Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 12:43 AM EDT

PDB ID	:	1XES
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 (i) 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 (i)) were used in the production of this report:

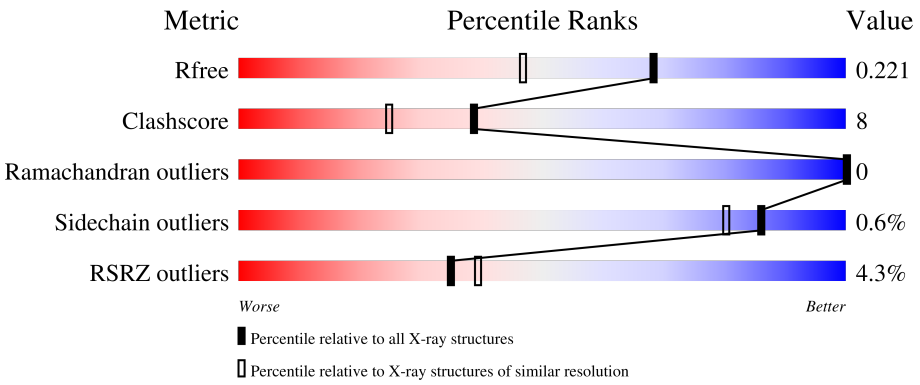
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	.% 81% 13% 6%
1	B	413	2% 83% 11% 6%
1	C	413	6% 76% 15% • 8%
1	D	413	7% 76% 16% 8%

2 Entry composition (i)

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

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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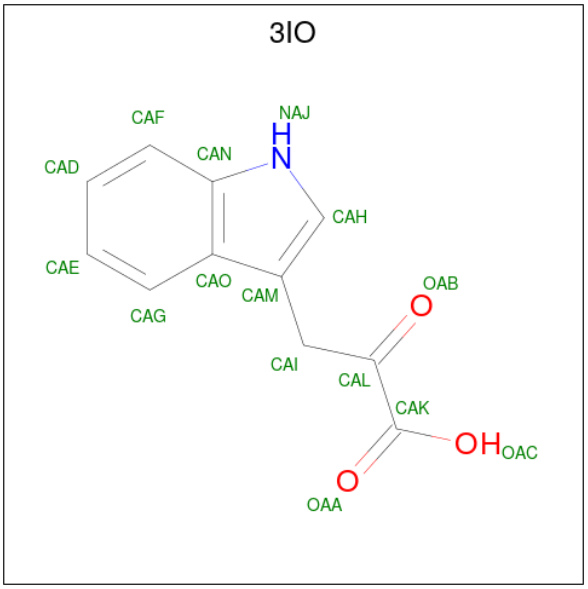
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	cloning artifact	UNP Q02323
D	-15	HIS	-	cloning artifact	UNP Q02323
D	-14	HIS	-	cloning artifact	UNP Q02323
D	-13	HIS	-	cloning artifact	UNP Q02323
D	-12	HIS	-	cloning artifact	UNP Q02323
D	-11	HIS	-	cloning artifact	UNP Q02323
D	-10	HIS	-	cloning 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 (three-letter code: 3IO) (formula: $C_{11}H_9NO_3$).



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

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

- Molecule 3 is water.

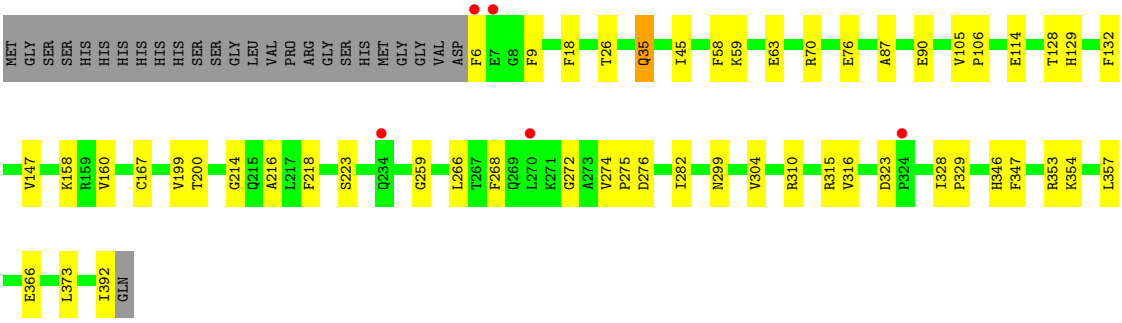
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	334	334	334	0	0
			Total	O		
3	B	324	324	324	0	0
			Total	O		
3	C	230	230	230	0	0
			Total	O		
3	D	189	189	189	0	0

