Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 03:03 am GMT

PDB ID	:	6H01
Title	:	Crystal structure of a domain-swapped dark-state sfGFP containing the unnatural amino acid ortho-nitrobenzyl-tyrosine (ONBY) at residue 66
Authors	:	Kesgin-Schaefer, S.; Tidow, H.
Deposited on	:	2018-07-06
Resolution	:	2.78 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:

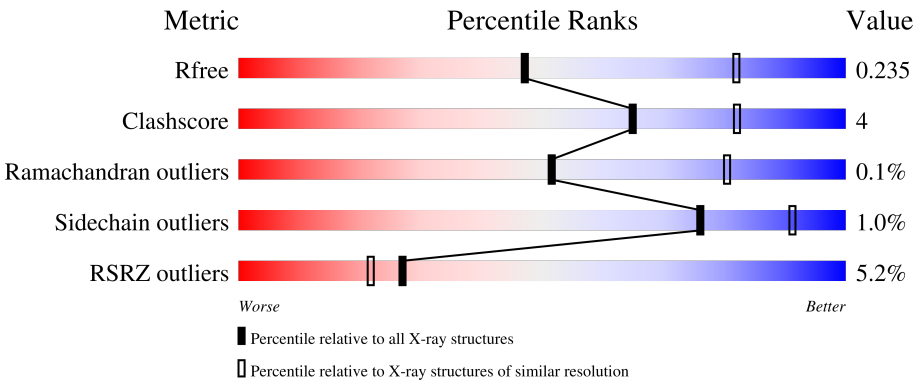
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	264	80% 7% • 12%
1	B	264	8% 75% 12% 12%
1	C	264	% 78% 8% • 12%
1	D	264	9% 77% 10% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7534 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1857	1175	316	360	6	0	0	0
			Total	C	N	O	S			
1	B	231	1848	1170	315	357	6	0	0	0
			Total	C	N	O	S			
1	C	231	1848	1170	315	357	6	0	0	0
			Total	C	N	O	S			
1	D	231	1848	1170	315	357	6	0	0	0

