Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2016 – 03:47 PM EST

PDB ID	:	5FHP
Title	:	SeMet regulator of nicotine degradation
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Deposited on	:	2015-12-22
Resolution	:	2.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

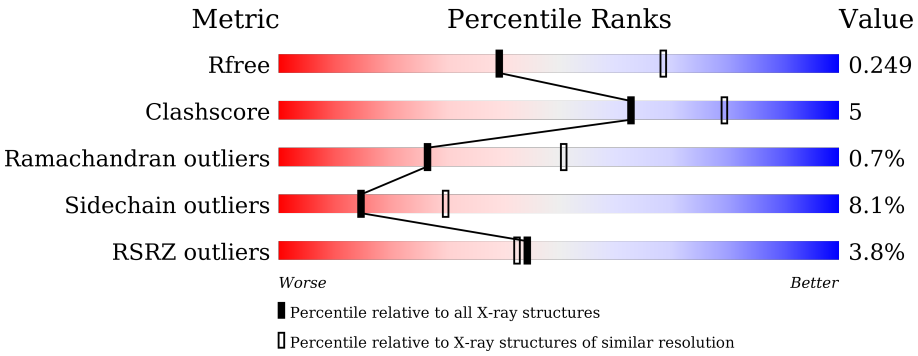
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.65 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. 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	209	2% 81% 14%
1	B	209	2% 82% 12%
1	C	209	4% 85% 11%
1	D	209	6% 79% 14%
1	E	209	3% 78% 17%
1	F	209	4% 78% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	301	-	-	-	X
2	GOL	F	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10162 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.

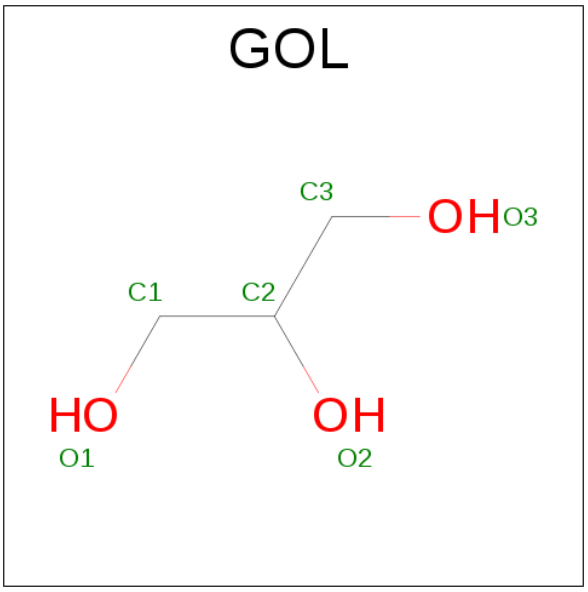
- Molecule 1 is a protein called NicR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	Se	0	0	0
			1675	1058	289	318	1	9			
1	B	206	Total	C	N	O	S	Se	0	0	0
			1662	1050	287	315	1	9			
1	C	209	Total	C	N	O	S	Se	0	0	0
			1696	1073	292	321	1	9			
1	D	201	Total	C	N	O	S	Se	0	0	0
			1626	1031	278	307	1	9			
1	E	205	Total	C	N	O	S	Se	0	0	0
			1658	1047	286	316	1	8			
1	F	201	Total	C	N	O	S	Se	0	0	0
			1623	1026	279	308	1	9			

There are 6 discrepancies between the modelled and reference sequences:

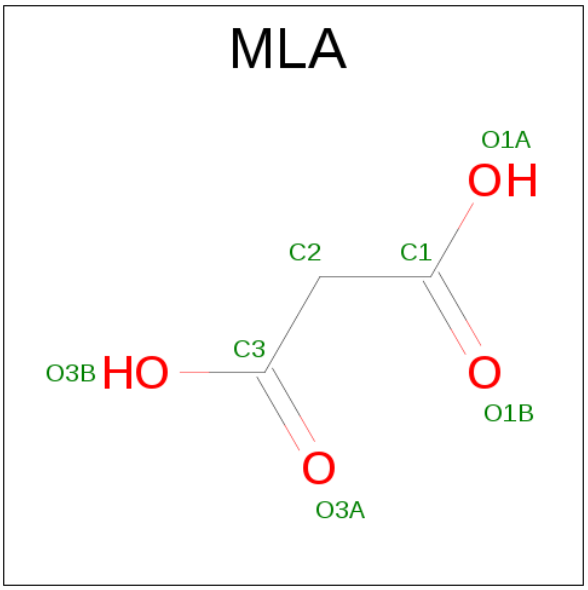
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MSE	-	initiating methionine	UNP A0A0B4KIF6
B	30	MSE	-	initiating methionine	UNP A0A0B4KIF6
C	30	MSE	-	initiating methionine	UNP A0A0B4KIF6
D	30	MSE	-	initiating methionine	UNP A0A0B4KIF6
E	30	MSE	-	initiating methionine	UNP A0A0B4KIF6
F	30	MSE	-	initiating methionine	UNP A0A0B4KIF6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 7 3 4	0	0
3	E	1	Total C O 7 3 4	0	0

- Molecule 4 is water.

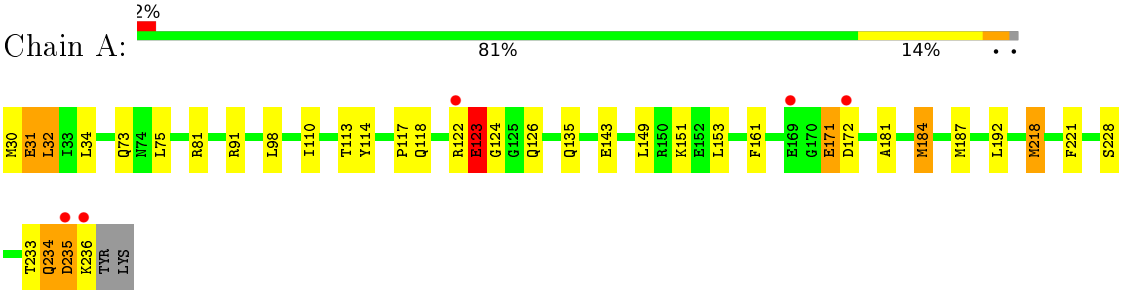
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	30	Total O 30 30	0	0
4	C	30	Total O 30 30	0	0
4	D	27	Total O 27 27	0	0
4	E	33	Total O 33 33	0	0
4	F	24	Total O 24 24	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

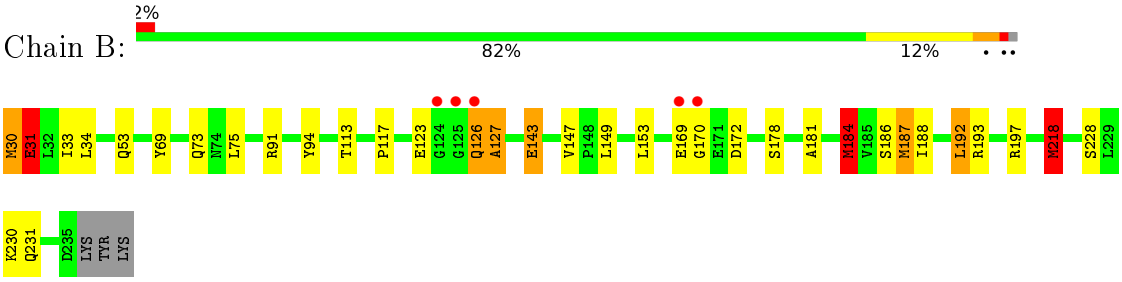
- Molecule 1: NicR

Chain A:



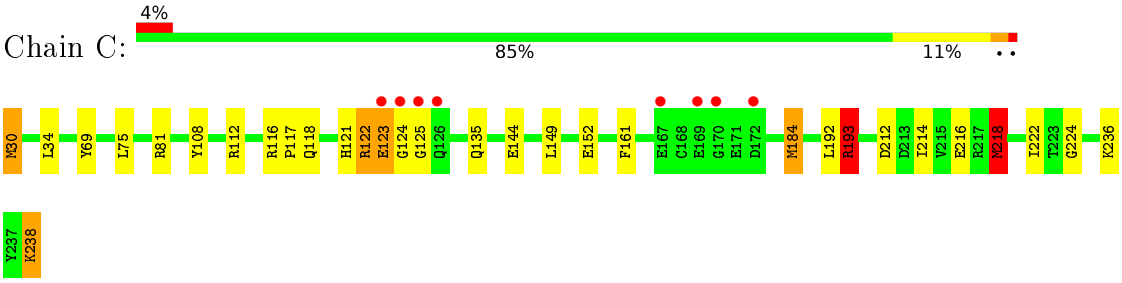
- Molecule 1: NicR

Chain B:



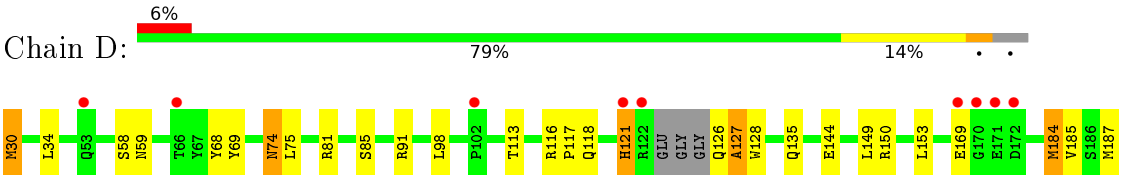
- Molecule 1: NicR

Chain C:

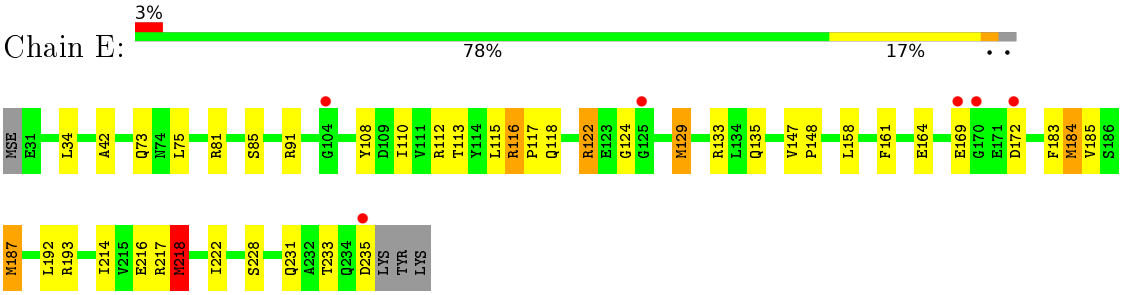


- Molecule 1: NicR

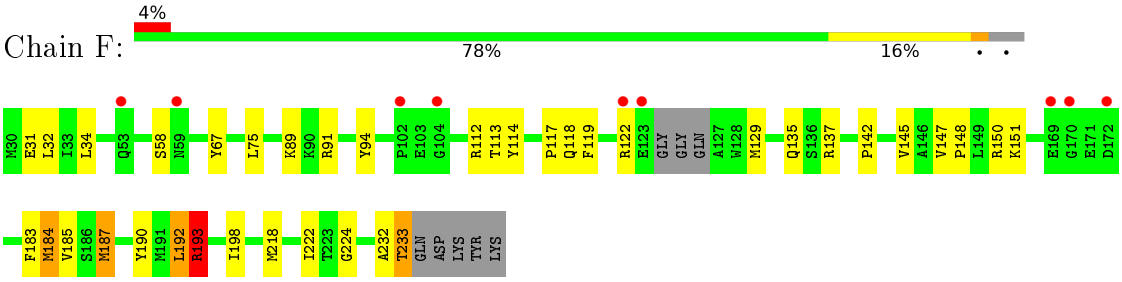
Chain D:



- Molecule 1: NicR



- Molecule 1: NicR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	150.01Å 150.01Å 156.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.61 – 2.65 37.90 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.61-2.65) 99.9 (37.90-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.197 , 0.251 0.199 , 0.249	Depositor DCC
R_{free} test set	2672 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k 0.012 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10162	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

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

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	0.81	1/1699 (0.1%)	1.00	6/2276 (0.3%)
1	B	0.79	1/1686 (0.1%)	0.94	3/2260 (0.1%)
1	C	0.75	0/1721	0.91	5/2305 (0.2%)
1	D	0.74	0/1649	0.86	1/2210 (0.0%)
1	E	0.74	0/1682	0.96	7/2255 (0.3%)
1	F	0.74	0/1644	0.92	7/2201 (0.3%)
All	All	0.76	2/10081 (0.0%)	0.93	29/13507 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	GLU	CG-CD	5.54	1.60	1.51
1	B	143	GLU	CG-CD	5.46	1.60	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	MSE	CB-CA-C	-10.61	89.19	110.40
1	E	122	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	184	MSE	CA-CB-CG	8.61	127.94	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184	MSE	CB-CA-C	-6.89	96.62	110.40
1	B	187	MSE	CG-SE-CE	-6.88	83.77	98.90
1	F	193	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	193	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	E	184	MSE	CB-CA-C	-6.51	97.38	110.40
1	A	81	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	218	MSE	N-CA-CB	6.13	121.64	110.60
1	F	193	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	184	MSE	CB-CA-C	-5.91	98.58	110.40
1	E	129	MSE	CG-SE-CE	5.88	111.84	98.90
1	B	218	MSE	N-CA-CB	5.84	121.12	110.60
1	F	193	ARG	CG-CD-NE	5.78	123.94	111.80
1	A	122	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	124	GLY	N-CA-C	-5.58	99.16	113.10
1	F	184	MSE	CB-CA-C	-5.48	99.45	110.40
1	E	116	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	137	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	218	MSE	N-CA-CB	5.33	120.20	110.60
1	E	217	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	122	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	143	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	D	150	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	112	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	30	MSE	CG-SE-CE	5.05	110.01	98.90
1	C	193	ARG	CG-CD-NE	5.05	122.40	111.80
1	F	150	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	GLU	Peptide
1	C	123	GLU	Peptide

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	1675	0	1639	20	0
1	B	1662	0	1622	20	0
1	C	1696	0	1661	15	0
1	D	1626	0	1590	21	0
1	E	1658	0	1617	18	0
1	F	1623	0	1591	20	0
2	A	6	0	8	0	0
2	D	6	0	8	1	0
2	E	6	0	8	0	0
2	F	6	0	8	2	0
3	B	7	0	2	0	0
3	E	7	0	2	0	0
4	A	40	0	0	3	0
4	B	30	0	0	0	0
4	C	30	0	0	1	0
4	D	27	0	0	2	0
4	E	33	0	0	2	0
4	F	24	0	0	0	0
All	All	10162	0	9756	105	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 5.

