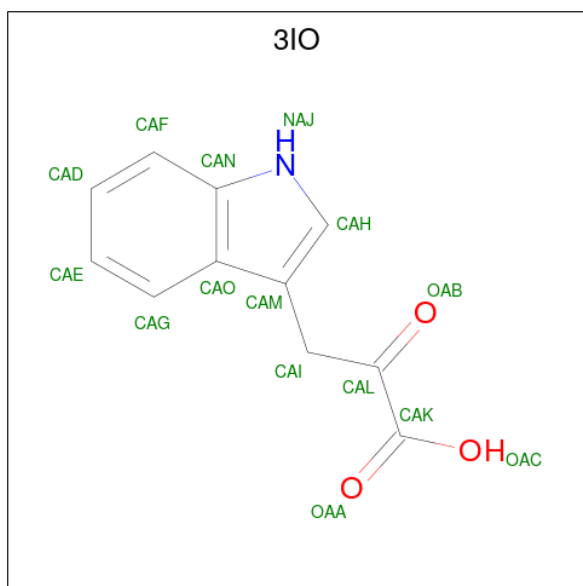
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	cloning artifact	UNP Q02323
B	-17	SER	-	cloning artifact	UNP Q02323
B	-16	SER	-	cloning artifact	UNP Q02323
B	-15	HIS	-	cloning artifact	UNP Q02323
B	-14	HIS	-	cloning artifact	UNP Q02323
B	-13	HIS	-	cloning artifact	UNP Q02323
B	-12	HIS	-	cloning artifact	UNP Q02323
B	-11	HIS	-	cloning artifact	UNP Q02323
B	-10	HIS	-	cloning artifact	UNP Q02323
B	-9	SER	-	cloning artifact	UNP Q02323
B	-8	SER	-	cloning artifact	UNP Q02323
B	-7	GLY	-	cloning artifact	UNP Q02323
B	-6	LEU	-	cloning artifact	UNP Q02323
B	-5	VAL	-	cloning artifact	UNP Q02323
B	-4	PRO	-	cloning artifact	UNP Q02323
B	-3	ARG	-	cloning artifact	UNP Q02323
B	-2	GLY	-	cloning artifact	UNP Q02323
B	-1	SER	-	cloning artifact	UNP Q02323
B	0	HIS	-	cloning artifact	UNP Q02323
C	-19	MET	-	cloning artifact	UNP Q02323
C	-18	GLY	-	cloning artifact	UNP Q02323
C	-17	SER	-	cloning artifact	UNP Q02323
C	-16	SER	-	cloning artifact	UNP Q02323
C	-15	HIS	-	cloning artifact	UNP Q02323
C	-14	HIS	-	cloning artifact	UNP Q02323
C	-13	HIS	-	cloning artifact	UNP Q02323
C	-12	HIS	-	cloning artifact	UNP Q02323
C	-11	HIS	-	cloning artifact	UNP Q02323
C	-10	HIS	-	cloning artifact	UNP Q02323
C	-9	SER	-	cloning artifact	UNP Q02323
C	-8	SER	-	cloning artifact	UNP Q02323
C	-7	GLY	-	cloning artifact	UNP Q02323
C	-6	LEU	-	cloning artifact	UNP Q02323
C	-5	VAL	-	cloning artifact	UNP Q02323
C	-4	PRO	-	cloning artifact	UNP Q02323
C	-3	ARG	-	cloning artifact	UNP Q02323
C	-2	GLY	-	cloning artifact	UNP Q02323
C	-1	SER	-	cloning artifact	UNP Q02323
C	0	HIS	-	cloning artifact	UNP Q02323
D	-19	MET	-	cloning artifact	UNP Q02323
D	-18	GLY	-	cloning artifact	UNP Q02323
D	-17	SER	-	cloning artifact	UNP Q02323

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	cloning artifact	UNP Q02323
D	-15	HIS	-	cloning artifact	UNP Q02323
D	-14	HIS	-	cloning artifact	UNP Q02323
D	-13	HIS	-	cloning artifact	UNP Q02323
D	-12	HIS	-	cloning artifact	UNP Q02323
D	-11	HIS	-	cloning artifact	UNP Q02323
D	-10	HIS	-	cloning artifact	UNP Q02323