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP A0A059PIQ0
A	-11	GLY	-	expression tag	UNP A0A059PIQ0
A	-10	SER	-	expression tag	UNP A0A059PIQ0
A	-9	SER	-	expression tag	UNP A0A059PIQ0
A	-8	HIS	-	expression tag	UNP A0A059PIQ0
A	-7	HIS	-	expression tag	UNP A0A059PIQ0
A	-6	HIS	-	expression tag	UNP A0A059PIQ0
A	-5	HIS	-	expression tag	UNP A0A059PIQ0
A	-4	HIS	-	expression tag	UNP A0A059PIQ0
A	-3	HIS	-	expression tag	UNP A0A059PIQ0
A	-2	GLY	-	expression tag	UNP A0A059PIQ0
A	-1	SER	-	expression tag	UNP A0A059PIQ0
A	0	SER	-	expression tag	UNP A0A059PIQ0
A	1	VAL	-	expression tag	UNP A0A059PIQ0
A	2	SER	-	expression tag	UNP A0A059PIQ0
A	30	ARG	SER	conflict	UNP A0A059PIQ0
A	66	FHE	THR	chromophore	UNP A0A059PIQ0
A	66	FHE	TYR	chromophore	UNP A0A059PIQ0
A	66	FHE	GLY	chromophore	UNP A0A059PIQ0
A	72	SER	ALA	conflict	UNP A0A059PIQ0
A	206	LYS	ALA	conflict	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	231	LEU	HIS	conflict	UNP A0A059PIQ0
A	239	GLY	-	expression tag	UNP A0A059PIQ0
A	240	ILE	-	expression tag	UNP A0A059PIQ0
A	241	GLU	-	expression tag	UNP A0A059PIQ0
A	242	GLU	-	expression tag	UNP A0A059PIQ0
A	243	ASN	-	expression tag	UNP A0A059PIQ0
A	244	LEU	-	expression tag	UNP A0A059PIQ0
A	245	TYR	-	expression tag	UNP A0A059PIQ0
A	246	PHE	-	expression tag	UNP A0A059PIQ0
A	247	GLN	-	expression tag	UNP A0A059PIQ0
A	248	SER	-	expression tag	UNP A0A059PIQ0
A	249	ASN	-	expression tag	UNP A0A059PIQ0
A	250	ILE	-	expression tag	UNP A0A059PIQ0
A	251	GLY	-	expression tag	UNP A0A059PIQ0
A	252	SER	-	expression tag	UNP A0A059PIQ0
A	253	GLY	-	expression tag	UNP A0A059PIQ0
B	-12	MET	-	initiating methionine	UNP A0A059PIQ0
B	-11	GLY	-	expression tag	UNP A0A059PIQ0
B	-10	SER	-	expression tag	UNP A0A059PIQ0
B	-9	SER	-	expression tag	UNP A0A059PIQ0
B	-8	HIS	-	expression tag	UNP A0A059PIQ0
B	-7	HIS	-	expression tag	UNP A0A059PIQ0
B	-6	HIS	-	expression tag	UNP A0A059PIQ0
B	-5	HIS	-	expression tag	UNP A0A059PIQ0
B	-4	HIS	-	expression tag	UNP A0A059PIQ0
B	-3	HIS	-	expression tag	UNP A0A059PIQ0
B	-2	GLY	-	expression tag	UNP A0A059PIQ0
B	-1	SER	-	expression tag	UNP A0A059PIQ0
B	0	SER	-	expression tag	UNP A0A059PIQ0
B	1	VAL	-	expression tag	UNP A0A059PIQ0
B	2	SER	-	expression tag	UNP A0A059PIQ0
B	30	ARG	SER	conflict	UNP A0A059PIQ0
B	66	FHE	THR	chromophore	UNP A0A059PIQ0
B	66	FHE	TYR	chromophore	UNP A0A059PIQ0
B	66	FHE	GLY	chromophore	UNP A0A059PIQ0
B	72	SER	ALA	conflict	UNP A0A059PIQ0
B	206	LYS	ALA	conflict	UNP A0A059PIQ0
B	231	LEU	HIS	conflict	UNP A0A059PIQ0
B	239	GLY	-	expression tag	UNP A0A059PIQ0
B	240	ILE	-	expression tag	UNP A0A059PIQ0
B	241	GLU	-	expression tag	UNP A0A059PIQ0
B	242	GLU	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	243	ASN	-	expression tag	UNP A0A059PIQ0
B	244	LEU	-	expression tag	UNP A0A059PIQ0
B	245	TYR	-	expression tag	UNP A0A059PIQ0
B	246	PHE	-	expression tag	UNP A0A059PIQ0
B	247	GLN	-	expression tag	UNP A0A059PIQ0
B	248	SER	-	expression tag	UNP A0A059PIQ0
B	249	ASN	-	expression tag	UNP A0A059PIQ0
B	250	ILE	-	expression tag	UNP A0A059PIQ0
B	251	GLY	-	expression tag	UNP A0A059PIQ0
B	252	SER	-	expression tag	UNP A0A059PIQ0
B	253	GLY	-	expression tag	UNP A0A059PIQ0
