Full wwPDB X-ray Structure Validation Report (i)

May 3, 2016 – 11:00 AM EDT

PDB ID	:	5DWZ
Title	:	Structural and functional characterization of PqsBC, a condensing enzyme in the biosynthesis of the Pseudomonas aeruginosa quinolone signal
Authors	:	Drees, S.L.; Li, C.; Prasetya, F.; Saleem, M.; Dreveny, I.; Hennecke, U.; Williams, P.; Emsley, J.; Fetzner, S.
Deposited on	:	2015-09-23
Resolution	:	2.04 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:

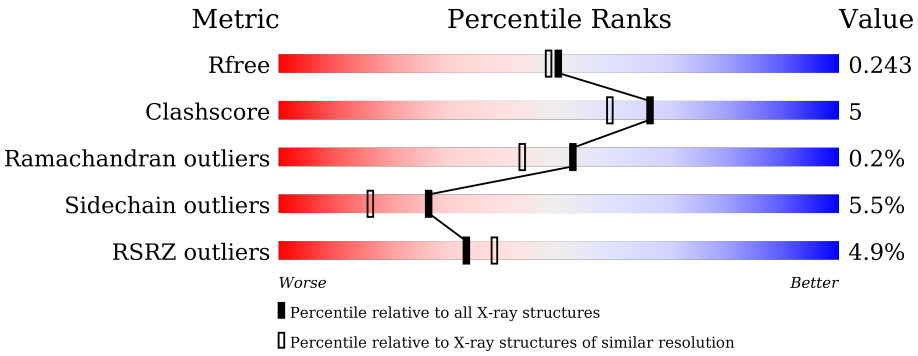
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	C	350	3% 87% 9%
1	D	350	5% 87% 9%
1	F	350	7% 85% 10%
1	H	350	7% 85% 11%
2	A	283	2% 91% 7%
2	B	283	3% 89% 9%

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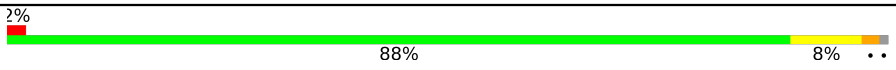
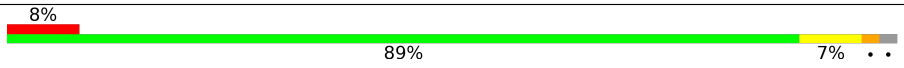
Mol	Chain	Length	Quality of chain
2	E	283	
2	G	283	

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
10	NA	E	402	-	-	-	X
3	PO4	A	401	-	-	-	X
3	PO4	E	401	-	-	-	X
3	PO4	F	405	-	-	-	X
3	PO4	H	404	-	-	-	X
4	GOL	B	501	-	-	-	X
4	GOL	B	502	-	-	-	X
4	GOL	B	503	-	-	-	X
4	GOL	C	404	-	-	-	X
4	GOL	C	405	-	-	-	X
4	GOL	D	405	-	-	-	X
5	MPO	C	407	-	-	-	X
5	MPO	H	406	-	-	-	X
6	TRS	C	408	-	-	-	X
8	PGE	B	505	-	-	-	X
9	PEG	D	407	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20303 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 3-oxoacyl-[acyl-carrier-protein] synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	340	Total	C	N	O	S	1	1	0
			2625	1663	453	491	18			
1	D	340	Total	C	N	O	S	2	3	0
			2637	1672	454	493	18			
1	F	340	Total	C	N	O	S	12	0	0
			2622	1661	454	490	17			
1	H	341	Total	C	N	O	S	3	1	0
			2633	1667	455	493	18			

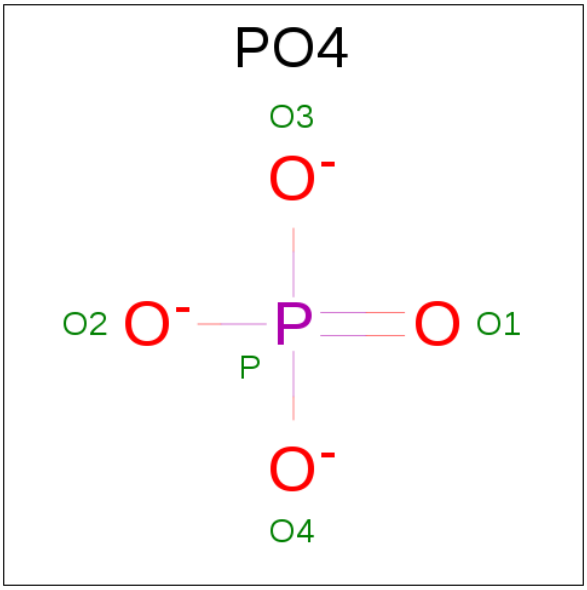
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP A0A0C6EZ24
C	0	ALA	-	expression tag	UNP A0A0C6EZ24
C	1	GLY	-	expression tag	UNP A0A0C6EZ24
C	129	ALA	CYS	engineered mutation	UNP A0A0C6EZ24
D	-1	SER	-	expression tag	UNP A0A0C6EZ24
D	0	ALA	-	expression tag	UNP A0A0C6EZ24
D	1	GLY	-	expression tag	UNP A0A0C6EZ24
D	129	ALA	CYS	engineered mutation	UNP A0A0C6EZ24
F	-1	SER	-	expression tag	UNP A0A0C6EZ24
F	0	ALA	-	expression tag	UNP A0A0C6EZ24
F	1	GLY	-	expression tag	UNP A0A0C6EZ24
F	129	ALA	CYS	engineered mutation	UNP A0A0C6EZ24
H	-1	SER	-	expression tag	UNP A0A0C6EZ24
H	0	ALA	-	expression tag	UNP A0A0C6EZ24
H	1	GLY	-	expression tag	UNP A0A0C6EZ24
H	129	ALA	CYS	engineered mutation	UNP A0A0C6EZ24

- Molecule 2 is a protein called 3-oxoacyl-(Acyl carrier protein) synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	1	0	0
			2113	1333	377	395	8			
2	A	278	Total	C	N	O	S	7	0	0
			2113	1333	377	395	8			
2	E	279	Total	C	N	O	S	4	0	0
			2117	1335	378	396	8			
2	G	278	Total	C	N	O	S	9	0	0
			2112	1332	377	395	8			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