D	-9	SER	-	cloning artifact	UNP Q02323
D	-8	SER	-	cloning artifact	UNP Q02323
D	-7	GLY	-	cloning artifact	UNP Q02323
D	-6	LEU	-	cloning artifact	UNP Q02323
D	-5	VAL	-	cloning artifact	UNP Q02323
D	-4	PRO	-	cloning artifact	UNP Q02323
D	-3	ARG	-	cloning artifact	UNP Q02323
D	-2	GLY	-	cloning artifact	UNP Q02323
D	-1	SER	-	cloning artifact	UNP Q02323
D	0	HIS	-	cloning artifact	UNP Q02323

- Molecule 2 is 3-(1H-INDOL-3-YL)-2-OXOPROPANOIC ACID (CCD ID: 3IO) (formula: $C_{11}H_9NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	11	1	3		
2	B	1	Total	C	N	O	0	0
			15	11	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	1	3		
2	D	1	Total	C	N	O	0	0
			15	11	1	3		

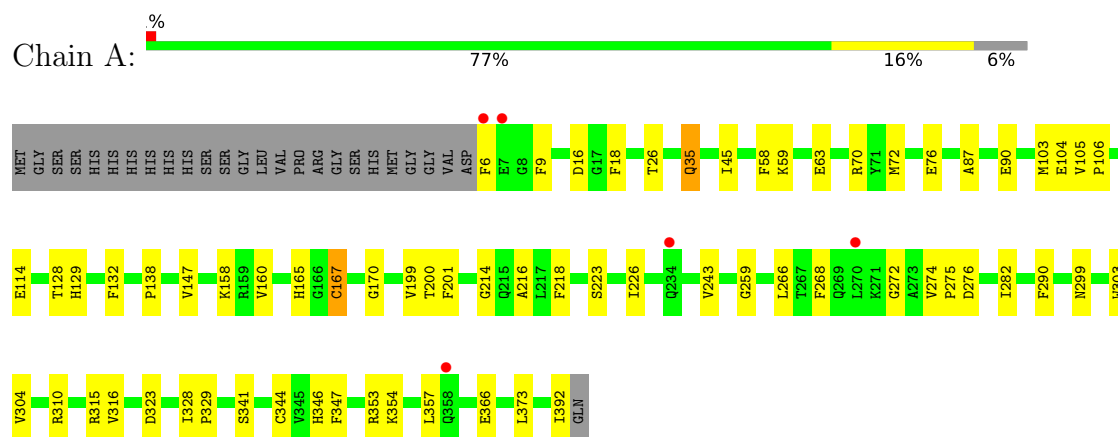
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total	O	0	0
			334	334		
3	B	324	Total	O	0	0
			324	324		
3	C	230	Total	O	0	0
			230	230		
3	D	189	Total	O	0	0
			189	189		

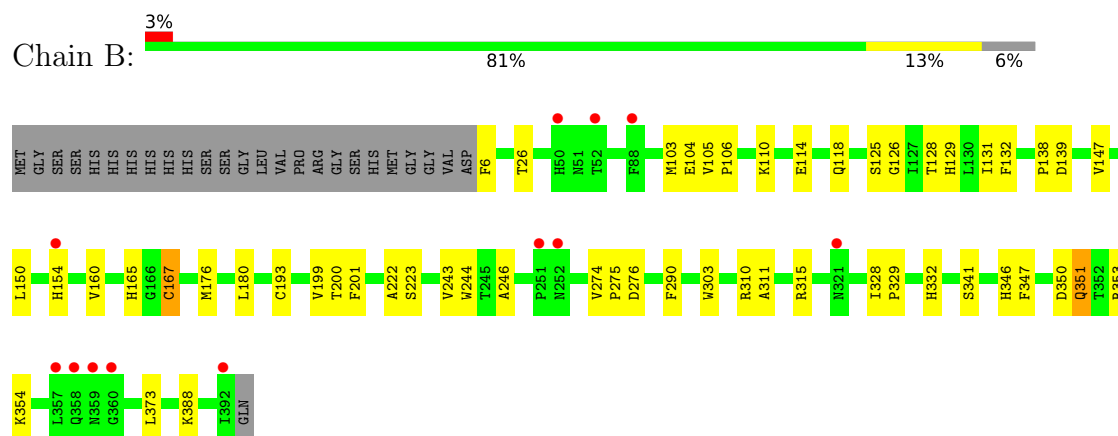
3 Residue-property plots [i](#)

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.

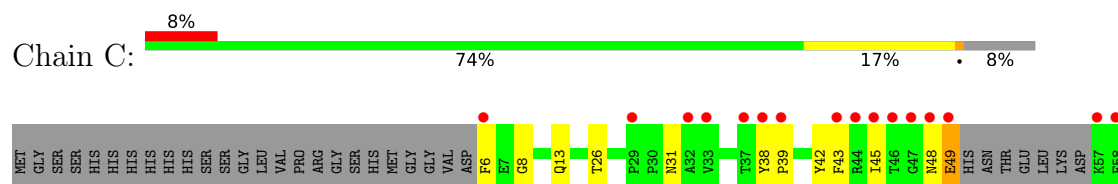
- Molecule 1: Dihydropinosylvin synthase

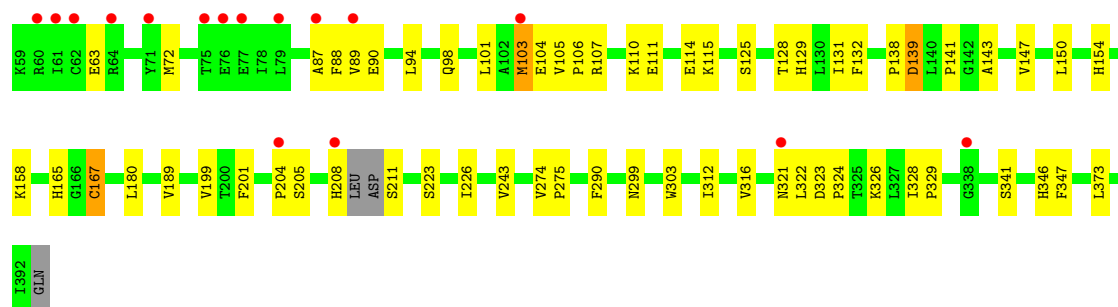


- Molecule 1: Dihydropinosylvin synthase

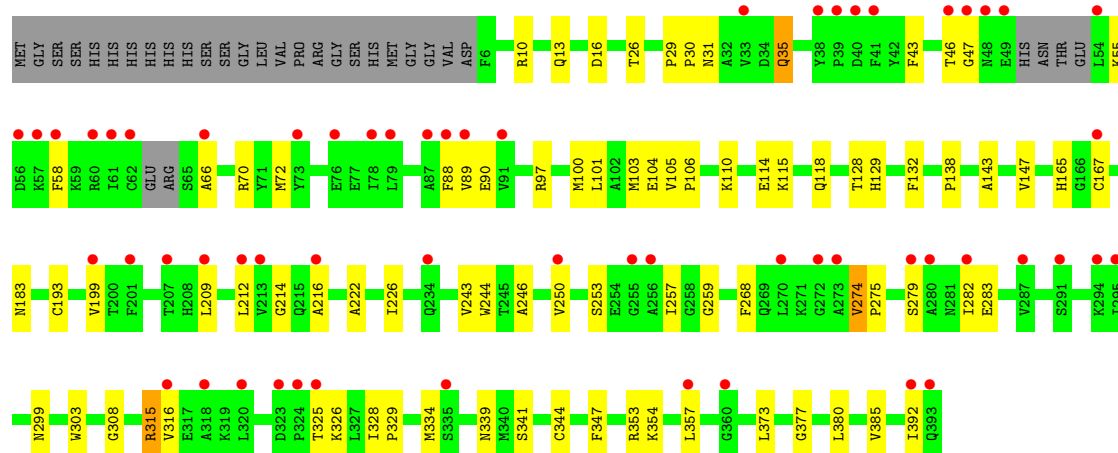
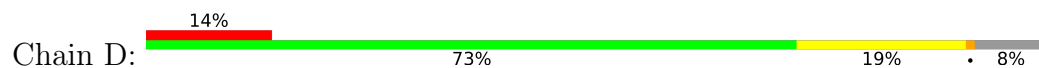


- Molecule 1: Dihydropinosylvin synthase





● Molecule 1: Dihydropinosylvin synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.37Å 111.37Å 131.69Å 90.00° 93.05° 90.00°	Depositor
Resolution (Å)	19.95 – 1.70 19.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.95-1.70) 99.7 (19.95-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.225 0.202 , 0.225	Depositor DCC
R_{free} test set	8585 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12492	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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: 3IO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/2960	0.90	12/4021 (0.3%)
1	B	0.36	0/2955	0.91	8/4013 (0.2%)
1	C	0.35	0/2844	0.90	12/3867 (0.3%)
1	D	0.34	0/2826	0.88	10/3849 (0.3%)