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.

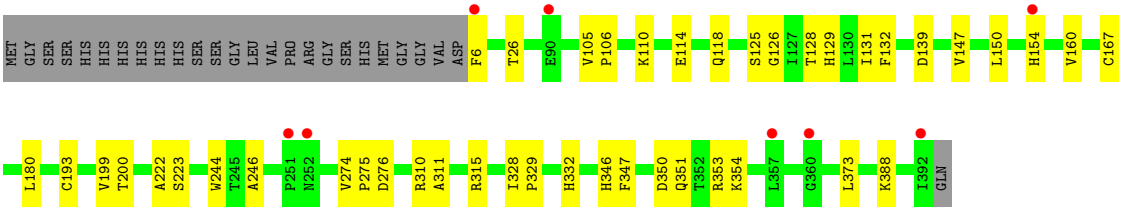
• Molecule 1: Dihydropinosylvin synthase

Chain A:



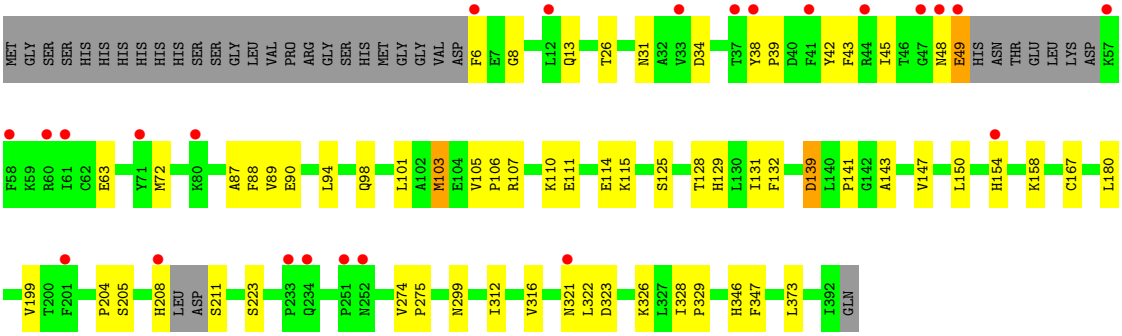
• Molecule 1: Dihydropinosylvin synthase

Chain B:



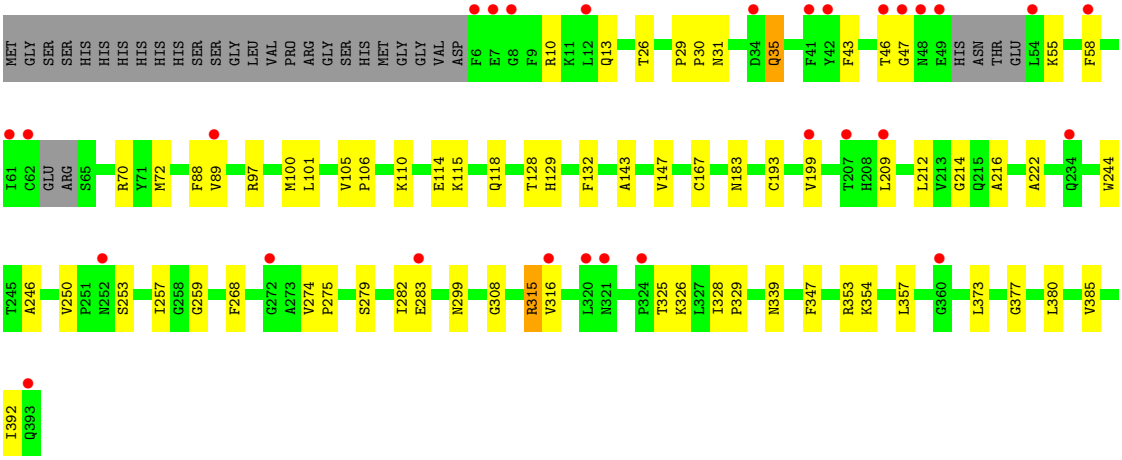
• Molecule 1: Dihydropinosylvin synthase