All (105) 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:D:118:GLN:HE22	1:D:135:GLN:HE22	1.17	0.88
1:A:123:GLU:OE1	1:A:124:GLY:HA2	1.78	0.84
1:C:81:ARG:NH2	1:C:152:GLU:OE2	2.10	0.83
1:C:118:GLN:HE22	1:C:135:GLN:HE22	1.31	0.78
1:F:193:ARG:HH11	1:F:193:ARG:HG2	1.58	0.69
1:A:221:PHE:HE2	1:D:187:MSE:HE1	1.57	0.69
1:A:118:GLN:HE22	1:A:135:GLN:HE22	1.41	0.68
1:A:161:PHE:CE1	1:A:184:MSE:HE2	2.28	0.68
1:C:238:LYS:HE3	1:C:238:LYS:HA	1.75	0.68
1:F:184:MSE:HG2	1:F:222:ILE:HD13	1.77	0.66
1:A:171:GLU:HB3	4:A:403:HOH:O	1.96	0.65
1:E:233:THR:HG21	4:E:411:HOH:O	1.98	0.64
1:A:114:TYR:HB3	1:A:184:MSE:HE1	1.81	0.62
1:A:181:ALA:O	1:A:184:MSE:HB2	2.00	0.62
1:C:112:ARG:NH2	1:C:212:ASP:OD1	2.33	0.61
1:F:118:GLN:HE22	1:F:135:GLN:HE22	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ARG:HH11	1:C:193:ARG:HG2	1.66	0.60
1:D:149:LEU:HD23	1:D:153:LEU:HD12	1.83	0.60
1:A:161:PHE:CZ	1:A:184:MSE:HE2	2.37	0.59
1:B:30:MSE:HA	1:B:31:GLU:HB2	1.85	0.59
1:D:121:HIS:HB2	1:D:128:TRP:CG	2.38	0.59
1:E:214:ILE:O	1:E:218:MSE:HG2	2.03	0.59
1:C:184:MSE:HG2	1:C:222:ILE:HD13	1.85	0.58
1:D:30:MSE:HA	1:D:30:MSE:HE3	1.85	0.58
1:D:184:MSE:HG2	1:D:222:ILE:HD13	1.86	0.58
1:D:127:ALA:O	4:D:401:HOH:O	2.16	0.58
1:D:118:GLN:NE2	1:D:135:GLN:HE22	1.98	0.57
1:D:30:MSE:HE1	1:D:68:TYR:CG	2.40	0.57
1:E:161:PHE:CE2	1:E:184:MSE:HE2	2.40	0.56
1:B:170:GLY:O	1:B:230:LYS:HE2	2.06	0.56
1:D:126:GLN:O	1:D:127:ALA:C	2.44	0.56
1:C:238:LYS:HE3	1:C:238:LYS:CA	2.36	0.55
1:C:30:MSE:N	1:C:69:TYR:HH	2.04	0.55
1:E:133:ARG:HG3	4:E:414:HOH:O	2.06	0.55
1:E:118:GLN:HE22	1:E:135:GLN:HE22	1.55	0.55
1:B:91:ARG:HG3	1:B:117:PRO:HG2	1.87	0.54
1:A:31:GLU:C	4:A:404:HOH:O	2.47	0.53
1:B:94:TYR:HB2	1:B:113:THR:HG23	1.91	0.52
1:B:149:LEU:HD23	1:B:153:LEU:HD12	1.92	0.51
1:B:187:MSE:HE2	1:F:183:PHE:HB3	1.92	0.51
1:F:185:VAL:HG11	2:F:301:GOL:H31	1.92	0.51
1:A:32:LEU:N	4:A:404:HOH:O	2.42	0.51
1:B:186:SER:HB2	1:F:190:TYR:HB2	1.92	0.51
1:F:232:ALA:N	1:F:233:THR:HA	2.26	0.50
1:D:30:MSE:HE1	1:D:68:TYR:CD1	2.47	0.50
1:E:183:PHE:O	1:E:187:MSE:HG2	2.12	0.49
1:C:214:ILE:O	1:C:218:MSE:HG2	2.13	0.48
1:E:115:LEU:HD13	1:E:218:MSE:HG3	1.96	0.48
1:A:228:SER:OG	1:D:224:GLY:HA3	2.13	0.48
1:F:184:MSE:HG2	1:F:222:ILE:CD1	2.43	0.48
1:A:110:ILE:O	1:A:113:THR:HB	2.13	0.47
1:A:91:ARG:HG3	1:A:117:PRO:HG2	1.97	0.47
1:E:42:ALA:HB1	1:E:133:ARG:HD3	1.96	0.47
1:A:187:MSE:HE2	1:A:218:MSE:HB3	1.96	0.47
1:B:186:SER:HB2	1:F:190:TYR:CB	2.44	0.47
1:E:147:VAL:HB	1:E:148:PRO:HD3	1.97	0.47
1:B:30:MSE:HA	1:B:31:GLU:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ARG:N	1:C:122:ARG:CD	2.78	0.47