All	All	0.36	0/11585	0.90	42/15750 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	243	VAL	N-CA-C	8.71	119.26	110.82
1	B	243	VAL	N-CA-C	8.46	119.03	110.82
1	D	243	VAL	N-CA-C	8.45	119.02	110.82
1	A	243	VAL	N-CA-C	8.34	118.91	110.82
1	A	165	HIS	N-CA-C	-7.40	102.84	112.68
1	B	104	GLU	N-CA-C	7.30	119.32	111.36
1	B	138	PRO	N-CA-C	7.18	122.98	113.57
1	A	104	GLU	N-CA-C	6.67	118.63	111.36
1	C	321	ASN	CB-CA-C	6.55	121.20	111.89
1	B	165	HIS	N-CA-C	-6.54	103.99	112.68
1	C	104	GLU	N-CA-C	6.47	118.13	111.14
1	A	138	PRO	N-CA-C	6.46	122.03	113.57
1	C	303	TRP	N-CA-C	6.32	119.71	109.40
1	C	290	PHE	N-CA-C	6.28	121.11	113.38
1	B	167	CYS	N-CA-C	6.27	120.03	112.38
1	A	226	ILE	N-CA-C	-6.19	98.71	107.75
1	D	165	HIS	N-CA-C	-6.16	105.42	113.12
1	D	104	GLU	N-CA-C	6.07	117.69	111.14
1	D	303	TRP	N-CA-C	6.07	119.43	109.72
1	D	344	CYS	N-CA-C	6.03	118.38	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	PHE	N-CA-C	5.94	120.68	113.38
1	C	138	PRO	N-CA-C	5.92	121.34	113.40
1	C	165	HIS	N-CA-C	-5.91	103.53	112.04
1	A	290	PHE	N-CA-C	5.87	120.60	113.38
1	B	303	TRP	N-CA-C	5.81	119.01	109.72
1	D	138	PRO	N-CA-C	5.70	121.04	113.57
1	B	341	SER	CB-CA-C	-5.69	110.03	116.63
1	C	324	PRO	N-CA-CB	5.67	109.20	103.25
1	A	303	TRP	N-CA-C	5.54	118.59	109.72
1	A	167	CYS	N-CA-C	5.53	119.13	112.38
1	C	167	CYS	N-CA-C	5.50	119.08	112.38
1	C	189	VAL	N-CA-C	5.45	116.15	108.36
1	D	341	SER	CB-CA-C	-5.44	110.32	116.63
1	C	341	SER	CB-CA-C	-5.39	110.34	116.54
1	A	341	SER	CB-CA-C	-5.31	110.44	116.54
1	A	16	ASP	N-CA-C	5.26	119.61	112.04
1	C	226	ILE	N-CA-C	-5.17	100.21	107.75
1	D	226	ILE	N-CA-C	-5.15	100.23	107.75
1	D	16	ASP	N-CA-C	5.10	119.39	112.04
1	A	344	CYS	N-CA-C	5.04	117.17	111.02
1	A	170	GLY	N-CA-C	-5.04	106.62	113.37
1	D	274	VAL	CB-CA-C	-5.00	108.95	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2900	0	2866	44	0
1	B	2896	0	2870	35	0
1	C	2788	0	2727	49	0
1	D	2771	0	2666	56	0
2	A	15	0	8	2	0
2	B	15	0	8	3	0
2	C	15	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	8	1	0
3	A	334	0	0	7	0
3	B	324	0	0	6	0
3	C	230	0	0	8	0
3	D	189	0	0	3	0
All	All	12492	0	11161	180	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 8.