C	-12	MET	-	initiating methionine	UNP A0A059PIQ0
C	-11	GLY	-	expression tag	UNP A0A059PIQ0
C	-10	SER	-	expression tag	UNP A0A059PIQ0
C	-9	SER	-	expression tag	UNP A0A059PIQ0
C	-8	HIS	-	expression tag	UNP A0A059PIQ0
C	-7	HIS	-	expression tag	UNP A0A059PIQ0
C	-6	HIS	-	expression tag	UNP A0A059PIQ0
C	-5	HIS	-	expression tag	UNP A0A059PIQ0
C	-4	HIS	-	expression tag	UNP A0A059PIQ0
C	-3	HIS	-	expression tag	UNP A0A059PIQ0
C	-2	GLY	-	expression tag	UNP A0A059PIQ0
C	-1	SER	-	expression tag	UNP A0A059PIQ0
C	0	SER	-	expression tag	UNP A0A059PIQ0
C	1	VAL	-	expression tag	UNP A0A059PIQ0
C	2	SER	-	expression tag	UNP A0A059PIQ0
C	30	ARG	SER	conflict	UNP A0A059PIQ0
C	66	FHE	THR	chromophore	UNP A0A059PIQ0
C	66	FHE	TYR	chromophore	UNP A0A059PIQ0
C	66	FHE	GLY	chromophore	UNP A0A059PIQ0
C	72	SER	ALA	conflict	UNP A0A059PIQ0
C	206	LYS	ALA	conflict	UNP A0A059PIQ0
C	231	LEU	HIS	conflict	UNP A0A059PIQ0
C	239	GLY	-	expression tag	UNP A0A059PIQ0
C	240	ILE	-	expression tag	UNP A0A059PIQ0
C	241	GLU	-	expression tag	UNP A0A059PIQ0
C	242	GLU	-	expression tag	UNP A0A059PIQ0
C	243	ASN	-	expression tag	UNP A0A059PIQ0
C	244	LEU	-	expression tag	UNP A0A059PIQ0
C	245	TYR	-	expression tag	UNP A0A059PIQ0
C	246	PHE	-	expression tag	UNP A0A059PIQ0
C	247	GLN	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	248	SER	-	expression tag	UNP A0A059PIQ0
C	249	ASN	-	expression tag	UNP A0A059PIQ0
C	250	ILE	-	expression tag	UNP A0A059PIQ0
C	251	GLY	-	expression tag	UNP A0A059PIQ0
C	252	SER	-	expression tag	UNP A0A059PIQ0
C	253	GLY	-	expression tag	UNP A0A059PIQ0
D	-12	MET	-	initiating methionine	UNP A0A059PIQ0
D	-11	GLY	-	expression tag	UNP A0A059PIQ0
D	-10	SER	-	expression tag	UNP A0A059PIQ0
D	-9	SER	-	expression tag	UNP A0A059PIQ0
D	-8	HIS	-	expression tag	UNP A0A059PIQ0
D	-7	HIS	-	expression tag	UNP A0A059PIQ0
D	-6	HIS	-	expression tag	UNP A0A059PIQ0
D	-5	HIS	-	expression tag	UNP A0A059PIQ0
D	-4	HIS	-	expression tag	UNP A0A059PIQ0
D	-3	HIS	-	expression tag	UNP A0A059PIQ0
D	-2	GLY	-	expression tag	UNP A0A059PIQ0
D	-1	SER	-	expression tag	UNP A0A059PIQ0
D	0	SER	-	expression tag	UNP A0A059PIQ0
D	1	VAL	-	expression tag	UNP A0A059PIQ0
D	2	SER	-	expression tag	UNP A0A059PIQ0
D	30	ARG	SER	conflict	UNP A0A059PIQ0
D	66	FHE	THR	chromophore	UNP A0A059PIQ0
D	66	FHE	TYR	chromophore	UNP A0A059PIQ0
D	66	FHE	GLY	chromophore	UNP A0A059PIQ0
D	72	SER	ALA	conflict	UNP A0A059PIQ0
D	206	LYS	ALA	conflict	UNP A0A059PIQ0
D	231	LEU	HIS	conflict	UNP A0A059PIQ0
D	239	GLY	-	expression tag	UNP A0A059PIQ0
D	240	ILE	-	expression tag	UNP A0A059PIQ0
D	241	GLU	-	expression tag	UNP A0A059PIQ0
D	242	GLU	-	expression tag	UNP A0A059PIQ0
D	243	ASN	-	expression tag	UNP A0A059PIQ0
D	244	LEU	-	expression tag	UNP A0A059PIQ0
D	245	TYR	-	expression tag	UNP A0A059PIQ0
D	246	PHE	-	expression tag	UNP A0A059PIQ0
D	247	GLN	-	expression tag	UNP A0A059PIQ0
D	248	SER	-	expression tag	UNP A0A059PIQ0
D	249	ASN	-	expression tag	UNP A0A059PIQ0
D	250	ILE	-	expression tag	UNP A0A059PIQ0
D	251	GLY	-	expression tag	UNP A0A059PIQ0
D	252	SER	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	253	GLY	-	expression tag	UNP A0A059PIQ0