1:E:91:ARG:HG3	1:E:117:PRO:HG2	1.97	0.47
1:B:188:ILE:HG22	1:B:192:LEU:HD22	1.96	0.46
1:D:116:ARG:HG2	1:F:67:TYR:OH	2.15	0.46
1:C:122:ARG:N	1:C:122:ARG:HD3	2.29	0.46
1:F:91:ARG:HG3	1:F:117:PRO:HG2	1.97	0.46
1:E:158:LEU:HD11	1:E:185:VAL:HG21	1.97	0.46
1:B:181:ALA:O	1:B:184:MSE:HB2	2.16	0.46
1:A:234:GLN:N	1:A:234:GLN:HE21	2.14	0.46
1:B:149:LEU:CD2	1:B:153:LEU:HD12	2.45	0.45
1:E:81:ARG:O	1:E:85:SER:HB2	2.16	0.45
1:A:114:TYR:CD1	1:A:184:MSE:HE3	2.51	0.45
1:E:108:TYR:OH	1:E:216:GLU:OE1	2.33	0.45
1:D:218:MSE:O	1:D:222:ILE:HD12	2.16	0.45
1:D:69:TYR:O	1:D:74:ASN:HB3	2.16	0.45
1:F:187:MSE:HB2	1:F:218:MSE:HE3	1.98	0.45
1:E:184:MSE:HG2	1:E:222:ILE:HD13	2.00	0.44
1:F:193:ARG:CG	1:F:193:ARG:HH11	2.26	0.44
1:F:119:PHE:CE1	1:F:192:LEU:HD13	2.53	0.44
1:F:147:VAL:HB	1:F:148:PRO:HD3	1.98	0.44
1:D:91:ARG:HG3	1:D:117:PRO:HG2	1.99	0.43
1:A:234:GLN:CA	1:A:234:GLN:HE21	2.32	0.43
1:E:112:ARG:O	1:E:116:ARG:HG3	2.18	0.43
1:B:187:MSE:HB3	1:B:218:MSE:HE3	2.01	0.43
1:A:149:LEU:CD2	1:A:153:LEU:HD12	2.49	0.43
1:C:108:TYR:OH	1:C:216:GLU:OE1	2.37	0.43
1:F:94:TYR:HB2	1:F:113:THR:HG23	2.00	0.43
1:D:149:LEU:CD2	1:D:153:LEU:HD12	2.48	0.43
1:B:197:ARG:HE	2:F:301:GOL:H32	1.84	0.42
1:D:185:VAL:HG13	2:D:301:GOL:H12	2.01	0.42
1:A:114:TYR:CG	1:A:184:MSE:HE3	2.54	0.42
1:B:126:GLN:HG2	1:B:126:GLN:O	2.20	0.42
1:A:149:LEU:HD23	1:A:153:LEU:HD12	2.00	0.42
1:E:110:ILE:HD12	1:E:164:GLU:HB3	2.02	0.42
1:B:30:MSE:O	1:B:69:TYR:OH	2.37	0.42
1:D:81:ARG:O	1:D:85:SER:HB2	2.20	0.42
1:F:114:TYR:CD2	1:F:184:MSE:HE1	2.54	0.42
1:C:116:ARG:HB3	1:C:117:PRO:HD3	2.00	0.42
1:D:30:MSE:HA	1:D:30:MSE:CE	2.50	0.41
1:F:142:PRO:HD2	1:F:145:VAL:HG22	2.02	0.41
1:C:161:PHE:HB3	4:C:322:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:GLU:HG3	4:D:420:HOH:O	2.20	0.41
1:E:161:PHE:CZ	1:E:184:MSE:HE2	2.55	0.41
1:B:178:SER:HB3	1:F:198:ILE:HD12	2.02	0.41
1:B:143:GLU:HG3	1:B:147:VAL:HG23	2.03	0.41
1:C:224:GLY:HA3	1:E:228:SER:OG	2.20	0.41
1:B:126:GLN:O	1:B:127:ALA:HB2	2.21	0.40
1:B:228:SER:OG	1:F:224:GLY:HA3	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	205/209 (98%)	197 (96%)	6 (3%)	2 (1%)	19	41
1	B	204/209 (98%)	197 (97%)	4 (2%)	3 (2%)	13	28
1	C	207/209 (99%)	201 (97%)	4 (2%)	2 (1%)	19	41
1	D	197/209 (94%)	194 (98%)	2 (1%)	1 (0%)	34	59
1	E	203/209 (97%)	199 (98%)	3 (2%)	1 (0%)	34	59
1	F	197/209 (94%)	192 (98%)	5 (2%)	0	100	100
All	All	1213/1254 (97%)	1180 (97%)	24 (2%)	9 (1%)	26	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	126	GLN
1	B	127	ALA
1	D	127	ALA
1	B	31	GLU
1	C	123	GLU