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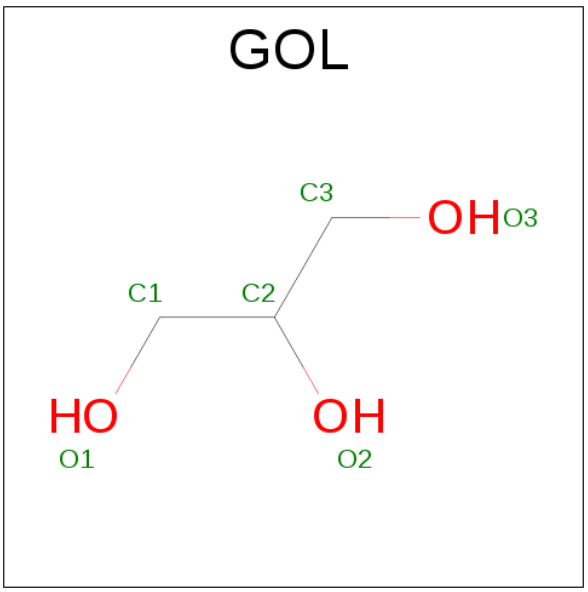
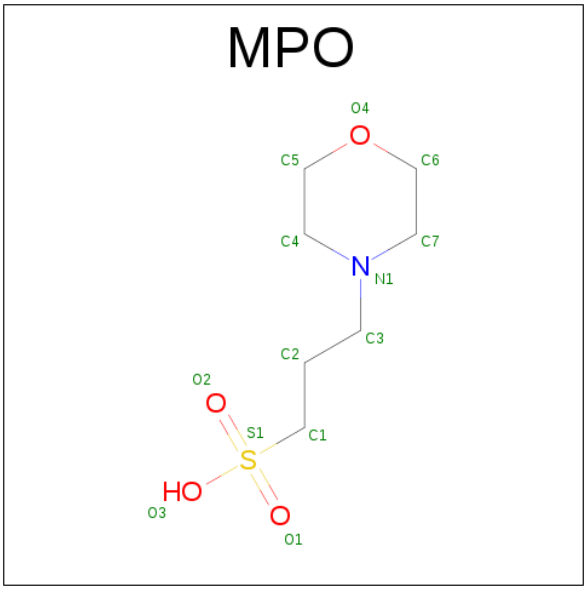
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



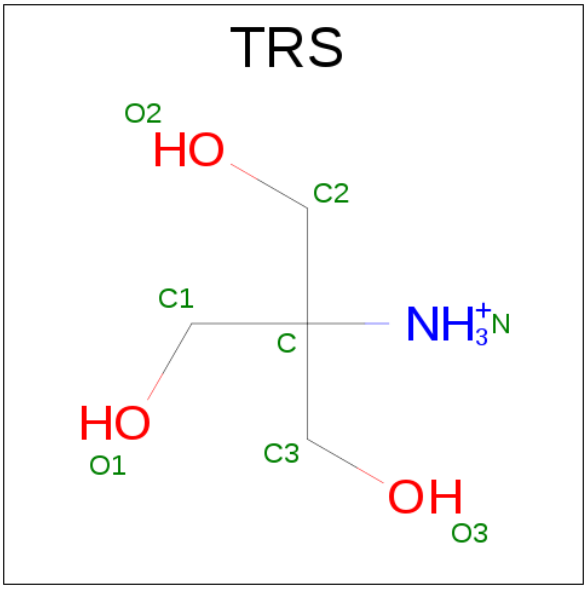
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O S 13 7 1 4 1	0	0
5	C	1	Total C N O S 13 7 1 4 1	0	0
5	D	1	Total C N O S 13 7 1 4 1	0	0
5	H	1	Total C N O S 13 7 1 4 1	1	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

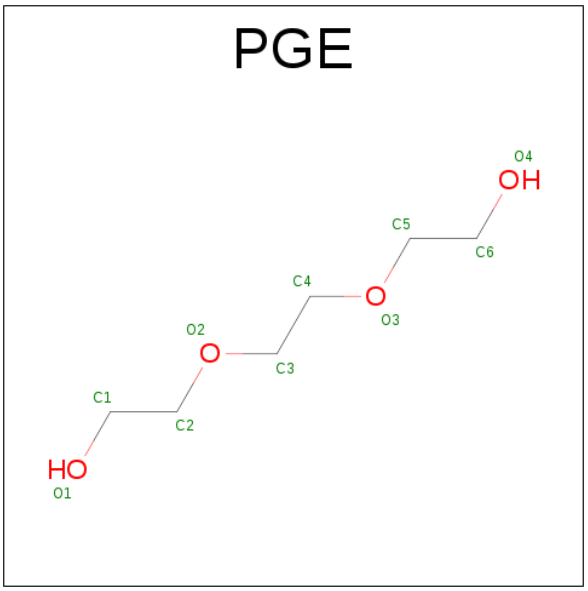


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

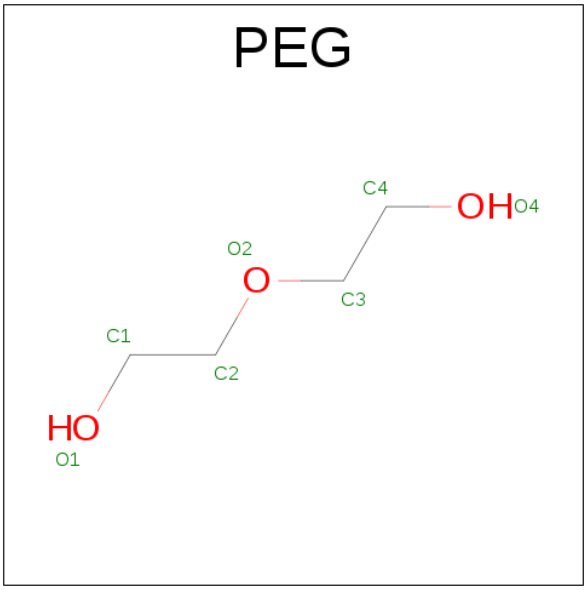
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 10 6 4	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	H	1	Total C O 7 4 3	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total Na 1 1	0	0

- Molecule 11 is water.

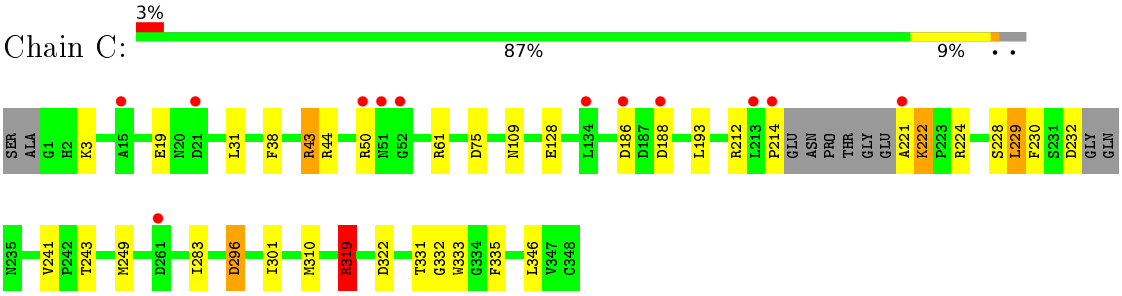
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	184	Total O 184 184	0	0
11	B	167	Total O 167 167	0	0
11	D	158	Total O 158 158	0	0
11	A	141	Total O 141 141	0	0
11	F	94	Total O 94 94	0	0
11	E	140	Total O 140 140	0	0
11	H	112	Total O 112 112	0	0
11	G	99	Total O 99 99	0	0

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.

