Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:30 am BST

PDB ID	:	3D7J
Title	:	SCO6650, a 6-pyruvoyltetrahydropterin synthase homolog from Streptomyces coelicolor
Authors	:	Spoonamore, J.E.; Roberts, S.A.; Heroux, A.; Bandarian, V.
Deposited on	:	2008-05-21
Resolution	:	1.45 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 following versions of software and data (see references ①) were used in the production of this report:

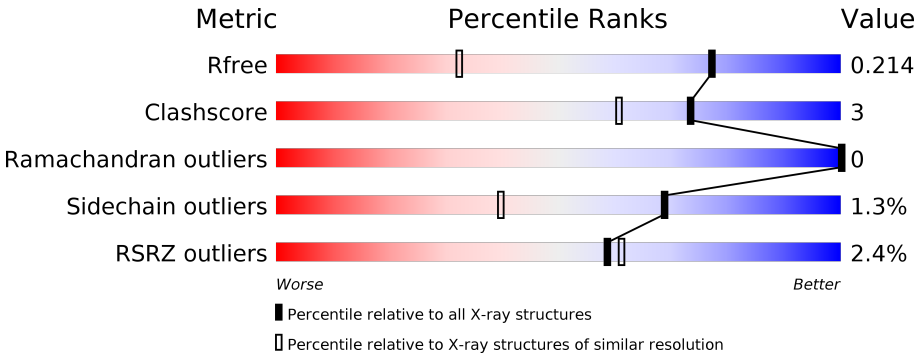
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on 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	152	80% 9% 12%
1	B	152	3% 85% 12%
1	C	152	2% 82% 7% 11%
1	D	152	2% 83% 5% 12%
1	E	152	2% 79% 9% 12%
1	F	152	3% 85% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7026 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 Uncharacterized protein SCO6650.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	Se	0	2	0
			1053	658	194	199	2			
1	B	134	Total	C	N	O	Se	0	3	0
			1057	662	191	202	2			
1	C	135	Total	C	N	O	Se	0	1	0
			1040	651	190	197	2			
1	D	134	Total	C	N	O	Se	0	1	0
			1042	652	190	198	2			
1	E	134	Total	C	N	O	Se	0	8	0
			1101	689	202	208	2			
1	F	135	Total	C	N	O	Se	0	2	0
			1051	657	194	198	2			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	EXPRESSION TAG	UNP O86696
A	-17	SER	-	EXPRESSION TAG	UNP O86696
A	-16	SER	-	EXPRESSION TAG	UNP O86696
A	-15	HIS	-	EXPRESSION TAG	UNP O86696
A	-14	HIS	-	EXPRESSION TAG	UNP O86696
A	-13	HIS	-	EXPRESSION TAG	UNP O86696
A	-12	HIS	-	EXPRESSION TAG	UNP O86696
A	-11	HIS	-	EXPRESSION TAG	UNP O86696
A	-10	HIS	-	EXPRESSION TAG	UNP O86696
A	-9	SER	-	EXPRESSION TAG	UNP O86696
A	-8	SER	-	EXPRESSION TAG	UNP O86696
A	-7	GLY	-	EXPRESSION TAG	UNP O86696
A	-6	LEU	-	EXPRESSION TAG	UNP O86696
A	-5	VAL	-	EXPRESSION TAG	UNP O86696
A	-4	PRO	-	EXPRESSION TAG	UNP O86696
A	-3	ARG	-	EXPRESSION TAG	UNP O86696
A	-2	GLY	-	EXPRESSION TAG	UNP O86696