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Mol	Chain	Res	Type
1	C	125	GLY
1	A	123	GLU
1	A	235	ASP
1	E	124	GLY

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	177/170 (104%)	160 (90%)	17 (10%)	10	21
1	B	175/170 (103%)	161 (92%)	14 (8%)	15	31
1	C	179/170 (105%)	167 (93%)	12 (7%)	20	41
1	D	172/170 (101%)	157 (91%)	15 (9%)	13	26
1	E	175/170 (103%)	161 (92%)	14 (8%)	15	31
1	F	172/170 (101%)	159 (92%)	13 (8%)	16	34
All	All	1050/1020 (103%)	965 (92%)	85 (8%)	15	30

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	32	LEU
1	A	34	LEU
1	A	73	GLN
1	A	75	LEU
1	A	98	LEU
1	A	123	GLU
1	A	126	GLN
1	A	151	LYS
1	A	171	GLU
1	A	172	ASP
1	A	192	LEU
1	A	218	MSE
1	A	233	THR

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	235	ASP
1	A	236	LYS
1	B	30	MSE
1	B	31	GLU
1	B	33	ILE
1	B	34	LEU
1	B	53	GLN
1	B	73	GLN
1	B	75	LEU
1	B	169	GLU
1	B	172	ASP
1	B	184	MSE
1	B	192	LEU
1	B	193	ARG
1	B	218	MSE
1	B	231	GLN
1	C	30	MSE
1	C	34	LEU
1	C	75	LEU
1	C	121	HIS
1	C	122	ARG
1	C	144	GLU
1	C	149	LEU
1	C	192	LEU
1	C	193	ARG
1	C	218	MSE
1	C	236	LYS
1	C	238	LYS
1	D	30	MSE
1	D	34	LEU
1	D	58	SER
1	D	59	ASN
1	D	74	ASN
1	D	75	LEU
1	D	98	LEU
1	D	113	THR
1	D	121	HIS
1	D	144	GLU
1	D	169	GLU
1	D	184	MSE
1	D	192	LEU

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Mol	Chain	Res	Type
1	D	206	LEU
1	D	218	MSE
1	E	34	LEU
1	E	73	GLN
1	E	75	LEU
1	E	113	THR
1	E	122	ARG
1	E	129	MSE
1	E	169	GLU
1	E	172	ASP
1	E	187	MSE
1	E	192	LEU
1	E	193	ARG
1	E	218	MSE
1	E	231	GLN
1	E	235	ASP
1	F	31	GLU
1	F	32	LEU
1	F	34	LEU
1	F	58	SER
1	F	75	LEU
1	F	89	LYS
1	F	122	ARG
1	F	129	MSE
1	F	151	LYS
1	F	187	MSE
1	F	192	LEU
1	F	193	ARG
1	F	233	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	121	HIS
1	A	135	GLN
1	A	207	HIS
1	A	234	GLN
1	B	57	ASN
1	B	74	ASN
1	B	93	ASN
1	B	135	GLN

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Mol	Chain	Res	Type
1	C	53	GLN
1	C	57	ASN
1	C	62	GLN
1	C	74	ASN
1	C	93	ASN
1	C	135	GLN
1	D	93	ASN
1	D	135	GLN
1	E	53	GLN
1	E	57	ASN
1	E	93	ASN
1	E	135	GLN
1	F	74	ASN
1	F	93	ASN
1	F	121	HIS
1	F	135	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