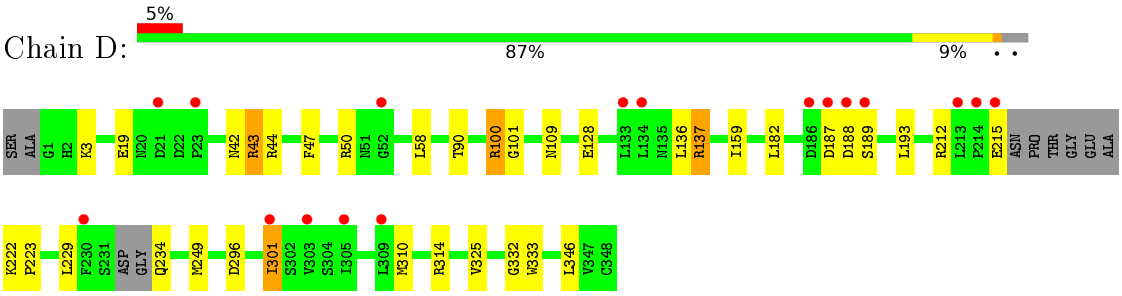
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain C:



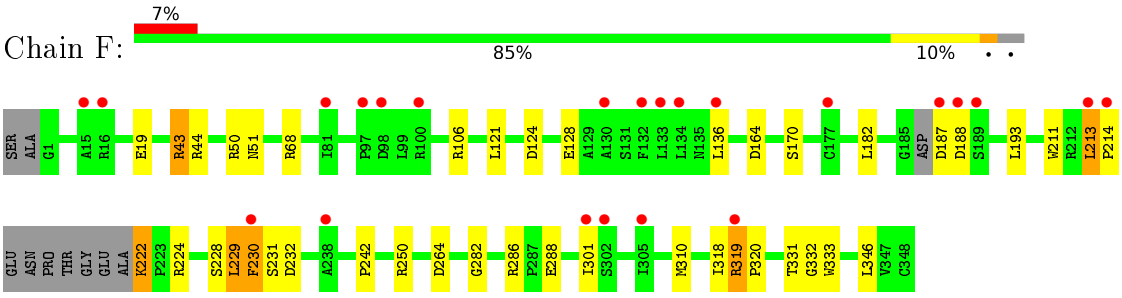
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain D:



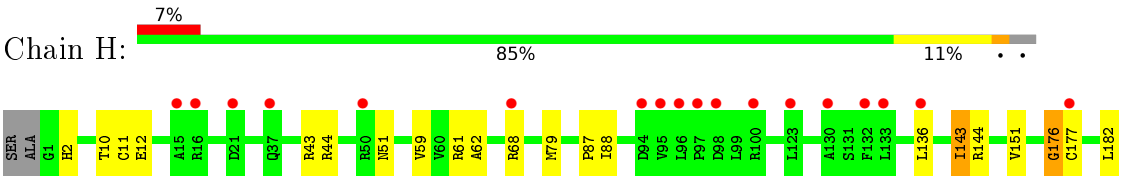
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

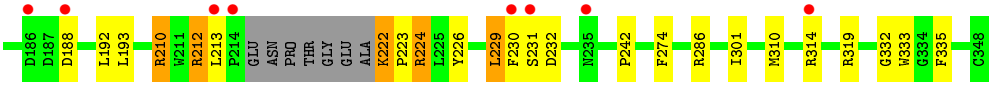
Chain F:



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

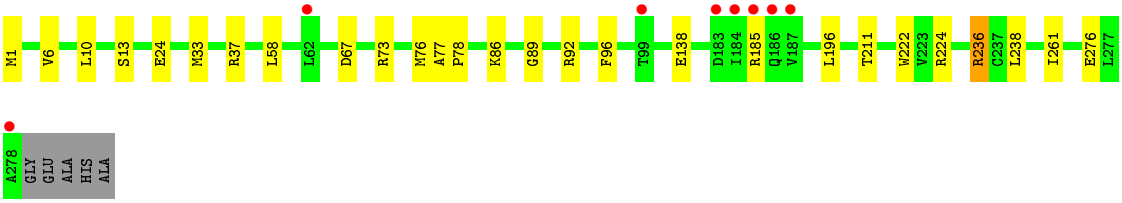
Chain H:





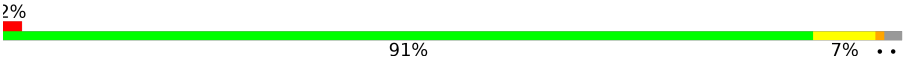
• Molecule 2: 3-oxoacyl-(Acyl carrier protein) synthase III

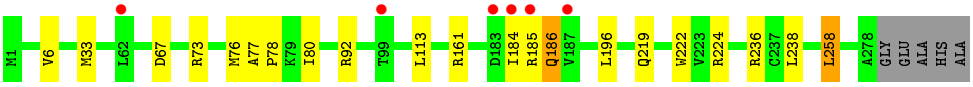
Chain B:



• Molecule 2: 3-oxoacyl-(Acyl carrier protein) synthase III

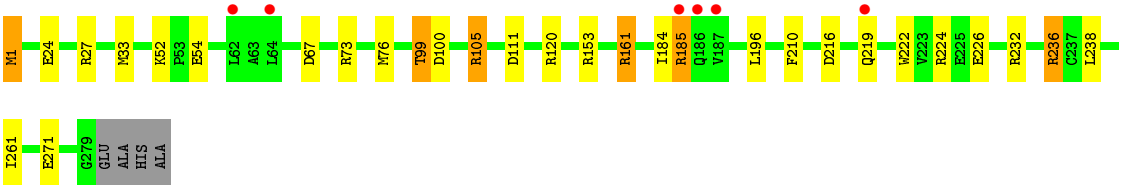
Chain A:





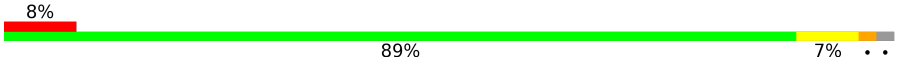
• Molecule 2: 3-oxoacyl-(Acyl carrier protein) synthase III

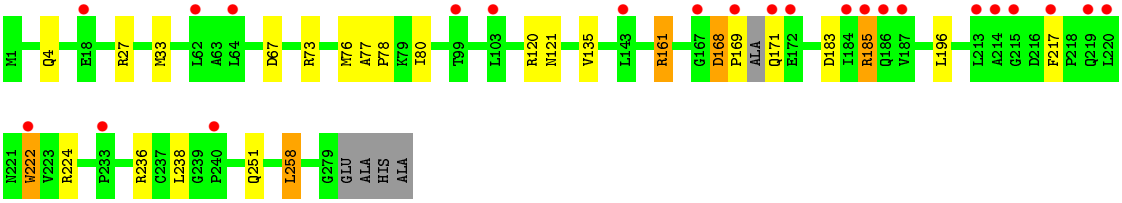
Chain E:



• Molecule 2: 3-oxoacyl-(Acyl carrier protein) synthase III

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.49Å 114.96Å 289.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	144.84 – 2.04 29.60 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.1 (144.84-2.04) 99.2 (29.60-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.190 , 0.237 0.199 , 0.243	Depositor DCC
R_{free} test set	8364 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20303	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 20.32 % 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 8.9095e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, PGE, CL, MPO, PO4, NA, TRS, PEG

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	C	0.83	0/2684	0.92	2/3640 (0.1%)
1	D	0.81	0/2702	0.90	2/3664 (0.1%)
1	F	0.76	0/2678	0.90	0/3631
1	H	0.82	0/2693	0.92	2/3653 (0.1%)
2	A	0.80	0/2154	0.90	1/2927 (0.0%)
2	B	0.86	0/2154	0.92	0/2927
2	E	0.80	0/2158	0.92	1/2932 (0.0%)
2	G	0.76	0/2152	0.91	0/2922
All	All	0.81	0/19375	0.91	8/26296 (0.0%)

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	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	176	GLY	C-N-CA	6.29	137.41	121.70
1	D	100	ARG	N-CA-C	6.09	127.45	111.00
1	C	75	ASP	CB-CA-C	-5.91	98.58	110.40
1	D	101	GLY	N-CA-C	-5.89	98.36	113.10
1	C	243	THR	N-CA-C	5.51	125.88	111.00
2	E	105	ARG	NE-CZ-NH1	-5.48	117.56	120.30
2	A	258	LEU	CA-CB-CG	5.33	127.56	115.30
1	H	222	LYS	C-N-CD	5.16	139.24	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	319	ARG	Sidechain