- Molecule 2 is water.

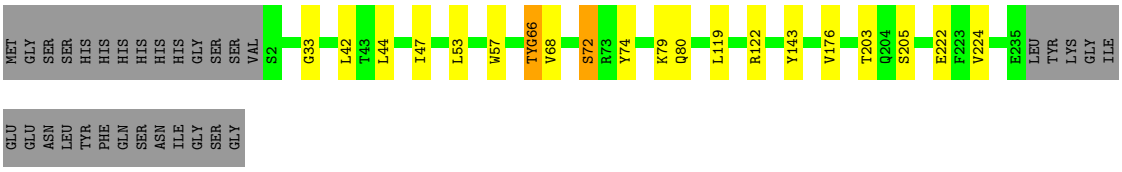
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	40	Total O 40 40	0	0
2	B	33	Total O 33 33	0	0
2	C	39	Total O 39 39	0	0
2	D	21	Total O 21 21	0	0

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.

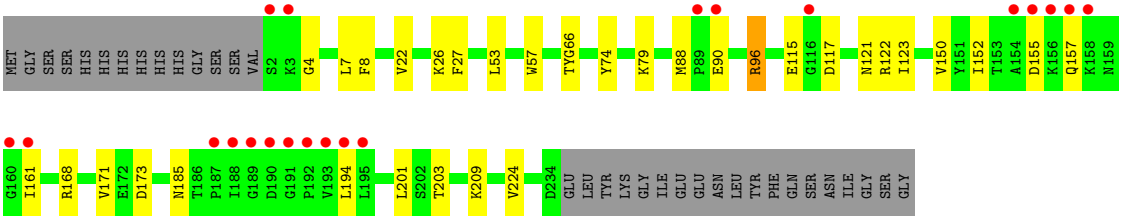
• Molecule 1: Green fluorescent protein

Chain A:



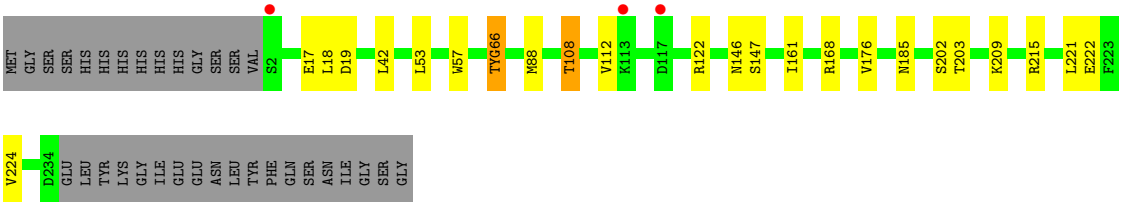
• Molecule 1: Green fluorescent protein

Chain B:



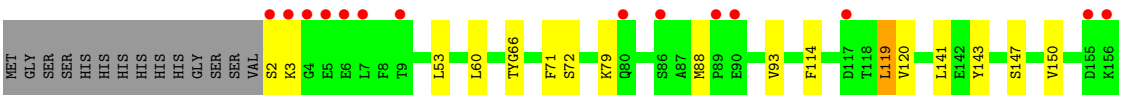
• Molecule 1: Green fluorescent protein

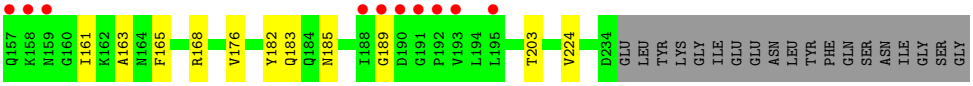
Chain C:



• Molecule 1: Green fluorescent protein

Chain D:




Q157
K158
N159
G160
I161
K162
A163
N164
F165
R168
V176
Y182
Q183
Q184
N185
I188
G189
D190
G191
P192
V193
L194
L195
T203
V224
D234
GLU
LEU
TYR
LYS
GLY
ILE
GLU
GLU
ASN
LEU
TYR
PHE
GLN
SER
ASN
ILE
GLY
SER
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	155.32Å 155.32Å 161.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.78 49.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.32-2.78) 100.0 (49.32-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.201 , 0.239 0.196 , 0.235	Depositor DCC
R_{free} test set	2903 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k 0.016 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7534	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: FHE

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	0.48	0/1863	0.63	1/2515 (0.0%)
1	B	0.47	0/1854	0.63	1/2503 (0.0%)
1	C	0.48	0/1854	0.63	0/2503
1	D	0.46	0/1854	0.61	1/2503 (0.0%)
All	All	0.47	0/7425	0.62	3/10024 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	119	LEU	CA-CB-CG	-5.39	102.91	115.30
1	D	119	LEU	CA-CB-CG	-5.25	103.22	115.30

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	1857	0	1785	15	0
1	B	1848	0	1778	22	0
1	C	1848	0	1779	19	0
1	D	1848	0	1777	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	40	0	0	0	0
2	B	33	0	0	0	0
2	C	39	0	0	1	0
2	D	21	0	0	0	0
All	All	7534	0	7119	60	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 4.