6 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	GOL	A	301	-	5,5,5	0.29	0	5,5,5	0.73	0
3	MLA	B	301	-	0,6,6	0.00	-	0,7,7	0.00	-
2	GOL	D	301	-	5,5,5	0.69	0	5,5,5	1.01	0
3	MLA	E	301	-	0,6,6	0.00	-	0,7,7	0.00	-
2	GOL	E	302	-	5,5,5	0.28	0	5,5,5	0.16	0
2	GOL	F	301	-	5,5,5	1.21	0	5,5,5	1.52	1 (20%)

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	GOL	A	301	-	-	0/4/4/4	0/0/0/0
3	MLA	B	301	-	-	0/0/4/4	0/0/0/0
2	GOL	D	301	-	-	0/4/4/4	0/0/0/0
3	MLA	E	301	-	-	0/0/4/4	0/0/0/0
2	GOL	E	302	-	-	0/4/4/4	0/0/0/0
2	GOL	F	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	GOL	O3-C3-C2	2.05	120.36	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GOL	1	0
2	F	301	GOL	2	0

5.7 Other polymers (i)

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	198/209 (94%)	-0.28	5 (2%)	61	59	16, 28, 63, 120	1 (0%)
1	B	197/209 (94%)	-0.26	5 (2%)	61	59	17, 32, 76, 112	0
1	C	200/209 (95%)	-0.06	8 (4%)	42	40	17, 36, 82, 133	2 (1%)
1	D	192/209 (91%)	-0.00	12 (6%)	23	21	16, 36, 90, 210	1 (0%)
1	E	197/209 (94%)	-0.14	6 (3%)	54	52	17, 35, 91, 118	1 (0%)
1	F	192/209 (91%)	-0.06	9 (4%)	35	33	21, 39, 77, 111	0
All	All	1176/1254 (93%)	-0.13	45 (3%)	44	42	16, 34, 83, 210	5 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	GLU	7.5
1	F	123	GLU	5.6
1	A	169	GLU	5.3
1	D	169	GLU	5.2
1	B	125	GLY	4.8
1	A	235	ASP	4.4
1	C	169	GLU	4.2
1	F	170	GLY	3.6
1	F	102	PRO	3.6
1	C	124	GLY	3.4
1	D	121	HIS	3.3
1	D	172	ASP	3.3
1	D	170	GLY	3.3
1	B	124	GLY	3.3
1	E	170	GLY	3.2
1	C	125	GLY	3.1
1	E	235	ASP	3.1
1	F	169	GLU	3.1
1	D	122	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	125	GLY	3.0
1	C	172	ASP	2.9
1	C	170	GLY	2.7
1	C	126	GLN	2.7
1	A	122	ARG	2.7
1	D	66	THR	2.5
1	E	172	ASP	2.5
1	D	232	ALA	2.4
1	A	172	ASP	2.4
1	D	233	THR	2.3
1	B	170	GLY	2.3
1	E	169	GLU	2.3
1	C	167	GLU	2.3
1	F	104	GLY	2.3
1	D	171	GLU	2.3
1	B	126	GLN	2.2
1	A	236	LYS	2.2
1	F	122	ARG	2.2
1	D	53	GLN	2.2
1	D	231	GLN	2.2
1	F	59	ASN	2.2
1	F	172	ASP	2.2
1	D	102	PRO	2.1
1	E	104	GLY	2.1
1	F	53	GLN	2.1
1	B	169	GLU	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	A	301	6/6	0.88	0.31	4.37	50,53,62,69	0
2	GOL	F	301	6/6	0.86	0.30	3.83	40,41,43,43	0
3	MLA	E	301	7/7	0.87	0.22	0.49	51,62,65,68	0
2	GOL	D	301	6/6	0.96	0.16	-0.02	26,33,36,41	0
2	GOL	E	302	6/6	0.78	0.20	-1.32	79,80,83,84	0
3	MLA	B	301	7/7	0.85	0.31	-	66,76,79,84	0

6.5 Other polymers (i)

There are no such residues in this entry.