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	C	2625	0	2600	28	0
1	D	2637	0	2619	28	0
1	F	2622	0	2597	36	0
1	H	2633	0	2607	36	0
2	A	2113	0	2123	6	0
2	B	2113	0	2123	15	0
2	E	2117	0	2126	31	0
2	G	2112	0	2120	25	0
3	A	5	0	0	0	0
3	C	15	0	0	0	0
3	D	20	0	0	0	0
3	E	5	0	0	0	0
3	F	30	0	0	0	0
3	H	25	0	0	0	0
4	B	24	0	32	3	0
4	C	12	0	16	2	0
4	D	6	0	8	0	0
5	C	26	0	29	5	0
5	D	13	0	14	1	0
5	H	13	0	14	3	0
6	C	8	0	12	3	0
7	C	1	0	0	0	0
7	D	1	0	0	1	0
8	B	10	0	14	3	0
9	D	14	0	20	0	0
9	H	7	0	10	0	0
10	E	1	0	0	0	0
11	A	141	0	0	1	0
11	B	167	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	184	0	0	4	1
11	D	158	0	0	3	0
11	E	140	0	0	1	0
11	F	94	0	0	2	0
11	G	99	0	0	1	0
11	H	112	0	0	1	0
All	All	20303	0	19084	188	1