All (180) 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:167:CYS:SG	2:B:3000:3IO:CAL	2.60	0.89
1:A:167:CYS:SG	2:A:2000:3IO:CAL	2.63	0.87
1:D:46:THR:OG1	1:D:47:GLY:HA3	1.74	0.86
1:D:315:ARG:HH21	1:D:315:ARG:HB2	1.43	0.82
1:D:315:ARG:HB2	1:D:315:ARG:NH2	1.96	0.80
1:C:167:CYS:SG	2:C:4000:3IO:CAL	2.71	0.78
1:A:310:ARG:NH1	1:A:310:ARG:HB3	2.02	0.75
1:D:35:GLN:HA	1:D:35:GLN:HE21	1.49	0.75
1:A:35:GLN:HE21	1:A:35:GLN:HA	1.51	0.74
1:D:167:CYS:SG	2:D:5000:3IO:CAL	2.77	0.73
1:D:250:VAL:HG22	1:D:380:LEU:HB3	1.72	0.70
1:D:97:ARG:HA	1:D:100:MET:HE2	1.74	0.68
1:A:299:ASN:HD21	1:A:323:ASP:H	1.42	0.67
1:A:366:GLU:HG3	3:A:2276:HOH:O	1.92	0.67
1:B:276:ASP:OD2	1:B:315:ARG:NH1	2.28	0.66
1:C:299:ASN:HD21	1:C:323:ASP:H	1.41	0.66
1:D:250:VAL:CG2	1:D:380:LEU:HB3	2.27	0.65
1:A:158:LYS:HE3	1:B:246:ALA:HA	1.80	0.64
1:C:105:VAL:HB	1:C:106:PRO:HD3	1.80	0.64
1:D:328:ILE:HB	1:D:329:PRO:HD3	1.79	0.64
1:C:110:LYS:O	1:C:114:GLU:HG3	1.98	0.63
1:A:310:ARG:HB3	1:A:310:ARG:HH11	1.61	0.63
1:D:35:GLN:HE22	1:D:70:ARG:HH11	1.48	0.62
1:C:107:ARG:O	1:C:111:GLU:HG3	2.01	0.61
1:A:128:THR:OG1	1:A:129:HIS:HD2	1.83	0.60
1:A:35:GLN:HE22	1:A:70:ARG:HH21	1.47	0.60
1:D:282:ILE:HD13	1:D:316:VAL:HG13	1.83	0.60
1:D:105:VAL:HB	1:D:106:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ARG:HH21	1:D:315:ARG:CB	2.11	0.60
1:D:299:ASN:HA	1:D:326:LYS:HE3	1.84	0.60
1:A:357:LEU:HD23	1:A:392:ILE:HD13	1.84	0.59
1:C:132:PHE:CE2	1:C:147:VAL:HG21	2.36	0.59
1:A:199:VAL:HG13	1:A:200:THR:HG23	1.84	0.59
1:D:357:LEU:HD23	1:D:392:ILE:HD13	1.85	0.59
1:D:132:PHE:CE2	1:D:147:VAL:HG21	2.37	0.59
1:D:46:THR:CB	1:D:47:GLY:CA	2.80	0.58
1:A:18:PHE:HE2	1:B:6:PHE:HB3	1.68	0.58
1:D:97:ARG:HA	1:D:100:MET:CE	2.33	0.58
1:D:46:THR:CB	1:D:47:GLY:HA3	2.34	0.57
1:B:105:VAL:HB	1:B:106:PRO:HD3	1.85	0.57
1:D:377:GLY:O	1:D:380:LEU:HD12	2.05	0.57
1:B:128:THR:OG1	1:B:129:HIS:HD2	1.87	0.57
1:A:59:LYS:HG2	1:A:63:GLU:OE2	2.04	0.57
1:C:274:VAL:HB	1:C:275:PRO:HD3	1.86	0.56
1:C:328:ILE:HB	1:C:329:PRO:HD3	1.87	0.56
1:A:105:VAL:HB	1:A:106:PRO:HD3	1.88	0.56
1:B:160:VAL:HG23	3:B:3225:HOH:O	2.06	0.56
1:C:139:ASP:HB3	1:D:259:GLY:O	2.07	0.54
1:D:274:VAL:HB	1:D:275:PRO:HD3	1.88	0.54
1:B:125:SER:HB2	1:B:154:HIS:NE2	2.22	0.54
1:C:128:THR:OG1	1:C:129:HIS:HD2	1.89	0.54
1:A:114:GLU:HG3	3:A:2286:HOH:O	2.08	0.54
1:A:167:CYS:SG	2:A:2000:3IO:CAK	2.96	0.54
1:B:353:ARG:HG3	1:B:354:LYS:N	2.22	0.53
1:C:87:ALA:HB1	1:C:90:GLU:OE2	2.08	0.53
1:B:167:CYS:SG	2:B:3000:3IO:CAK	2.97	0.53
1:C:180:LEU:HD21	3:C:4084:HOH:O	2.07	0.53
1:A:158:LYS:HE2	3:B:3205:HOH:O	2.08	0.52
1:C:110:LYS:HD2	1:C:150:LEU:HB3	1.90	0.52
1:C:299:ASN:ND2	1:C:323:ASP:H	2.06	0.52
1:A:282:ILE:HD13	1:A:316:VAL:HG13	1.91	0.52