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP O86696
A	0	HIS	-	EXPRESSION TAG	UNP O86696
A	1	MSE	-	EXPRESSION TAG	UNP O86696
B	-18	GLY	-	EXPRESSION TAG	UNP O86696
B	-17	SER	-	EXPRESSION TAG	UNP O86696
B	-16	SER	-	EXPRESSION TAG	UNP O86696
B	-15	HIS	-	EXPRESSION TAG	UNP O86696
B	-14	HIS	-	EXPRESSION TAG	UNP O86696
B	-13	HIS	-	EXPRESSION TAG	UNP O86696
B	-12	HIS	-	EXPRESSION TAG	UNP O86696
B	-11	HIS	-	EXPRESSION TAG	UNP O86696
B	-10	HIS	-	EXPRESSION TAG	UNP O86696
B	-9	SER	-	EXPRESSION TAG	UNP O86696
B	-8	SER	-	EXPRESSION TAG	UNP O86696
B	-7	GLY	-	EXPRESSION TAG	UNP O86696
B	-6	LEU	-	EXPRESSION TAG	UNP O86696
B	-5	VAL	-	EXPRESSION TAG	UNP O86696
B	-4	PRO	-	EXPRESSION TAG	UNP O86696
B	-3	ARG	-	EXPRESSION TAG	UNP O86696
B	-2	GLY	-	EXPRESSION TAG	UNP O86696
B	-1	SER	-	EXPRESSION TAG	UNP O86696
B	0	HIS	-	EXPRESSION TAG	UNP O86696
B	1	MSE	-	EXPRESSION TAG	UNP O86696
C	-18	GLY	-	EXPRESSION TAG	UNP O86696
C	-17	SER	-	EXPRESSION TAG	UNP O86696
C	-16	SER	-	EXPRESSION TAG	UNP O86696
C	-15	HIS	-	EXPRESSION TAG	UNP O86696
C	-14	HIS	-	EXPRESSION TAG	UNP O86696
C	-13	HIS	-	EXPRESSION TAG	UNP O86696
C	-12	HIS	-	EXPRESSION TAG	UNP O86696
C	-11	HIS	-	EXPRESSION TAG	UNP O86696
C	-10	HIS	-	EXPRESSION TAG	UNP O86696
C	-9	SER	-	EXPRESSION TAG	UNP O86696
C	-8	SER	-	EXPRESSION TAG	UNP O86696
C	-7	GLY	-	EXPRESSION TAG	UNP O86696
C	-6	LEU	-	EXPRESSION TAG	UNP O86696
C	-5	VAL	-	EXPRESSION TAG	UNP O86696
C	-4	PRO	-	EXPRESSION TAG	UNP O86696
C	-3	ARG	-	EXPRESSION TAG	UNP O86696
C	-2	GLY	-	EXPRESSION TAG	UNP O86696
C	-1	SER	-	EXPRESSION TAG	UNP O86696
C	0	HIS	-	EXPRESSION TAG	UNP O86696