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 (188) 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)
2:E:99:THR:CG2	2:E:100:ASP:H	1.49	1.15
1:F:319:ARG:HE	1:F:319:ARG:HA	1.13	1.10
2:E:99:THR:HG22	2:E:100:ASP:H	0.98	1.06
1:D:43:ARG:HG2	1:D:43:ARG:HH11	1.22	1.04
2:G:169:PRO:HA	2:G:171:GLN:HB2	1.37	1.03
1:H:59:VAL:CG2	1:H:177[A]:CYS:SG	2.52	0.98
2:G:185:ARG:HH21	2:G:185:ARG:HG2	1.31	0.95
2:E:99:THR:HG22	2:E:100:ASP:N	1.78	0.95
1:F:106:ARG:HG3	2:E:99:THR:CG2	1.98	0.93
2:E:99:THR:CG2	2:E:100:ASP:N	2.26	0.92
1:H:59:VAL:HG22	1:H:177[A]:CYS:SG	2.09	0.92
1:F:106:ARG:HG3	2:E:99:THR:HG23	1.55	0.89
1:F:121:LEU:HD11	2:E:105:ARG:HD2	1.56	0.87
1:F:319:ARG:HA	1:F:319:ARG:NE	1.88	0.87
2:G:169:PRO:CA	2:G:171:GLN:HB2	2.04	0.86
1:H:59:VAL:HG23	1:H:177[A]:CYS:SG	2.16	0.84
1:F:213:LEU:HD23	1:F:214:PRO:HD2	1.60	0.83
2:G:169:PRO:HB2	2:G:171:GLN:N	1.97	0.80
2:E:222:TRP:CZ3	2:E:224:ARG:HD3	2.17	0.79
1:C:335:PHE:HE1	5:C:407:MPO:H12	1.50	0.76
1:F:213:LEU:HD21	2:E:185:ARG:O	1.87	0.73
1:C:319:ARG:NH2	1:C:322:ASP:OD1	2.22	0.73
1:D:43:ARG:HG2	1:D:43:ARG:NH1	2.01	0.73
2:G:4:GLN:HE22	2:G:121:ASN:HD22	1.37	0.72
1:F:106:ARG:HG3	2:E:99:THR:HG21	1.72	0.71
2:E:226:GLU:HG2	2:E:232:ARG:NE	2.05	0.71
1:F:319:ARG:NE	1:F:320:PRO:HD3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASP:OD2	1:D:189:SER:HB3	1.90	0.70
2:G:222:TRP:H	2:G:222:TRP:HE3	1.39	0.69
1:H:61:ARG:HH11	1:H:61:ARG:HG3	1.57	0.69
1:F:319:ARG:HE	1:F:319:ARG:CA	1.98	0.68
2:B:276:GLU:HG3	4:B:501:GOL:H32	1.73	0.68
2:G:185:ARG:CG	2:G:185:ARG:HH21	2.03	0.68
1:H:212:ARG:HD2	1:H:224:ARG:HG3	1.77	0.67
1:F:124:ASP:HB2	2:E:99:THR:HG21	1.76	0.67
2:E:210:PHE:CD2	2:E:224:ARG:HD2	2.31	0.66
1:H:222:LYS:N	1:H:223:PRO:HD3	2.11	0.66
2:B:92:ARG:O	4:B:502:GOL:H11	1.95	0.65
1:C:109:ASN:HB2	11:C:507:HOH:O	1.96	0.65
1:H:229:LEU:HD12	1:H:230:PHE:N	2.12	0.64
1:C:229:LEU:O	1:C:230:PHE:HD1	1.81	0.63
1:C:230:PHE:CE1	1:F:230:PHE:HD1	2.18	0.62
1:D:222:LYS:HB2	1:D:223:PRO:HD3	1.82	0.61
2:G:169:PRO:CB	2:G:171:GLN:N	2.64	0.61
1:H:335:PHE:HE1	5:H:406:MPO:H12	1.66	0.61
6:C:408:TRS:C2	1:F:242:PRO:HD3	2.31	0.61
2:E:24:GLU:OE1	2:E:236:ARG:NH1	2.34	0.61
1:H:143:ILE:HD11	1:H:151:VAL:HG23	1.85	0.59
1:C:212:ARG:HB2	1:C:224:ARG:HD2	1.85	0.59
1:D:42:ASN:HB3	1:D:43:ARG:HH12	1.68	0.59
2:G:258:LEU:HD23	2:G:258:LEU:C	2.24	0.59
1:H:10:THR:HA	1:H:310:MET:CE	2.33	0.58
1:H:136:LEU:HD22	1:H:182:LEU:HD11	1.86	0.58
1:C:296:ASP:HB3	11:C:627:HOH:O	2.04	0.58
1:D:314:ARG:HH11	1:D:314:ARG:HG3	1.69	0.57
1:H:87:PRO:HG2	1:H:223:PRO:HG2	1.85	0.57
1:F:250:ARG:NH1	1:F:282:GLY:O	2.37	0.57
2:E:99:THR:HG23	2:E:100:ASP:H	1.55	0.57
1:D:222:LYS:HE3	2:A:184:ILE:HD12	1.85	0.57
1:D:187:ASP:OD2	1:D:189:SER:CB	2.52	0.57
2:G:120:ARG:NH1	11:G:301:HOH:O	2.30	0.57
1:C:241:VAL:HG22	5:C:407:MPO:H22	1.87	0.56
2:G:185:ARG:NH2	2:G:185:ARG:HG2	2.08	0.56
1:F:164:ASP:O	1:F:170:SER:HB3	2.05	0.56
1:F:19:GLU:OE1	1:F:43:ARG:NH1	2.39	0.56
1:F:128:GLU:HG2	1:F:331:THR:OG1	2.06	0.56
1:H:212:ARG:HG3	1:H:226:TYR:OH	2.06	0.55
1:C:335:PHE:CE1	5:C:407:MPO:H12	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:ARG:HG3	1:H:226:TYR:CD1	2.42	0.55
1:F:318:ILE:O	1:F:319:ARG:HG2	2.08	0.54
1:H:10:THR:HA	1:H:310:MET:HE2	1.88	0.54
1:C:222:LYS:HE3	11:C:502:HOH:O	2.07	0.54
2:E:1:MET:HG2	2:E:111:ASP:HB2	1.89	0.54
2:G:168:ASP:CA	2:G:169:PRO:C	2.76	0.54
1:C:230:PHE:HE1	1:F:230:PHE:HD1	1.54	0.54
1:C:214:PRO:HD3	1:C:221:ALA:HB2	1.90	0.54
1:D:109:ASN:HB3	7:D:409:CL:CL	2.44	0.54
1:C:222:LYS:N	1:C:222:LYS:HD3	2.22	0.54
1:F:228:SER:HG	1:F:230:PHE:HE1	1.54	0.54
2:B:185:ARG:HH11	2:B:185:ARG:HB2	1.72	0.54
2:B:276:GLU:HG3	4:B:501:GOL:C3	2.38	0.54
1:F:128:GLU:HB3	11:F:513:HOH:O	2.08	0.54
1:F:213:LEU:HD23	1:F:214:PRO:CD	2.34	0.53
2:E:99:THR:HG23	2:E:100:ASP:N	2.19	0.53
2:B:37:ARG:NH1	8:B:505:PGE:H32	2.24	0.53
2:G:169:PRO:C	2:G:171:GLN:N	2.63	0.53
1:H:222:LYS:N	1:H:223:PRO:CD	2.71	0.52
4:C:405:GOL:H2	2:B:86:LYS:HA	1.91	0.52
1:D:222:LYS:CB	1:D:223:PRO:HD3	2.40	0.52
1:H:229:LEU:HD12	1:H:230:PHE:H	1.74	0.52
1:H:61:ARG:HG3	1:H:61:ARG:NH1	2.25	0.52
2:B:24:GLU:OE2	2:B:236:ARG:HD3	2.10	0.52
1:H:176:GLY:O	1:H:177[B]:CYS:SG	2.65	0.51
1:H:335:PHE:CE1	5:H:406:MPO:H12	2.46	0.51
1:D:42:ASN:HB3	1:D:43:ARG:NH1	2.26	0.50
1:C:222:LYS:H	1:C:222:LYS:HD3	1.76	0.50
2:G:67:ASP:HB2	2:G:73:ARG:O	2.12	0.50
2:G:4:GLN:HE22	2:G:121:ASN:ND2	2.07	0.50
2:G:222:TRP:CE3	2:G:222:TRP:N	2.74	0.50
1:C:38:PHE:HE1	5:C:406:MPO:H72	1.77	0.49
2:B:10:LEU:O	8:B:505:PGE:H2	2.13	0.49
2:G:27:ARG:HH22	2:G:135:VAL:HG11	1.78	0.49
2:B:37:ARG:HH12	8:B:505:PGE:H32	1.78	0.49
1:D:234:GLN:NE2	11:D:506:HOH:O	2.46	0.49
1:D:137:ARG:HD3	2:A:113:LEU:CD1	2.43	0.48
2:G:161:ARG:HD2	2:G:217:PHE:CZ	2.48	0.48
2:E:27:ARG:NH1	11:E:503:HOH:O	2.46	0.48
1:F:332:GLY:N	1:F:333:TRP:HA	2.29	0.48
1:H:210:ARG:CG	1:H:226:TYR:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LYS:HA	11:D:624:HOH:O	2.13	0.48
1:D:19:GLU:HB3	11:D:556:HOH:O	2.13	0.48
1:C:222:LYS:HE2	1:C:224:ARG:NH1	2.29	0.48
1:D:212:ARG:HD3	1:H:232:ASP:OD2	2.13	0.48
1:C:224:ARG:HD3	1:F:232:ASP:OD1	2.14	0.48
2:B:24:GLU:O	2:B:236:ARG:HG3	2.14	0.47
1:C:222:LYS:HE2	1:C:224:ARG:CZ	2.43	0.47
1:H:11:CYS:H	1:H:310:MET:HE1	1.78	0.47
6:C:408:TRS:H22	1:F:242:PRO:HD3	1.96	0.47
2:E:105:ARG:HD3	2:E:271:GLU:OE2	2.14	0.47
2:E:222:TRP:HZ3	2:E:224:ARG:HD3	1.77	0.47
1:C:19:GLU:OE1	1:C:43:ARG:NH1	2.47	0.47
1:D:332:GLY:N	1:D:333:TRP:HA	2.29	0.47
2:E:222:TRP:CE3	2:E:261:ILE:HD12	2.51	0.46
2:A:222:TRP:HZ3	2:A:224:ARG:HD2	1.81	0.46
2:E:222:TRP:CZ3	2:E:224:ARG:CD	2.94	0.46
1:D:159:ILE:HG21	1:D:301:ILE:CD1	2.45	0.46
2:E:67:ASP:HB2	2:E:73:ARG:O	2.16	0.46
1:H:332:GLY:N	1:H:333:TRP:HA	2.30	0.46
4:C:405:GOL:H32	2:B:89:GLY:HA2	1.98	0.46
1:C:38:PHE:HE1	5:C:406:MPO:C7	2.30	0.45
1:F:136:LEU:HD22	1:F:182:LEU:HD11	1.98	0.45
5:D:406:MPO:H41	1:H:274:PHE:HE2	1.80	0.45
2:E:1:MET:HG2	2:E:111:ASP:CB	2.45	0.45
1:H:88:ILE:HD11	1:H:223:PRO:HD3	1.97	0.45
1:D:249:MET:HE2	1:D:325:VAL:HG11	1.98	0.45
1:F:128:GLU:HG2	1:F:331:THR:HG1	1.82	0.45
1:C:109:ASN:HB2	11:C:642:HOH:O	2.16	0.45
1:H:333:TRP:CD2	5:H:406:MPO:H42	2.52	0.45
1:H:144:ARG:NH1	1:H:192:LEU:O	2.46	0.45
2:E:54:GLU:CD	2:E:54:GLU:H	2.21	0.45
1:C:229:LEU:CD1	1:F:229:LEU:HB3	2.47	0.44
2:E:222:TRP:HZ3	2:E:224:ARG:CD	2.30	0.44
1:F:319:ARG:CD	1:F:320:PRO:HD3	2.46	0.44
2:G:222:TRP:N	2:G:222:TRP:HE3	2.11	0.44
2:A:67:ASP:HB2	2:A:73:ARG:O	2.18	0.44
2:G:222:TRP:O	2:G:222:TRP:CE3	2.70	0.44
2:A:77:ALA:HA	2:A:78:PRO:C	2.38	0.44
1:F:264:ASP:OD1	1:H:286:ARG:NH2	2.50	0.44
1:D:19:GLU:OE1	1:D:43:ARG:NH2	2.51	0.44
2:E:226:GLU:HG2	2:E:232:ARG:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:GLU:HG2	1:C:331:THR:OG1	2.18	0.43
2:E:52:LYS:HB3	2:E:54:GLU:OE1	2.18	0.43
2:B:77:ALA:HA	2:B:78:PRO:C	2.37	0.43
1:H:11:CYS:N	1:H:310:MET:HE1	2.33	0.43
2:B:222:TRP:CE3	2:B:261:ILE:HD12	2.54	0.43
2:G:77:ALA:HA	2:G:78:PRO:C	2.39	0.43
1:D:222:LYS:HB2	1:D:223:PRO:CD	2.47	0.43
1:C:249:MET:HE3	1:C:283:ILE:HB	2.00	0.42
1:D:128:GLU:HG2	11:A:588:HOH:O	2.19	0.42
2:G:161:ARG:HD2	2:G:217:PHE:HZ	1.83	0.42
1:D:43:ARG:NH1	1:D:43:ARG:CG	2.71	0.42
1:F:124:ASP:O	2:E:99:THR:HB	2.20	0.42
1:D:47:PHE:CE1	1:D:58:LEU:HD22	2.54	0.42
1:H:79:MET:HB3	1:H:151:VAL:HG22	2.01	0.42
1:H:231:SER:OG	11:H:501:HOH:O	2.21	0.42
1:C:229:LEU:HD12	1:F:229:LEU:HB3	2.02	0.42
1:D:222:LYS:CB	1:D:223:PRO:CD	2.97	0.42
6:C:408:TRS:H21	1:F:242:PRO:HD3	2.01	0.42
1:H:2:HIS:O	1:H:144:ARG:HD3	2.19	0.42
2:B:58:LEU:HD11	2:B:96:PHE:CE1	2.55	0.42
2:A:186:GLN:H	2:A:186:GLN:HG2	1.71	0.41
1:F:222:LYS:CE	2:E:184:ILE:HD12	2.50	0.41
1:H:12:GLU:HB2	1:H:62:ALA:HB2	2.02	0.41
1:D:90:THR:HA	1:D:100:ARG:O	2.20	0.41
2:E:161:ARG:HD3	2:E:216:ASP:OD2	2.20	0.41
2:B:67:ASP:HB2	2:B:73:ARG:O	2.19	0.41
1:C:229:LEU:C	1:C:230:PHE:CD1	2.93	0.41
1:F:319:ARG:CA	11:F:533:HOH:O	2.69	0.41
2:G:222:TRP:O	2:G:222:TRP:HE3	2.02	0.41
1:D:136:LEU:HD22	1:D:182:LEU:HD11	2.01	0.41
1:H:210:ARG:HD3	1:H:226:TYR:HB2	2.02	0.41
2:G:183:ASP:OD1	2:G:185:ARG:NH2	2.54	0.41
1:C:222:LYS:HE3	1:C:224:ARG:HG2	2.03	0.41
1:F:211:TRP:CZ3	1:F:222:LYS:HB2	2.56	0.41
1:C:332:GLY:N	1:C:333:TRP:HA	2.36	0.41
2:G:169:PRO:C	2:G:171:GLN:HB2	2.41	0.40
1:D:3:LYS:HE2	1:D:188:ASP:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:546:HOH:O	11:B:744:HOH:O[4_565]	2.01	0.19