1:D:250:VAL:HG23	1:D:253:SER:OG	2.10	0.52
1:D:101:LEU:HD11	1:D:199:VAL:HB	1.92	0.52
1:A:87:ALA:HB1	1:A:90:GLU:CD	2.34	0.52
1:C:103:MET:HE1	3:C:4168:HOH:O	2.10	0.52
1:B:328:ILE:HB	1:B:329:PRO:HD3	1.91	0.51
1:B:114:GLU:O	1:B:118:GLN:HG3	2.10	0.51
1:C:42:TYR:O	1:C:45:ILE:HG22	2.11	0.51
1:A:35:GLN:HE22	1:A:70:ARG:NH2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD1	1:A:315:ARG:NH2	2.33	0.50
1:A:328:ILE:HB	1:A:329:PRO:HD3	1.93	0.50
1:A:274:VAL:HB	1:A:275:PRO:HD3	1.92	0.50
1:C:48:ASN:O	1:C:49:GLU:HG3	2.10	0.50
1:D:66:ALA:HB3	1:D:334:MET:HE3	1.93	0.50
3:C:4090:HOH:O	1:D:129:HIS:HE1	1.94	0.50
1:A:132:PHE:CE2	1:A:147:VAL:HG21	2.47	0.50
1:B:132:PHE:CE2	1:B:147:VAL:HG21	2.47	0.49
1:D:58:PHE:CE1	1:D:216:ALA:HB2	2.47	0.49
1:D:128:THR:OG1	1:D:129:HIS:HD2	1.95	0.49
1:D:46:THR:OG1	1:D:47:GLY:CA	2.53	0.49
1:A:299:ASN:ND2	1:A:323:ASP:H	2.09	0.49
1:C:125:SER:HB2	1:C:154:HIS:NE2	2.27	0.49
1:C:13:GLN:HG2	3:C:4070:HOH:O	2.13	0.48
1:D:10:ARG:HH12	1:D:183:ASN:HD21	1.61	0.48
1:D:257:ILE:HD12	1:D:380:LEU:CD1	2.42	0.48
1:C:26:THR:O	1:C:115:LYS:HD2	2.14	0.48
1:D:13:GLN:HG2	3:D:5106:HOH:O	2.14	0.47
1:C:88:PHE:CD2	1:C:89:VAL:HG22	2.49	0.47
1:C:131:ILE:HD11	1:C:180:LEU:HD22	1.95	0.47
1:C:223:SER:OG	1:C:346:HIS:HD2	1.97	0.47
1:D:114:GLU:O	1:D:118:GLN:HG3	2.14	0.47
1:C:205:SER:HB3	1:C:208:HIS:HB2	1.96	0.47
1:B:110:LYS:HD2	1:B:150:LEU:HB3	1.97	0.47
1:A:272:GLY:O	1:A:275:PRO:HD2	2.15	0.46
1:B:199:VAL:HG13	1:B:200:THR:HG23	1.95	0.46
1:D:279:SER:CB	1:D:315:ARG:HG3	2.46	0.46
1:A:160:VAL:HG23	3:A:2179:HOH:O	2.15	0.46
1:A:214:GLY:HA3	1:A:268:PHE:CZ	2.51	0.46
1:C:43:PHE:O	1:C:48:ASN:O	2.34	0.46
1:B:274:VAL:HB	1:B:275:PRO:HD3	1.98	0.46
1:C:167:CYS:SG	2:C:4000:3IO:CAK	3.04	0.46
1:B:373:LEU:C	1:B:373:LEU:HD23	2.41	0.46
1:D:35:GLN:HE22	1:D:70:ARG:NH1	2.12	0.46
1:B:353:ARG:HD2	3:B:3253:HOH:O	2.15	0.45
1:C:373:LEU:C	1:C:373:LEU:HD23	2.42	0.45
1:D:214:GLY:HA3	1:D:268:PHE:CZ	2.51	0.45
1:C:199:VAL:HG22	1:C:199:VAL:O	2.17	0.45
1:B:160:VAL:HG11	1:B:176:MET:HE1	1.98	0.45
1:D:143:ALA:O	1:D:147:VAL:HG23	2.16	0.45
1:D:325:THR:HA	1:D:328:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2116:HOH:O	1:B:129:HIS:HE1	1.99	0.45
1:C:141:PRO:HA	3:D:5038:HOH:O	2.16	0.45
1:C:129:HIS:HE1	3:C:4156:HOH:O	1.99	0.45
1:D:283:GLU:HB2	3:D:5119:HOH:O	2.17	0.45
1:B:193:CYS:O	1:B:222:ALA:HA	2.17	0.45
1:B:388:LYS:HE3	3:B:3317:HOH:O	2.16	0.45
1:A:201:PHE:C	1:A:201:PHE:CD1	2.94	0.44
1:A:223:SER:OG	1:A:346:HIS:HD2	2.01	0.44
1:C:6:PHE:O	1:C:8:GLY:N	2.49	0.44
1:D:35:GLN:HE21	1:D:35:GLN:CA	2.19	0.44
1:A:199:VAL:HG23	3:A:2264:HOH:O	2.16	0.44
1:A:103:MET:SD	1:A:103:MET:C	3.00	0.44
1:C:94:LEU:O	1:C:98:GLN:HG2	2.17	0.44