All (60) 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:A:222:GLU:HB3	1:C:42:LEU:HB2	1.66	0.78
1:B:203:THR:HG23	1:B:224:VAL:HG22	1.71	0.73
1:A:176:VAL:HG21	1:C:168:ARG:HD2	1.73	0.70
1:B:171:VAL:HG12	1:D:141:LEU:HD23	1.74	0.69
1:B:168:ARG:HD2	1:D:176:VAL:HG21	1.78	0.66
1:C:161:ILE:HG13	1:C:185:ASN:HB2	1.84	0.60
1:A:66:FHE:C10	1:C:146:ASN:HB2	2.31	0.59
1:D:203:THR:HG23	1:D:224:VAL:HG22	1.83	0.59
1:D:71:PHE:HE2	1:D:119:LEU:HD22	1.68	0.58
1:B:171:VAL:HG23	1:B:173:ASP:OD1	2.07	0.55
1:C:168:ARG:HB3	1:C:176:VAL:HG21	1.88	0.54
1:A:74:TYR:O	1:A:79:LYS:NZ	2.40	0.54
1:B:171:VAL:HG12	1:D:141:LEU:CD2	2.36	0.54
1:A:53:LEU:HD22	1:A:57:TRP:CE2	2.42	0.53
1:B:150:VAL:HG22	1:B:201:LEU:HB2	1.89	0.53
1:B:155:ASP:CG	1:B:157:GLN:HE22	2.12	0.53
1:B:209:LYS:HE2	1:D:143:TYR:CZ	2.44	0.53
1:D:88:MET:HE2	1:D:114:PHE:HD1	1.72	0.53
1:D:53:LEU:HD21	1:D:60:LEU:HD12	1.91	0.52
1:A:203:THR:HG23	1:A:224:VAL:HG22	1.90	0.52
1:B:152:ILE:HG23	1:B:161:ILE:HG23	1.92	0.52
1:D:163:ALA:HB3	1:D:183:GLN:HB3	1.92	0.52
1:D:168:ARG:HB3	1:D:176:VAL:HG11	1.91	0.51
1:B:74:TYR:O	1:B:79:LYS:HE3	2.11	0.51
1:C:17:GLU:OE1	1:C:122:ARG:NH1	2.37	0.50
1:C:88:MET:HE1	1:C:112:VAL:HG12	1.95	0.49
1:D:71:PHE:CE2	1:D:119:LEU:HD22	2.48	0.48
1:C:168:ARG:HB3	1:C:176:VAL:CG2	2.43	0.48
1:A:42:LEU:HB2	1:C:222:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:HB3	1:C:224:VAL:HG12	1.96	0.47
1:B:185:ASN:HA	1:D:93:VAL:O	2.14	0.47
1:B:117:ASP:N	1:B:117:ASP:OD1	2.48	0.47
1:D:161:ILE:HG12	1:D:185:ASN:HB2	1.97	0.47
1:B:90:GLU:HG3	1:D:189:GLY:HA3	1.98	0.46
1:B:4:GLY:HA2	1:B:7:LEU:HD12	1.99	0.45
1:B:121:ASN:ND2	1:B:123:ILE:HD11	2.32	0.45
1:C:53:LEU:HD22	1:C:57:TRP:CE2	2.51	0.45
1:C:161:ILE:CG1	1:C:185:ASN:HB2	2.47	0.44
1:B:115:GLU:OE2	1:B:122:ARG:NH1	2.36	0.44
1:A:80:GLN:H	1:A:80:GLN:HG2	1.55	0.44
1:C:18:LEU:HD23	1:C:19:ASP:N	2.34	0.43
1:A:42:LEU:HD21	1:A:68:VAL:HG23	2.00	0.43
1:B:194:LEU:HD11	1:D:2:SER:HB2	2.01	0.43
1:B:22:VAL:HG23	1:B:27:PHE:HE1	1.84	0.43
1:B:26:LYS:HB3	1:B:26:LYS:HE3	1.73	0.42
1:B:96:ARG:HA	1:D:182:TYR:O	2.20	0.42
1:D:168:ARG:HB3	1:D:176:VAL:CG1	2.49	0.42
1:D:119:LEU:HG	1:D:120:VAL:N	2.32	0.42
1:C:108:THR:HG21	2:C:329:HOH:O	2.19	0.42
1:B:8:PHE:CE2	1:B:88:MET:HG3	2.55	0.41
1:A:33:GLY:HA3	1:A:44:LEU:HD23	2.02	0.41
1:C:53:LEU:HD12	1:C:53:LEU:HA	1.95	0.41
1:B:53:LEU:HD22	1:B:57:TRP:CE2	2.55	0.41
1:C:203:THR:HG22	1:C:224:VAL:HG13	2.01	0.41
1:D:53:LEU:HD12	1:D:53:LEU:HA	1.92	0.41
1:A:122:ARG:HH11	1:A:122:ARG:HD2	1.74	0.41
1:A:143:TYR:CZ	1:C:209:LYS:HE2	2.55	0.41
1:A:205:SER:HB2	1:C:66:FHE:C11	2.50	0.41
1:D:150:VAL:HG13	1:D:165:PHE:CD1	2.56	0.41
1:A:47:ILE:HD13	1:C:215:ARG:CZ	2.51	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	227/264 (86%)	220 (97%)	7 (3%)	0	100	100
1	B	226/264 (86%)	217 (96%)	9 (4%)	0	100	100
1	C	226/264 (86%)	220 (97%)	6 (3%)	0	100	100
1	D	226/264 (86%)	218 (96%)	7 (3%)	1 (0%)	34	64
All	All	905/1056 (86%)	875 (97%)	29 (3%)	1 (0%)	51	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	79	LYS