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	C	335/350 (96%)	326 (97%)	8 (2%)	1 (0%)	46	36
1	D	337/350 (96%)	329 (98%)	7 (2%)	1 (0%)	46	36
1	F	334/350 (95%)	325 (97%)	8 (2%)	1 (0%)	46	36
1	H	338/350 (97%)	328 (97%)	9 (3%)	1 (0%)	46	36
2	A	276/283 (98%)	273 (99%)	3 (1%)	0	100	100
2	B	276/283 (98%)	273 (99%)	3 (1%)	0	100	100
2	E	277/283 (98%)	272 (98%)	5 (2%)	0	100	100
2	G	274/283 (97%)	268 (98%)	6 (2%)	0	100	100
All	All	2447/2532 (97%)	2394 (98%)	49 (2%)	4 (0%)	52	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	301	ILE
1	F	301	ILE
1	H	301	ILE
1	C	301	ILE

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	C	279/285 (98%)	262 (94%)	17 (6%)	23 13
1	D	282/285 (99%)	272 (96%)	10 (4%)	43 35
1	F	278/285 (98%)	259 (93%)	19 (7%)	20 11
1	H	280/285 (98%)	265 (95%)	15 (5%)	27 17
2	A	221/223 (99%)	208 (94%)	13 (6%)	24 14
2	B	221/223 (99%)	210 (95%)	11 (5%)	30 20
2	E	221/223 (99%)	209 (95%)	12 (5%)	27 17
2	G	221/223 (99%)	208 (94%)	13 (6%)	24 14
All	All	2003/2032 (99%)	1893 (94%)	110 (6%)	27 16

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	LYS
1	C	31	LEU
1	C	43	ARG
1	C	44	ARG
1	C	50	ARG
1	C	61	ARG
1	C	186	ASP
1	C	188	ASP
1	C	193	LEU
1	C	222	LYS
1	C	228	SER
1	C	229	LEU
1	C	232	ASP
1	C	296	ASP
1	C	310	MET
1	C	319	ARG
1	C	346	LEU
2	B	1	MET
2	B	6	VAL
2	B	13	SER
2	B	33	MET
2	B	76	MET
2	B	138	GLU
2	B	196	LEU
2	B	211	THR

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Mol	Chain	Res	Type
2	B	224	ARG
2	B	236	ARG
2	B	238	LEU
1	D	43	ARG
1	D	44	ARG
1	D	50	ARG
1	D	137	ARG
1	D	193	LEU
1	D	215	GLU
1	D	229	LEU
1	D	296	ASP
1	D	310	MET
1	D	346	LEU
2	A	6	VAL
2	A	33	MET
2	A	76	MET
2	A	80	ILE
2	A	92	ARG
2	A	161	ARG
2	A	185	ARG
2	A	186	GLN
2	A	196	LEU
2	A	219	GLN
2	A	236	ARG
2	A	238	LEU
2	A	258	LEU
1	F	43	ARG
1	F	44	ARG
1	F	50	ARG
1	F	51	ASN
1	F	68	ARG
1	F	187	ASP
1	F	188	ASP
1	F	193	LEU
1	F	213	LEU
1	F	222	LYS
1	F	224	ARG
1	F	229	LEU
1	F	230	PHE
1	F	231	SER
1	F	286	ARG
1	F	288	GLU

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Mol	Chain	Res	Type
1	F	310	MET
1	F	319	ARG
1	F	346	LEU
2	E	1	MET
2	E	33	MET
2	E	76	MET
2	E	99	THR
2	E	120	ARG
2	E	153	ARG
2	E	161	ARG
2	E	185	ARG
2	E	196	LEU
2	E	219	GLN
2	E	236	ARG
2	E	238	LEU
1	H	43	ARG
1	H	44	ARG
1	H	51	ASN
1	H	68	ARG
1	H	143	ILE
1	H	188	ASP
1	H	193	LEU
1	H	210	ARG
1	H	212	ARG
1	H	213	LEU
1	H	224	ARG
1	H	229	LEU
1	H	242	PRO
1	H	314	ARG
1	H	319	ARG
2	G	33	MET
2	G	76	MET
2	G	80	ILE
2	G	161	ARG
2	G	168	ASP
2	G	185	ARG
2	G	196	LEU
2	G	222	TRP
2	G	224	ARG
2	G	236	ARG
2	G	238	LEU
2	G	251	GLN

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Mol	Chain	Res	Type
2	G	258	LEU

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

Mol	Chain	Res	Type
2	G	121	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 3 are monoatomic - leaving 36 for Mogul analysis.