1:D:88:PHE:CD2	1:D:89:VAL:HG22	2.52	0.44
1:B:201:PHE:CD1	1:B:201:PHE:C	2.95	0.44
1:C:38:TYR:N	1:C:39:PRO:CD	2.80	0.44
1:C:63:GLU:HA	3:C:4229:HOH:O	2.17	0.44
1:C:101:LEU:HD11	1:C:199:VAL:HB	1.99	0.44
1:D:26:THR:HB	1:D:347:PHE:CZ	2.53	0.44
1:D:353:ARG:HG3	1:D:354:LYS:N	2.31	0.43
1:D:373:LEU:HB3	1:D:385:VAL:HB	2.00	0.43
1:C:299:ASN:HD21	1:C:323:ASP:N	2.13	0.43
1:D:26:THR:O	1:D:115:LYS:HD2	2.18	0.43
1:A:259:GLY:O	1:B:139:ASP:HB3	2.19	0.43
1:B:26:THR:HB	1:B:347:PHE:CZ	2.54	0.43
1:C:31:ASN:HB3	1:C:72:MET:O	2.19	0.43
1:A:199:VAL:HG22	1:A:266:LEU:HB3	2.00	0.43
1:B:332:HIS:ND1	1:B:351:GLN:OE1	2.52	0.43
1:D:31:ASN:HB3	1:D:72:MET:O	2.18	0.43
1:D:193:CYS:O	1:D:222:ALA:HA	2.19	0.43
1:C:205:SER:OG	1:C:208:HIS:HD2	2.02	0.43
1:A:45:ILE:HD13	1:A:76:GLU:HG3	2.01	0.42
1:B:167:CYS:SG	2:B:3000:3IO:CAI	3.07	0.42
1:B:103:MET:C	1:B:103:MET:SD	3.03	0.42
1:D:244:TRP:CH2	1:D:246:ALA:HB2	2.54	0.42
1:D:110:LYS:O	1:D:114:GLU:HG2	2.19	0.42
1:A:315:ARG:HD2	3:A:2221:HOH:O	2.19	0.42
1:C:26:THR:HB	1:C:347:PHE:CZ	2.54	0.42
1:B:311:ALA:O	1:B:315:ARG:HG2	2.20	0.42
1:C:211:SER:HB3	3:C:4101:HOH:O	2.20	0.42
1:C:180:LEU:HD11	3:C:4084:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:VAL:O	1:A:373:LEU:HA	2.21	0.41
1:A:353:ARG:HG3	1:A:354:LYS:N	2.35	0.41
1:B:310:ARG:HB3	1:B:310:ARG:NH2	2.35	0.41
1:C:42:TYR:CZ	1:C:204:PRO:HD3	2.55	0.41
1:C:201:PHE:CD1	1:C:201:PHE:C	2.98	0.41
1:C:299:ASN:HA	1:C:326:LYS:HE3	2.02	0.41
1:A:58:PHE:CE1	1:A:216:ALA:HB2	2.55	0.41
1:B:223:SER:OG	1:B:346:HIS:HD2	2.03	0.41
1:D:43:PHE:CZ	1:D:55:LYS:HA	2.55	0.41
1:C:299:ASN:HD21	1:C:322:LEU:HA	1.85	0.41
1:C:129:HIS:CE1	1:C:158:LYS:HD2	2.55	0.41
1:C:312:ILE:O	1:C:316:VAL:HG23	2.21	0.41
1:D:29:PRO:HA	1:D:30:PRO:HD3	1.97	0.41
1:D:90:GLU:CD	1:D:90:GLU:H	2.29	0.41
1:C:48:ASN:O	1:C:49:GLU:CG	2.68	0.41
1:D:209:LEU:O	1:D:212:LEU:HB3	2.21	0.41
1:B:244:TRP:CH2	1:B:246:ALA:HB2	2.56	0.41
1:B:350:ASP:OD1	1:B:354:LYS:HE3	2.21	0.41
1:A:6:PHE:O	1:A:9:PHE:HB3	2.21	0.40
1:A:129:HIS:HE1	3:B:3127:HOH:O	2.03	0.40
1:A:218:PHE:N	1:A:218:PHE:CD1	2.86	0.40
1:D:103:MET:SD	1:D:103:MET:C	3.04	0.40
1:A:26:THR:HB	1:A:347:PHE:CZ	2.56	0.40
1:B:126:GLY:HA3	3:B:3090:HOH:O	2.21	0.40
1:C:143:ALA:O	1:C:147:VAL:HG23	2.21	0.40
1:D:35:GLN:HA	1:D:35:GLN:NE2	2.26	0.40
1:A:72:MET:HE3	3:A:2240:HOH:O	2.20	0.40
1:B:131:ILE:HD11	1:B:180:LEU:HD22	2.03	0.40
1:D:308:GLY:HA2	1:D:339:ASN:ND2	2.36	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	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	B	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	C	372/413 (90%)	359 (96%)	13 (4%)	0	100	100
1	D	376/413 (91%)	361 (96%)	15 (4%)	0	100	100