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	202/229 (88%)	201 (100%)	1 (0%)	88	95
1	B	201/229 (88%)	201 (100%)	0	100	100
1	C	201/229 (88%)	197 (98%)	4 (2%)	55	82
1	D	201/229 (88%)	198 (98%)	3 (2%)	65	87
All	All	805/916 (88%)	797 (99%)	8 (1%)	76	91

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

Mol	Chain	Res	Type
1	A	72	SER
1	C	108	THR
1	C	147	SER
1	C	202	SER
1	C	221	LEU
1	D	3	LYS
1	D	72	SER

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Mol	Chain	Res	Type
1	D	147	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	FHE	A	66	1	31,34,35	5.04	8 (25%)	38,47,49	3.23	15 (39%)
1	FHE	C	66	1	31,34,35	4.91	7 (22%)	38,47,49	2.92	10 (26%)
1	FHE	B	66	1	31,34,35	5.35	7 (22%)	38,47,49	3.52	14 (36%)
1	FHE	D	66	1	31,34,35	4.95	8 (25%)	38,47,49	2.78	12 (31%)

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
1	FHE	A	66	1	-	5/16/40/41	0/3/3/3
1	FHE	C	66	1	-	4/16/40/41	0/3/3/3
1	FHE	B	66	1	-	5/16/40/41	0/3/3/3
1	FHE	D	66	1	-	5/16/40/41	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	FHE	CB2-CA2	23.22	1.54	1.35
1	A	66	FHE	CB2-CA2	21.27	1.52	1.35
1	D	66	FHE	CB2-CA2	21.08	1.52	1.35
1	C	66	FHE	CB2-CA2	20.84	1.52	1.35
1	B	66	FHE	O15-N14	11.11	1.41	1.22
1	A	66	FHE	O15-N14	10.63	1.40	1.22
1	C	66	FHE	O15-N14	10.63	1.40	1.22
1	D	66	FHE	O15-N14	10.61	1.40	1.22
1	B	66	FHE	O2-C2	10.08	1.44	1.23
1	A	66	FHE	CA2-C2	-9.85	1.38	1.48
1	C	66	FHE	CA2-C2	-9.19	1.39	1.48
1	D	66	FHE	O2-C2	9.08	1.42	1.23
1	B	66	FHE	CA2-C2	-8.80	1.39	1.48
1	D	66	FHE	CA2-C2	-8.58	1.40	1.48
1	A	66	FHE	O2-C2	8.23	1.40	1.23
1	C	66	FHE	O2-C2	8.01	1.40	1.23
1	C	66	FHE	CG2-CB2	4.24	1.55	1.46
1	B	66	FHE	CG2-CB2	3.52	1.53	1.46
1	A	66	FHE	CG2-CB2	3.49	1.53	1.46
1	A	66	FHE	C2-N3	-3.45	1.31	1.39
1	D	66	FHE	CG2-CB2	3.17	1.53	1.46
1	D	66	FHE	C2-N3	-3.04	1.32	1.39
1	C	66	FHE	C2-N3	-2.79	1.33	1.39
1	A	66	FHE	C1-N3	-2.78	1.32	1.37
1	C	66	FHE	CA2-N2	-2.62	1.33	1.38
1	A	66	FHE	CA2-N2	-2.55	1.33	1.38
1	D	66	FHE	CA2-N2	-2.42	1.33	1.38
1	B	66	FHE	OH-C4	-2.12	1.36	1.43
1	B	66	FHE	C2-N3	-2.09	1.34	1.39
1	D	66	FHE	CA1-C1	2.04	1.54	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	FHE	O2-C2-CA2	-13.94	123.14	130.96