Chain C:



• Molecule 1: Dihydropinosylvin synthase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.15 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.225 0.198 , 0.221	Depositor DCC
R_{free} test set	8585 reflections (5.01%)	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)	0.36 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/2960	0.62	0/4021
1	B	0.31	0/2955	0.61	0/4013
1	C	0.31	0/2844	0.59	1/3867 (0.0%)
1	D	0.29	0/2826	0.57	0/3849
All	All	0.31	0/11585	0.60	1/15750 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	321	ASN	CB-CA-C	5.40	121.20	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2900	0	2866	41	0
1	B	2896	0	2870	32	0
1	C	2788	0	2727	48	0
1	D	2771	0	2666	53	0
2	A	15	0	8	2	0
2	B	15	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	8	2	0
2	D	15	0	8	1	0
3	A	334	0	0	6	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	170	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 (170) 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: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:97:ARG:HA	1:D:100:MET:CE	2.33	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: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:B:353:ARG:HG3	1:B:354:LYS:N	2.22	0.55
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:C:87:ALA:HB1	1:C:90:GLU:OE2	2.08	0.53
1:D:97:ARG:HA	1:D:100:MET:HE2	1.88	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: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:C:103:MET:HE1	3:C:4168:HOH:O	2.10	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
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:A:87:ALA:HB1	1:A:90:GLU:CD	2.34	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:A:353:ARG:HG3	1:A:354:LYS:N	2.35	0.41
1:C:180:LEU:HD11	3:C:4084:HOH:O	2.19	0.41
1:A:304:VAL:O	1:A:373:LEU:HA	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:373:LEU:C	1:B:373:LEU:HD23	2.41	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: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:C:373:LEU:C	1:C:373:LEU:HD23	2.42	0.40
1:A:218:PHE:N	1:A:218:PHE:CD1	2.86	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: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 (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	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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	304/340 (89%)	303 (100%)	1 (0%)	92 89
1	B	302/340 (89%)	302 (100%)	0	100 100
1	C	286/340 (84%)	282 (99%)	4 (1%)	67 53
1	D	276/340 (81%)	274 (99%)	2 (1%)	84 77
All	All	1168/1360 (86%)	1161 (99%)	7 (1%)	86 80

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

Mol	Chain	Res	Type
1	A	35	GLN
1	C	34	ASP
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	129	HIS
1	A	154	HIS
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

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Mol	Chain	Res	Type
1	B	321	ASN
1	B	346	HIS
1	B	359	ASN
1	C	129	HIS
1	C	208	HIS
1	C	281	ASN
1	C	299	ASN
1	C	346	HIS
1	C	359	ASN
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 (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 monosaccharides 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	C	4000	-	15,16,16	1.24	0	17,22,22	0.94	1 (5%)
2	3IO	B	3000	-	15,16,16	1.25	0	17,22,22	0.84	1 (5%)
2	3IO	A	2000	-	15,16,16	1.24	1 (6%)	17,22,22	0.98	1 (5%)
2	3IO	D	5000	-	15,16,16	1.25	0	17,22,22	1.00	1 (5%)