All	All	1518/1652 (92%)	1466 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	304/340 (89%)	303 (100%)	1 (0%)	86	83
1	B	302/340 (89%)	301 (100%)	1 (0%)	86	83
1	C	286/340 (84%)	283 (99%)	3 (1%)	68	58
1	D	276/340 (81%)	274 (99%)	2 (1%)	76	69
All	All	1168/1360 (86%)	1161 (99%)	7 (1%)	78	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	B	351	GLN
1	C	49	GLU
1	C	103	MET
1	C	139	ASP
1	D	35	GLN
1	D	315	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	129	HIS
1	A	234	GLN
1	A	281	ASN
1	A	299	ASN
1	A	346	HIS
1	A	358	GLN
1	B	51	ASN
1	B	129	HIS
1	B	208	HIS
1	B	215	GLN
1	B	269	GLN
1	B	321	ASN
1	B	346	HIS
1	B	359	ASN
1	C	31	ASN
1	C	129	HIS
1	C	208	HIS
1	C	281	ASN
1	C	299	ASN
1	C	346	HIS
1	D	31	ASN
1	D	35	GLN
1	D	69	GLN
1	D	129	HIS
1	D	183	ASN
1	D	234	GLN
1	D	281	ASN
1	D	346	HIS
1	D	358	GLN
1	D	359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3IO	D	5000	-	16,16,16	1.58	5 (31%)	21,22,22	1.07	2 (9%)
2	3IO	B	3000	-	16,16,16	1.59	5 (31%)	21,22,22	0.97	2 (9%)
2	3IO	C	4000	-	16,16,16	1.59	5 (31%)	21,22,22	1.03	2 (9%)
2	3IO	A	2000	-	16,16,16	1.58	5 (31%)	21,22,22	1.08	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3IO	D	5000	-	-	1/8/8/8	0/2/2/2
2	3IO	B	3000	-	-	1/8/8/8	0/2/2/2
2	3IO	C	4000	-	-	1/8/8/8	0/2/2/2
2	3IO	A	2000	-	-	1/8/8/8	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4000	3IO	CAO-CAM	-2.82	1.39	1.44
2	A	2000	3IO	CAO-CAM	-2.81	1.39	1.44
2	B	3000	3IO	CAO-CAM	-2.77	1.39	1.44
2	D	5000	3IO	CAO-CAM	-2.75	1.39	1.44
2	D	5000	3IO	CAN-NAJ	-2.74	1.33	1.37
2	C	4000	3IO	CAN-NAJ	-2.73	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	3IO	CAN-NAJ	-2.70	1.33	1.37
2	B	3000	3IO	CAI-CAM	2.68	1.53	1.50
2	C	4000	3IO	CAI-CAM	2.66	1.53	1.50
2	A	2000	3IO	CAN-NAJ	-2.65	1.33	1.37
2	A	2000	3IO	CAI-CAM	2.59	1.53	1.50
2	D	5000	3IO	CAI-CAM	2.53	1.53	1.50
2	A	2000	3IO	CAH-NAJ	-2.23	1.33	1.37
2	D	5000	3IO	CAH-NAJ	-2.23	1.33	1.37
2	B	3000	3IO	CAH-NAJ	-2.19	1.33	1.37
2	C	4000	3IO	CAH-CAM	-2.19	1.33	1.36
2	D	5000	3IO	CAH-CAM	-2.19	1.33	1.36
2	B	3000	3IO	CAH-CAM	-2.18	1.33	1.36
2	A	2000	3IO	CAH-CAM	-2.16	1.33	1.36
2	C	4000	3IO	CAH-NAJ	-2.16	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	3IO	OAA-CAK-CAL	-3.24	117.78	121.81
2	D	5000	3IO	OAA-CAK-CAL	-2.91	118.19	121.81
2	C	4000	3IO	OAA-CAK-CAL	-2.82	118.31	121.81
2	B	3000	3IO	OAA-CAK-CAL	-2.59	118.59	121.81
2	D	5000	3IO	CAF-CAN-CAO	-2.33	119.93	122.19
2	C	4000	3IO	CAF-CAN-CAO	-2.26	120.00	122.19
2	A	2000	3IO	CAF-CAN-CAO	-2.18	120.08	122.19
2	B	3000	3IO	CAF-CAN-CAO	-2.08	120.18	122.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3000	3IO	OAC-CAK-CAL-CAI
2	C	4000	3IO	OAC-CAK-CAL-CAI
2	D	5000	3IO	OAC-CAK-CAL-CAI