1	C	66	FHE	CG2-CB2-CA2	-8.95	118.98	129.94
1	A	66	FHE	CG2-CB2-CA2	-8.90	119.03	129.94
1	A	66	FHE	CA2-C2-N3	8.28	107.28	103.37
1	D	66	FHE	O2-C2-CA2	-8.12	126.40	130.96
1	A	66	FHE	O2-C2-CA2	-8.07	126.43	130.96
1	C	66	FHE	CA2-C2-N3	7.86	107.09	103.37
1	C	66	FHE	O2-C2-CA2	-7.85	126.55	130.96
1	D	66	FHE	CG2-CB2-CA2	-7.78	120.41	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	FHE	CG2-CB2-CA2	-7.71	120.50	129.94
1	D	66	FHE	C4-C8-C13	-7.35	119.86	123.94
1	A	66	FHE	C4-C8-C13	6.92	127.78	123.94
1	B	66	FHE	N3-C1-N2	-6.41	107.02	111.45
1	B	66	FHE	CA2-C2-N3	6.17	106.29	103.37
1	B	66	FHE	CA2-N2-C1	6.02	110.21	105.77
1	C	66	FHE	C4-C8-C13	-5.23	121.04	123.94
1	D	66	FHE	CA2-C2-N3	4.87	105.67	103.37
1	A	66	FHE	C4-OH-CZ	-4.61	106.27	117.65
1	C	66	FHE	CA2-N2-C1	4.22	108.88	105.77
1	A	66	FHE	N3-C1-N2	-4.11	108.61	111.45
1	C	66	FHE	N3-C1-N2	-4.09	108.62	111.45
1	B	66	FHE	C2-N3-C1	3.81	109.90	107.97
1	B	66	FHE	C12-C13-N14	-3.81	112.41	116.47
1	D	66	FHE	N3-C1-N2	-3.77	108.84	111.45
1	A	66	FHE	CA2-N2-C1	3.70	108.50	105.77
1	A	66	FHE	OH-C4-C8	3.44	119.53	109.38
1	A	66	FHE	C2-CA2-N2	-3.43	106.53	108.93
1	B	66	FHE	C2-CA2-N2	-3.36	106.58	108.93
1	A	66	FHE	C4-C8-C9	-3.14	112.69	119.52
1	B	66	FHE	O2-C2-N3	3.11	130.53	124.35
1	D	66	FHE	O15-N14-C13	3.04	124.23	119.03
1	C	66	FHE	C1-CA1-CB1	3.03	116.71	110.78
1	D	66	FHE	C1-CA1-CB1	3.02	116.68	110.78
1	C	66	FHE	C2-CA2-N2	-2.95	106.86	108.93
1	D	66	FHE	C2-N3-C1	2.91	109.44	107.97
1	B	66	FHE	CB2-CA2-N2	2.84	132.76	128.83
1	D	66	FHE	CA2-N2-C1	2.83	107.86	105.77
1	C	66	FHE	O3-C3-CA3	-2.73	118.14	126.39
1	B	66	FHE	O3-C3-CA3	-2.68	118.31	126.39
1	D	66	FHE	C4-OH-CZ	-2.57	111.29	117.65
1	A	66	FHE	O15-N14-C13	2.56	123.42	119.03
1	D	66	FHE	CD2-CG2-CD1	2.56	121.43	117.64
1	A	66	FHE	C12-C13-N14	-2.40	113.91	116.47
1	D	66	FHE	CE2-CD2-CG2	-2.25	118.31	121.25
1	C	66	FHE	C4-OH-CZ	-2.22	112.17	117.65
1	B	66	FHE	C4-C8-C9	-2.19	114.75	119.52
1	A	66	FHE	C2-N3-C1	2.19	109.07	107.97
1	A	66	FHE	C1-CA1-CB1	2.16	115.00	110.78
1	B	66	FHE	CD2-CG2-CD1	2.09	120.73	117.64
1	A	66	FHE	O3-C3-CA3	-2.08	120.12	126.39
1	B	66	FHE	C4-OH-CZ	-2.04	112.61	117.65