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	$\#\|Z\| > 2$
3	PO4	A	401	-	4,4,4	0.68	0	6,6,6	0.23	0
4	GOL	B	501	-	5,5,5	0.22	0	5,5,5	0.23	0
4	GOL	B	502	-	5,5,5	0.22	0	5,5,5	0.22	0
4	GOL	B	503	-	5,5,5	0.21	0	5,5,5	0.23	0
4	GOL	B	504	-	5,5,5	0.22	0	5,5,5	0.22	0
8	PGE	B	505	-	9,9,9	0.39	0	8,8,8	0.31	0
3	PO4	C	401	-	4,4,4	1.01	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	C	402	-	4,4,4	1.63	1 (25%)	6,6,6	0.28	0
3	PO4	C	403	-	4,4,4	1.82	2 (50%)	6,6,6	0.22	0
4	GOL	C	404	-	5,5,5	0.45	0	5,5,5	0.55	0
4	GOL	C	405	-	5,5,5	0.36	0	5,5,5	2.44	2 (40%)
5	MPO	C	406	-	13,13,13	2.77	2 (15%)	16,17,17	3.37	4 (25%)
5	MPO	C	407	-	13,13,13	2.45	2 (15%)	16,17,17	1.75	4 (25%)
6	TRS	C	408	-	7,7,7	2.08	2 (28%)	9,9,9	3.15	5 (55%)
3	PO4	D	401	-	4,4,4	1.65	1 (25%)	6,6,6	0.29	0
3	PO4	D	402	-	4,4,4	1.11	0	6,6,6	0.34	0
3	PO4	D	403	-	4,4,4	1.16	0	6,6,6	0.33	0
3	PO4	D	404	-	4,4,4	2.49	3 (75%)	6,6,6	0.31	0
4	GOL	D	405	-	5,5,5	0.24	0	5,5,5	0.36	0
5	MPO	D	406	-	13,13,13	3.05	4 (30%)	16,17,17	2.92	4 (25%)
9	PEG	D	407	-	6,6,6	0.24	0	5,5,5	0.59	0
9	PEG	D	408	-	6,6,6	0.73	0	5,5,5	0.68	0
3	PO4	E	401	-	4,4,4	0.68	0	6,6,6	0.23	0
3	PO4	F	401	-	4,4,4	1.36	1 (25%)	6,6,6	0.31	0
3	PO4	F	402	-	4,4,4	1.56	2 (50%)	6,6,6	0.26	0
3	PO4	F	403	-	4,4,4	1.84	1 (25%)	6,6,6	0.40	0
3	PO4	F	404	-	4,4,4	1.05	0	6,6,6	0.38	0
3	PO4	F	405	-	4,4,4	2.93	3 (75%)	6,6,6	0.23	0
3	PO4	F	406	-	4,4,4	1.60	2 (50%)	6,6,6	0.35	0
3	PO4	H	401	-	4,4,4	1.44	1 (25%)	6,6,6	0.27	0
3	PO4	H	402	-	4,4,4	1.97	3 (75%)	6,6,6	0.32	0
3	PO4	H	403	-	4,4,4	0.78	0	6,6,6	0.22	0
3	PO4	H	404	-	4,4,4	0.70	0	6,6,6	0.31	0
3	PO4	H	405	-	4,4,4	1.12	0	6,6,6	0.35	0
5	MPO	H	406	-	13,13,13	3.84	2 (15%)	16,17,17	2.91	5 (31%)
9	PEG	H	407	-	6,6,6	0.69	0	5,5,5	0.62	0

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
3	PO4	A	401	-	-	0/0/0/0	0/0/0/0
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	503	-	-	0/4/4/4	0/0/0/0
4	GOL	B	504	-	-	0/4/4/4	0/0/0/0
8	PGE	B	505	-	-	0/7/7/7	0/0/0/0
3	PO4	C	401	-	-	0/0/0/0	0/0/0/0
3	PO4	C	402	-	-	0/0/0/0	0/0/0/0
3	PO4	C	403	-	-	0/0/0/0	0/0/0/0
4	GOL	C	404	-	-	0/4/4/4	0/0/0/0
4	GOL	C	405	-	-	0/4/4/4	0/0/0/0
5	MPO	C	406	-	-	0/7/15/15	0/1/1/1
5	MPO	C	407	-	-	0/7/15/15	0/1/1/1
6	TRS	C	408	-	-	0/9/9/9	0/0/0/0
3	PO4	D	401	-	-	0/0/0/0	0/0/0/0
3	PO4	D	402	-	-	0/0/0/0	0/0/0/0
3	PO4	D	403	-	-	0/0/0/0	0/0/0/0
3	PO4	D	404	-	-	0/0/0/0	0/0/0/0
4	GOL	D	405	-	-	0/4/4/4	0/0/0/0
5	MPO	D	406	-	-	0/7/15/15	0/1/1/1
9	PEG	D	407	-	-	0/4/4/4	0/0/0/0
9	PEG	D	408	-	-	0/4/4/4	0/0/0/0
3	PO4	E	401	-	-	0/0/0/0	0/0/0/0
3	PO4	F	401	-	-	0/0/0/0	0/0/0/0
3	PO4	F	402	-	-	0/0/0/0	0/0/0/0
3	PO4	F	403	-	-	0/0/0/0	0/0/0/0
3	PO4	F	404	-	-	0/0/0/0	0/0/0/0
3	PO4	F	405	-	-	0/0/0/0	0/0/0/0
3	PO4	F	406	-	-	0/0/0/0	0/0/0/0
3	PO4	H	401	-	-	0/0/0/0	0/0/0/0
3	PO4	H	402	-	-	0/0/0/0	0/0/0/0
3	PO4	H	403	-	-	0/0/0/0	0/0/0/0
3	PO4	H	404	-	-	0/0/0/0	0/0/0/0
3	PO4	H	405	-	-	0/0/0/0	0/0/0/0
5	MPO	H	406	-	-	0/7/15/15	0/1/1/1
9	PEG	H	407	-	-	0/4/4/4	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	406	MPO	C1-S1	-12.34	1.59	1.77
5	D	406	MPO	C1-S1	-9.11	1.63	1.77
5	C	407	MPO	C1-S1	-7.26	1.66	1.77
5	C	406	MPO	C1-S1	-6.94	1.67	1.77
6	C	408	TRS	C-N	-4.21	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	405	PO4	P-O4	-3.64	1.42	1.53
5	D	406	MPO	O3-S1	-3.37	1.36	1.47
3	D	404	PO4	P-O3	-3.33	1.43	1.53
3	F	405	PO4	P-O2	-3.11	1.44	1.53
3	F	405	PO4	P-O3	-3.05	1.44	1.53
6	C	408	TRS	C3-C	-2.87	1.49	1.53
3	F	403	PO4	P-O2	-2.86	1.44	1.53
5	D	406	MPO	O2-S1	-2.85	1.36	1.45
3	D	404	PO4	P-O4	-2.84	1.45	1.53
3	H	401	PO4	P-O4	-2.54	1.45	1.53
3	H	402	PO4	P-O3	-2.49	1.46	1.53
3	D	401	PO4	P-O2	-2.46	1.46	1.53
3	C	402	PO4	P-O3	-2.35	1.46	1.53
3	F	406	PO4	P-O3	-2.29	1.46	1.53
3	C	403	PO4	P-O2	-2.28	1.46	1.53
3	H	402	PO4	P-O2	-2.20	1.46	1.53
3	C	403	PO4	P-O3	-2.19	1.47	1.53
3	F	401	PO4	P-O4	-2.16	1.47	1.53
3	F	406	PO4	P-O2	-2.16	1.47	1.53
3	F	402	PO4	P-O3	-2.15	1.47	1.53
3	F	402	PO4	P-O2	-2.11	1.47	1.53
3	H	402	PO4	P-O1	-2.10	1.45	1.53
3	D	404	PO4	P-O2	2.19	1.60	1.53
5	D	406	MPO	O1-S1	3.97	1.56	1.45
5	C	407	MPO	O3-S1	4.88	1.63	1.47
5	H	406	MPO	O1-S1	5.30	1.60	1.45
5	C	406	MPO	O1-S1	6.92	1.65	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	408	TRS	C3-C-N	-6.16	97.42	107.88
6	C	408	TRS	O3-C3-C	-4.63	99.94	110.92
4	C	405	GOL	C3-C2-C1	-4.13	93.64	111.06
5	D	406	MPO	O3-S1-O2	-4.06	102.27	111.26
5	D	406	MPO	C2-C1-S1	-3.37	107.64	113.15
5	C	406	MPO	O2-S1-O1	-3.18	104.98	113.96
5	H	406	MPO	O2-S1-O1	-2.61	106.58	113.96
5	C	407	MPO	C2-C1-S1	-2.23	109.52	113.15
5	C	407	MPO	O3-S1-C1	2.15	109.47	104.99
6	C	408	TRS	O2-C2-C	2.28	116.34	110.92
6	C	408	TRS	C3-C-C1	2.32	115.54	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	406	MPO	O4-C5-C4	2.58	117.79	111.83
4	C	405	GOL	O2-C2-C3	2.86	122.22	108.47
5	C	407	MPO	O2-S1-C1	3.63	109.44	106.87
5	C	407	MPO	O1-S1-C1	3.71	109.49	106.87
5	C	406	MPO	O2-S1-C1	3.86	109.59	106.87
5	H	406	MPO	O3-S1-C1	4.00	113.31	104.99
5	H	406	MPO	C6-C7-N1	4.09	116.36	110.11
6	C	408	TRS	C2-C-N	4.24	115.09	107.88
5	C	406	MPO	C6-C7-N1	4.32	116.72	110.11
5	D	406	MPO	O3-S1-C1	4.97	115.33	104.99
5	D	406	MPO	O2-S1-C1	8.63	112.97	106.87
5	H	406	MPO	O1-S1-C1	8.74	113.05	106.87
5	C	406	MPO	O1-S1-C1	11.38	114.91	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	GOL	2	0
4	B	502	GOL	1	0
8	B	505	PGE	3	0
4	C	405	GOL	2	0
5	C	406	MPO	2	0
5	C	407	MPO	3	0
6	C	408	TRS	3	0
5	D	406	MPO	1	0
5	H	406	MPO	3	0