2	A	2000	3IO	OAC-CAK-CAL-OAB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5000	3IO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	3IO	3	0
2	C	4000	3IO	2	0
2	A	2000	3IO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/413 (93%)	-0.05	5 (1%) 75 79	10, 18, 30, 37	7 (1%)
1	B	387/413 (93%)	0.06	12 (3%) 51 55	10, 19, 31, 44	3 (0%)
1	C	378/413 (91%)	0.59	32 (8%) 16 17	14, 25, 41, 50	2 (0%)
1	D	382/413 (92%)	0.90	58 (15%) 5 5	16, 29, 44, 47	2 (0%)
All	All	1534/1652 (92%)	0.37	107 (6%) 22 24	10, 23, 41, 50	14 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	GLY	5.9
1	C	321	ASN	5.8
1	D	48	ASN	5.3
1	C	48	ASN	4.3
1	D	318	ALA	4.2
1	D	324	PRO	4.0
1	D	54	LEU	3.9
1	C	32	ALA	3.9
1	C	33	VAL	3.7
1	B	357	LEU	3.6
1	D	89	VAL	3.5
1	B	392	ILE	3.4
1	D	46	THR	3.4
1	D	270	LEU	3.4
1	C	71	TYR	3.3
1	C	38	TYR	3.2
1	C	39	PRO	3.2
1	A	358	GLN	3.2
1	D	295	ILE	3.2
1	C	57	LYS	3.2
1	A	6	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	251	PRO	3.1
1	C	47	GLY	3.1
1	D	360	GLY	3.1
1	C	75	THR	3.1
1	D	282	ILE	3.1
1	C	208	HIS	3.0
1	D	213	VAL	3.0
1	D	49	GLU	3.0
1	C	6	PHE	3.0
1	D	255	GLY	2.9
1	D	279	SER	2.9
1	C	37	THR	2.8
1	C	43	PHE	2.8
1	C	45	ILE	2.8
1	D	323	ASP	2.8
1	A	270	LEU	2.8
1	D	199	VAL	2.7
1	B	360	GLY	2.7
1	C	76	GLU	2.7
1	D	280	ALA	2.7
1	C	46	THR	2.7
1	D	62	CYS	2.7
1	D	38	TYR	2.7
1	D	61	ILE	2.7
1	D	335	SER	2.6
1	D	209	LEU	2.6
1	D	91	VAL	2.6
1	B	252	ASN	2.6
1	D	291	SER	2.6
1	D	60	ARG	2.6
1	B	359	ASN	2.5
1	D	87	ALA	2.5
1	D	357	LEU	2.5
1	D	234	GLN	2.4
1	C	58	PHE	2.4
1	C	87	ALA	2.4
1	D	73	TYR	2.4
1	A	7	GLU	2.4
1	C	79	LEU	2.4
1	D	256	ALA	2.4
1	C	61	ILE	2.4
1	D	273	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	88	PHE	2.3
1	D	39	PRO	2.3
1	D	393	GLN	2.3
1	B	52	THR	2.3
1	A	234	GLN	2.3
1	B	358	GLN	2.3
1	D	79	LEU	2.3
1	D	320	LEU	2.3
1	D	57	LYS	2.3
1	D	392	ILE	2.3
1	D	207	THR	2.2
1	C	49	GLU	2.2
1	D	216	ALA	2.2
1	C	60	ARG	2.2
1	B	321	ASN	2.2
1	D	167	CYS	2.2
1	D	40	ASP	2.2
1	D	212	LEU	2.2
1	C	338	GLY	2.2
1	C	77	GLU	2.2
1	B	154	HIS	2.2
1	D	88	PHE	2.2
1	D	66	ALA	2.2
1	D	287	VAL	2.1
1	C	44	ARG	2.1
1	C	64	ARG	2.1
1	D	41	PHE	2.1
1	D	33	VAL	2.1
1	D	250	VAL	2.1
1	D	76	GLU	2.1
1	D	325	THR	2.1
1	C	204	PRO	2.1
1	D	58	PHE	2.1
1	D	272	GLY	2.1
1	B	50	HIS	2.0
1	C	29	PRO	2.0
1	C	103	MET	2.0
1	D	78	ILE	2.0
1	D	201	PHE	2.0
1	D	56	ASP	2.0
1	C	62	CYS	2.0
1	C	89	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	316	VAL	2.0
1	D	294	LYS	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($\text{\AA}^2$)	Q<0.9
2	3IO	D	5000	15/15	0.78	0.11	31,32,36,37	0
2	3IO	C	4000	15/15	0.83	0.10	26,27,30,31	0
2	3IO	A	2000	15/15	0.88	0.09	22,23,26,26	0
2	3IO	B	3000	15/15	0.91	0.08	17,19,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.