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	FHE	C2-CA2-CB2-CG2
1	D	66	FHE	C2-CA2-CB2-CG2
1	C	66	FHE	CE1-CZ-OH-C4
1	C	66	FHE	CE2-CZ-OH-C4
1	A	66	FHE	N2-CA2-CB2-CG2
1	B	66	FHE	N2-CA2-CB2-CG2
1	D	66	FHE	N2-CA2-CB2-CG2
1	B	66	FHE	CE2-CZ-OH-C4
1	B	66	FHE	CE1-CZ-OH-C4
1	A	66	FHE	C3-CA3-N3-C2
1	C	66	FHE	C3-CA3-N3-C2
1	B	66	FHE	C8-C4-OH-CZ
1	C	66	FHE	C8-C4-OH-CZ
1	A	66	FHE	C2-CA2-CB2-CG2
1	D	66	FHE	C8-C4-OH-CZ
1	A	66	FHE	CE2-CZ-OH-C4
1	A	66	FHE	CE1-CZ-OH-C4
1	D	66	FHE	C12-C13-N14-O15
1	D	66	FHE	N2-C1-CA1-CB1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	FHE	1	0
1	C	66	FHE	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	231/264 (87%)	0.06	0 100 100	35, 40, 57, 94	0
1	B	230/264 (87%)	0.54	21 (9%) 9 6	37, 48, 68, 92	0
1	C	230/264 (87%)	0.12	3 (1%) 77 75	35, 41, 56, 89	0
1	D	230/264 (87%)	0.64	24 (10%) 6 4	37, 51, 74, 94	0
All	All	921/1056 (87%)	0.34	48 (5%) 27 22	35, 45, 66, 94	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	SER	7.9
1	B	156	LYS	4.8
1	D	190	ASP	4.7
1	B	195	LEU	4.3
1	B	189	GLY	4.2
1	B	193	VAL	4.2
1	B	194	LEU	4.1
1	B	190	ASP	4.0
1	B	157	GLN	4.0
1	B	3	LYS	3.9
1	B	155	ASP	3.9
1	D	7	LEU	3.8
1	C	117	ASP	3.7
1	B	188	ILE	3.7
1	D	157	GLN	3.5
1	B	154	ALA	3.4
1	D	193	VAL	3.3
1	B	192	PRO	3.3
1	D	3	LYS	3.2
1	D	192	PRO	3.1
1	D	195	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	5	GLU	3.0
1	D	191	GLY	3.0
1	D	156	LYS	2.9
1	D	188	ILE	2.9
1	D	6	GLU	2.8
1	D	155	ASP	2.7
1	B	158	LYS	2.7
1	D	4	GLY	2.7
1	B	160	GLY	2.7
1	C	2	SER	2.7
1	B	90	GLU	2.7
1	D	86	SER	2.6
1	D	189	GLY	2.6
1	D	89	PRO	2.5
1	B	187	PRO	2.5
1	B	161	ILE	2.5
1	D	117	ASP	2.5
1	D	90	GLU	2.4
1	D	158	LYS	2.4
1	B	116	GLY	2.3
1	D	9	THR	2.3
1	D	80	GLN	2.2
1	C	113	LYS	2.2
1	D	159	ASN	2.1
1	B	89	PRO	2.1
1	B	2	SER	2.0
1	B	191	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	FHE	B	66	32/33	0.94	0.20	41,42,58,72	0
1	FHE	D	66	32/33	0.96	0.17	44,45,69,75	0
1	FHE	C	66	32/33	0.97	0.18	35,37,47,58	0
1	FHE	A	66	32/33	0.97	0.19	34,36,56,60	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.