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	EXPRESSION TAG	UNP O86696
D	-18	GLY	-	EXPRESSION TAG	UNP O86696
D	-17	SER	-	EXPRESSION TAG	UNP O86696
D	-16	SER	-	EXPRESSION TAG	UNP O86696
D	-15	HIS	-	EXPRESSION TAG	UNP O86696
D	-14	HIS	-	EXPRESSION TAG	UNP O86696
D	-13	HIS	-	EXPRESSION TAG	UNP O86696
D	-12	HIS	-	EXPRESSION TAG	UNP O86696
D	-11	HIS	-	EXPRESSION TAG	UNP O86696
D	-10	HIS	-	EXPRESSION TAG	UNP O86696
D	-9	SER	-	EXPRESSION TAG	UNP O86696
D	-8	SER	-	EXPRESSION TAG	UNP O86696
D	-7	GLY	-	EXPRESSION TAG	UNP O86696
D	-6	LEU	-	EXPRESSION TAG	UNP O86696
D	-5	VAL	-	EXPRESSION TAG	UNP O86696
D	-4	PRO	-	EXPRESSION TAG	UNP O86696
D	-3	ARG	-	EXPRESSION TAG	UNP O86696
D	-2	GLY	-	EXPRESSION TAG	UNP O86696
D	-1	SER	-	EXPRESSION TAG	UNP O86696
D	0	HIS	-	EXPRESSION TAG	UNP O86696
D	1	MSE	-	EXPRESSION TAG	UNP O86696
E	-18	GLY	-	EXPRESSION TAG	UNP O86696
E	-17	SER	-	EXPRESSION TAG	UNP O86696
E	-16	SER	-	EXPRESSION TAG	UNP O86696
E	-15	HIS	-	EXPRESSION TAG	UNP O86696
E	-14	HIS	-	EXPRESSION TAG	UNP O86696
E	-13	HIS	-	EXPRESSION TAG	UNP O86696
E	-12	HIS	-	EXPRESSION TAG	UNP O86696
E	-11	HIS	-	EXPRESSION TAG	UNP O86696
E	-10	HIS	-	EXPRESSION TAG	UNP O86696
E	-9	SER	-	EXPRESSION TAG	UNP O86696
E	-8	SER	-	EXPRESSION TAG	UNP O86696
E	-7	GLY	-	EXPRESSION TAG	UNP O86696
E	-6	LEU	-	EXPRESSION TAG	UNP O86696
E	-5	VAL	-	EXPRESSION TAG	UNP O86696
E	-4	PRO	-	EXPRESSION TAG	UNP O86696
E	-3	ARG	-	EXPRESSION TAG	UNP O86696
E	-2	GLY	-	EXPRESSION TAG	UNP O86696
E	-1	SER	-	EXPRESSION TAG	UNP O86696
E	0	HIS	-	EXPRESSION TAG	UNP O86696
E	1	MSE	-	EXPRESSION TAG	UNP O86696
F	-18	GLY	-	EXPRESSION TAG	UNP O86696

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	SER	-	EXPRESSION TAG	UNP O86696
F	-16	SER	-	EXPRESSION TAG	UNP O86696
F	-15	HIS	-	EXPRESSION TAG	UNP O86696
F	-14	HIS	-	EXPRESSION TAG	UNP O86696
F	-13	HIS	-	EXPRESSION TAG	UNP O86696
F	-12	HIS	-	EXPRESSION TAG	UNP O86696
F	-11	HIS	-	EXPRESSION TAG	UNP O86696
F	-10	HIS	-	EXPRESSION TAG	UNP O86696
F	-9	SER	-	EXPRESSION TAG	UNP O86696
F	-8	SER	-	EXPRESSION TAG	UNP O86696
F	-7	GLY	-	EXPRESSION TAG	UNP O86696
F	-6	LEU	-	EXPRESSION TAG	UNP O86696
F	-5	VAL	-	EXPRESSION TAG	UNP O86696
F	-4	PRO	-	EXPRESSION TAG	UNP O86696
F	-3	ARG	-	EXPRESSION TAG	UNP O86696
F	-2	GLY	-	EXPRESSION TAG	UNP O86696
F	-1	SER	-	EXPRESSION TAG	UNP O86696
F	0	HIS	-	EXPRESSION TAG	UNP O86696
F	1	MSE	-	EXPRESSION TAG	UNP O86696

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0

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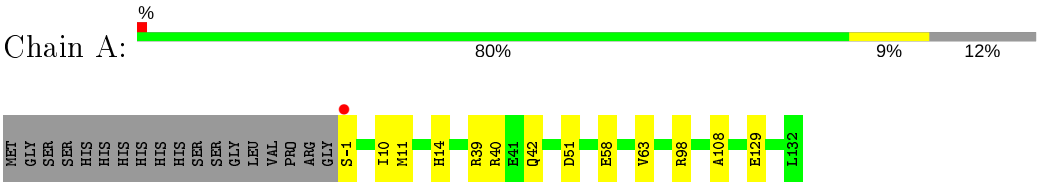
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	101	Total O 101 101	0	1
4	C	105	Total O 105 105	0	1
4	D	125	Total O 125 125	0	0
4	E	83	Total O 83 83	0	0
4	F	117	Total O 117 117	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