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	C	4000	-	-	1/8/8/8	0/2/2/2
2	3IO	B	3000	-	-	1/8/8/8	0/2/2/2
2	3IO	A	2000	-	-	1/8/8/8	0/2/2/2
2	3IO	D	5000	-	-	1/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	3IO	CAI-CAL	2.01	1.53	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2000	3IO	OAA-CAK-CAL	-2.95	117.78	121.72
2	D	5000	3IO	OAA-CAK-CAL	-2.64	118.19	121.72
2	C	4000	3IO	OAA-CAK-CAL	-2.56	118.31	121.72
2	B	3000	3IO	OAA-CAK-CAL	-2.34	118.59	121.72

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	C	4000	3IO	2	0
2	B	3000	3IO	3	0
2	A	2000	3IO	2	0
2	D	5000	3IO	1	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 (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	387/413 (93%)	-0.14	5 (1%)	77	81	10, 18, 30, 37	7 (1%)
1	B	387/413 (93%)	-0.03	8 (2%)	63	67	10, 19, 31, 44	3 (0%)
1	C	378/413 (91%)	0.33	24 (6%)	20	22	14, 25, 41, 50	2 (0%)
1	D	382/413 (92%)	0.56	29 (7%)	13	16	16, 29, 44, 47	2 (0%)
All	All	1534/1652 (92%)	0.18	66 (4%)	35	39	10, 23, 41, 50	14 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	GLY	6.4
1	C	321	ASN	6.1
1	D	207	THR	6.0
1	D	324	PRO	4.8
1	D	54	LEU	4.7
1	D	48	ASN	4.6
1	C	48	ASN	3.8
1	C	47	GLY	3.5
1	C	6	PHE	3.5
1	D	393	GLN	3.2
1	D	360	GLY	3.2
1	C	12	LEU	3.1
1	B	357	LEU	3.1
1	B	252	ASN	3.1
1	D	199	VAL	3.1
1	D	321	ASN	3.0
1	C	37	THR	3.0
1	C	38	TYR	2.9
1	D	6	PHE	2.9
1	D	12	LEU	2.8
1	D	272	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	61	ILE	2.8
1	C	57	LYS	2.8
1	D	46	THR	2.7
1	B	392	ILE	2.7
1	D	209	LEU	2.6
1	C	234	GLN	2.6
1	A	234	GLN	2.6
1	A	7	GLU	2.6
1	D	49	GLU	2.6
1	A	324	PRO	2.6
1	C	71	TYR	2.6
1	B	251	PRO	2.5
1	D	58	PHE	2.5
1	B	360	GLY	2.5
1	C	58	PHE	2.5
1	D	234	GLN	2.5
1	C	44	ARG	2.4
1	D	283	GLU	2.4
1	C	154	HIS	2.4
1	D	8	GLY	2.4
1	D	252	ASN	2.4
1	C	49	GLU	2.4
1	D	42	TYR	2.3
1	C	252	ASN	2.3
1	A	270	LEU	2.3
1	D	61	ILE	2.3
1	C	201	PHE	2.3
1	C	208	HIS	2.3
1	C	60	ARG	2.2
1	D	89	VAL	2.2
1	D	41	PHE	2.2
1	D	320	LEU	2.2
1	D	7	GLU	2.2
1	C	233	PRO	2.2
1	D	62	CYS	2.2
1	B	154	HIS	2.1
1	B	90	GLU	2.1
1	D	34	ASP	2.1
1	A	6	PHE	2.1
1	B	6	PHE	2.1
1	C	41	PHE	2.1
1	C	33	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	80	LYS	2.1
1	C	251	PRO	2.1
1	D	316	VAL	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 monosaccharides 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
2	3IO	D	5000	15/15	0.79	0.20	31,32,36,37	0
2	3IO	C	4000	15/15	0.83	0.14	26,27,30,31	0
2	3IO	A	2000	15/15	0.84	0.14	22,23,26,26	0
2	3IO	B	3000	15/15	0.91	0.11	17,19,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.