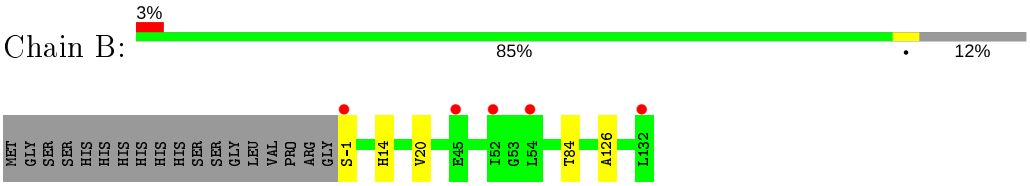
- Molecule 1: Uncharacterized protein SCO6650

Chain A:



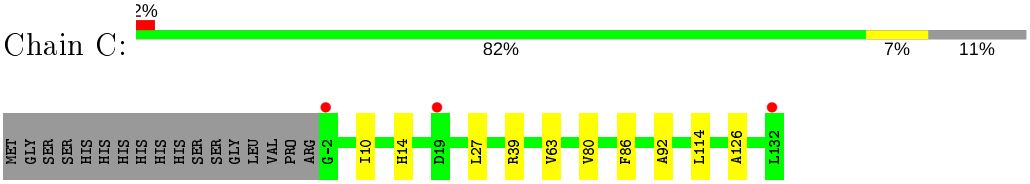
- Molecule 1: Uncharacterized protein SCO6650

Chain B:



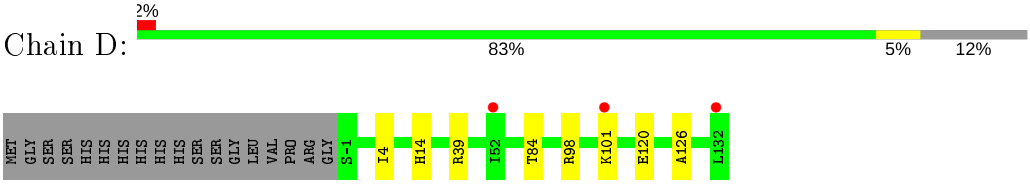
- Molecule 1: Uncharacterized protein SCO6650

Chain C:



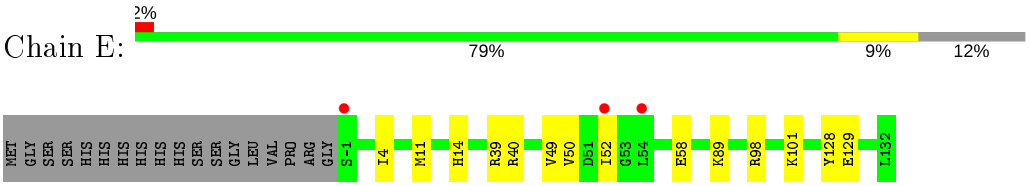
- Molecule 1: Uncharacterized protein SCO6650

Chain D:



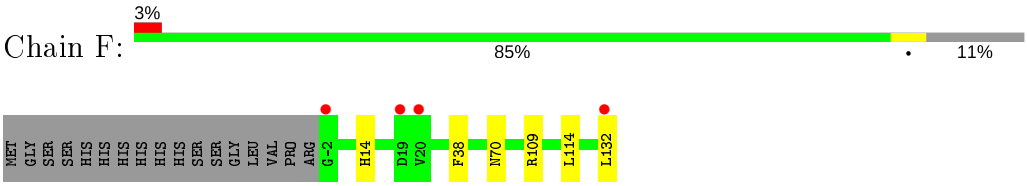
- Molecule 1: Uncharacterized protein SCO6650

Chain E:



- Molecule 1: Uncharacterized protein SCO6650

Chain F:


3%
85%
11%
MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
LEU
VAL
PRO
ARG
G-2
H14
D19
V20
F38
N70
R109
L114
L132

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.40Å 88.00Å 120.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.34 – 1.45 41.35 – 1.45	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.34-1.45) 93.4 (41.35-1.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.206 , 0.224 0.211 , 0.214	Depositor DCC
R_{free} test set	6900 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7026	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5186e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.49	0/1070	0.67	0/1444
1	B	0.50	0/1076	0.63	0/1450
1	C	0.47	0/1060	0.63	0/1431
1	D	0.49	0/1059	0.64	0/1430
1	E	0.50	0/1118	0.64	0/1509
1	F	0.48	0/1071	0.63	0/1445
All	All	0.49	0/6454	0.64	0/8709

There are no bond length outliers.

There are no bond angle outliers.

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	1053	0	1026	9	0
1	B	1057	0	1031	2	0
1	C	1040	0	1017	6	0
1	D	1042	0	1014	6	0
1	E	1101	0	1077	18	0
1	F	1051	0	1029	5	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	146	0	0	0	0
4	B	101	0	0	1	0
4	C	105	0	0	1	0
4	D	125	0	0	2	0
4	E	83	0	0	0	0
4	F	117	0	0	1	0
All	All	7026	0	6194	42	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 3.

All (42) 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:E:58:GLU:OE1	1:E:98:ARG:HD3	1.70	0.91
1:E:49[B]:VAL:CG2	1:E:50[B]:VAL:H	2.01	0.74
1:E:49[B]:VAL:CG2	1:E:50[B]:VAL:N	2.51	0.74
1:E:49[B]:VAL:HG23	1:E:50[B]:VAL:N	2.02	0.74
1:A:39:ARG:NH2	1:A:129:GLU:HG3	2.04	0.73
1:A:39:ARG:HH22	1:A:129:GLU:HG3	1.58	0.68
1:A:51:ASP:OD2	1:B:20:VAL:HG23	1.97	0.65
1:E:39:ARG:HH12	1:E:129:GLU:HG3	1.62	0.64
1:E:39:ARG:NH1	1:E:129:GLU:HG3	2.15	0.61
1:E:49[B]:VAL:HG23	1:E:50[B]:VAL:HG12	1.84	0.59
1:E:4:ILE:HG12	1:E:49[B]:VAL:CG2	2.33	0.58
1:E:49[B]:VAL:HG22	1:E:50[B]:VAL:H	1.67	0.58
1:E:89[A]:LYS:HD2	1:E:128:TYR:CZ	2.41	0.56
1:A:11:MSE:HE1	1:D:120[A]:GLU:OE2	2.07	0.54
1:C:39:ARG:NH1	4:C:218:HOH:O	2.39	0.53
1:D:84:THR:HG22	1:D:126:ALA:HB3	1.91	0.53
1:E:4:ILE:CG1	1:E:49[B]:VAL:HG21	2.39	0.52
1:B:84:THR:HG22	1:B:126:ALA:HB3	1.91	0.52
4:D:240:HOH:O	1:E:52[B]:ILE:HG21	2.09	0.52
1:E:40:ARG:HD3	1:E:49[B]:VAL:HA	1.92	0.51
1:C:126:ALA:HB2	1:D:4:ILE:HD12	1.93	0.49
1:F:109:ARG:NH2	4:F:201:HOH:O	2.45	0.49
1:A:40[B]:ARG:CD	1:A:42:GLN:O	2.61	0.49
1:C:92:ALA:HB1	1:C:114:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:HD12	1:F:70:ASN:HB2	1.96	0.47
1:D:98:ARG:HG2	1:D:101:LYS:HE2	1.98	0.46
1:F:114:LEU:CD2	1:F:132:LEU:HD11	2.46	0.45
1:F:38:PHE:CD1	1:F:114:LEU:CD2	3.00	0.45
1:C:10:ILE:CG2	1:C:63:VAL:HB	2.47	0.44
4:B:163:HOH:O	1:E:11:MSE:HE1	2.18	0.44
1:A:58:GLU:OE1	1:A:98:ARG:HD3	2.17	0.44
1:A:40[B]:ARG:HH22	1:A:108:ALA:HA	1.83	0.43
1:E:101:LYS:HB2	1:E:101:LYS:HE3	1.93	0.43
1:A:10:ILE:CG2	1:A:63:VAL:HB	2.48	0.42
1:C:80:VAL:HG11	1:C:86:PHE:CZ	2.54	0.42
1:E:4:ILE:CG1	1:E:49[B]:VAL:CG2	2.97	0.42
1:D:39:ARG:NH1	4:D:199:HOH:O	2.45	0.41
1:D:98:ARG:HA	1:D:101:LYS:HG2	2.01	0.41
1:E:58:GLU:OE1	1:E:98:ARG:CD	2.56	0.41
1:E:98:ARG:HA	1:E:101:LYS:HG2	2.02	0.41
1:F:38:PHE:CD1	1:F:114:LEU:HD22	2.55	0.40
1:A:40[B]:ARG:HD3	1:A:42:GLN:O	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	134/152 (88%)	131 (98%)	3 (2%)	0	100	100
1	B	134/152 (88%)	131 (98%)	3 (2%)	0	100	100
1	C	134/152 (88%)	131 (98%)	3 (2%)	0	100	100
1	D	133/152 (88%)	130 (98%)	3 (2%)	0	100	100
1	E	140/152 (92%)	138 (99%)	2 (1%)	0	100	100
1	F	135/152 (89%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	810/912 (89%)	793 (98%)	17 (2%)	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	107/118 (91%)	105 (98%)	2 (2%)	57 23
1	B	108/118 (92%)	106 (98%)	2 (2%)	57 23
1	C	106/118 (90%)	105 (99%)	1 (1%)	78 57
1	D	106/118 (90%)	105 (99%)	1 (1%)	78 57
1	E	113/118 (96%)	112 (99%)	1 (1%)	78 57
1	F	107/118 (91%)	106 (99%)	1 (1%)	78 57
All	All	647/708 (91%)	639 (99%)	8 (1%)	69 43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	14	HIS
1	B	-1	SER
1	B	14	HIS
1	C	14	HIS
1	D	14	HIS
1	E	14	HIS
1	F	14	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	42	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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, 95^{th} 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	132/152 (86%)	-0.03	1 (0%)	86	87	12, 16, 24, 32	7 (5%)
1	B	132/152 (86%)	0.15	5 (3%)	40	43	13, 20, 30, 31	8 (6%)
1	C	133/152 (87%)	0.05	3 (2%)	60	63	13, 20, 30, 35	3 (2%)
1	D	132/152 (86%)	0.01	3 (2%)	60	63	12, 18, 27, 33	8 (6%)
1	E	132/152 (86%)	0.13	3 (2%)	60	63	12, 18, 28, 33	5 (3%)
1	F	133/152 (87%)	-0.02	4 (3%)	50	53	13, 19, 28, 32	4 (3%)
All	All	794/912 (87%)	0.05	19 (2%)	59	61	12, 19, 28, 35	35 (4%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	SER	5.4
1	D	132	LEU	5.1
1	B	-1	SER	4.0
1	B	132[A]	LEU	3.6
1	E	52[A]	ILE	3.2
1	C	132	LEU	3.1
1	E	-1	SER	3.0
1	C	19	ASP	3.0
1	E	54	LEU	3.0
1	D	52	ILE	2.9
1	F	20	VAL	2.8
1	F	132	LEU	2.8
1	C	-2	GLY	2.8
1	F	19	ASP	2.6
1	F	-2	GLY	2.5
1	B	54	LEU	2.5
1	D	101	LYS	2.4
1	B	45	GLU	2.3
1	B	52	ILE	2.2

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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	135	1/1	0.98	0.06	22,22,22,22	0
2	NA	A	134	1/1	0.98	0.10	23,23,23,23	0
2	NA	A	133	1/1	0.98	0.05	20,20,20,20	0
3	CL	D	133	1/1	0.99	0.03	24,24,24,24	0
3	CL	B	133	1/1	0.99	0.04	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.