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	C	340/350 (97%)	0.08	12 (3%)	48	54	20, 31, 58, 77	2 (0%)
1	D	340/350 (97%)	0.30	17 (5%)	32	37	25, 35, 57, 76	3 (0%)
1	F	340/350 (97%)	0.52	23 (6%)	20	23	29, 42, 61, 94	10 (2%)
1	H	341/350 (97%)	0.58	26 (7%)	17	19	25, 41, 63, 93	2 (0%)
2	A	278/283 (98%)	0.05	6 (2%)	65	71	22, 30, 47, 72	2 (0%)
2	B	278/283 (98%)	-0.01	8 (2%)	55	62	19, 27, 44, 68	1 (0%)
2	E	279/283 (98%)	0.18	6 (2%)	65	71	25, 34, 50, 70	5 (1%)
2	G	278/283 (98%)	0.51	23 (8%)	14	16	27, 40, 64, 81	3 (1%)
All	All	2474/2532 (97%)	0.28	121 (4%)	33	38	19, 36, 58, 94	28 (1%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	188	ASP	6.6
1	H	230	PHE	5.1
2	E	187	VAL	5.0
1	F	214	PRO	4.8
2	G	184	ILE	4.7
1	D	215	GLU	4.7
2	G	187	VAL	4.7
2	G	215	GLY	4.7
1	F	213	LEU	4.6
1	F	188	ASP	4.5
1	F	187	ASP	4.3
2	G	219	GLN	4.3
1	H	50	ARG	4.3
1	H	186	ASP	4.3
1	D	230	PHE	4.2
2	B	185	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	A	187	VAL	4.2
2	A	185	ARG	4.2
2	G	167	GLY	4.0
1	H	214	PRO	4.0
1	C	186	ASP	4.0
1	D	188	ASP	3.7
1	D	213	LEU	3.7
1	C	214	PRO	3.7
2	G	185	ARG	3.5
2	G	186	GLN	3.4
2	G	172	GLU	3.4
2	G	222	TRP	3.4
1	D	189	SER	3.4
1	C	51	ASN	3.4
1	F	132	PHE	3.4
2	G	171	GLN	3.3
1	C	21	ASP	3.3
2	E	186	GLN	3.3
1	H	314	ARG	3.2
1	H	213	LEU	3.2
2	G	233	PRO	3.1
2	E	185	ARG	3.1
1	H	235	ASN	3.0
1	H	100	ARG	3.0
2	A	184	ILE	3.0
1	F	189	SER	2.9
1	F	230	PHE	2.9
2	B	187	VAL	2.9
2	G	240	PRO	2.9
1	D	187	ASP	2.9
1	D	214	PRO	2.9
1	F	305	ILE	2.9
1	F	319	ARG	2.8
1	C	188	ASP	2.8
1	H	96	LEU	2.8
1	F	130	ALA	2.8
1	D	23	PRO	2.7
2	B	184	ILE	2.7
1	C	221	ALA	2.7
1	C	50	ARG	2.6
1	F	100	ARG	2.6
1	H	21	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	177[A]	CYS	2.6
1	H	98	ASP	2.5
1	D	52	GLY	2.5
1	H	97	PRO	2.5
2	G	169	PRO	2.5
1	H	94	ASP	2.5
1	F	134	LEU	2.5
1	H	231	SER	2.5
2	B	183	ASP	2.5
1	C	213	LEU	2.4
1	D	305	ILE	2.4
1	F	133	LEU	2.4
1	F	97	PRO	2.4
1	F	16	ARG	2.4
2	B	278	ALA	2.4
1	D	309	LEU	2.4
1	F	136	LEU	2.4
2	B	99	THR	2.4
1	H	123	LEU	2.4
2	G	99	THR	2.4
1	H	136	LEU	2.3
2	G	213	LEU	2.3
2	G	217	PHE	2.3
1	D	186	ASP	2.3
2	G	18	GLU	2.3
1	D	301	ILE	2.3
2	G	220	LEU	2.3
1	F	302	SER	2.3
1	F	15	ALA	2.3
1	H	132	PHE	2.3
2	A	183	ASP	2.2
1	C	15	ALA	2.2
2	G	214	ALA	2.2
1	H	16	ARG	2.2
1	H	95	VAL	2.2
1	H	130	ALA	2.2
2	E	62	LEU	2.2
2	G	103	LEU	2.2
2	E	219	GLN	2.2
1	F	301	ILE	2.2
1	C	52	GLY	2.2
1	F	177	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	98	ASP	2.2
2	E	64	LEU	2.2
1	H	68	ARG	2.2
2	B	186	GLN	2.2
1	D	303	VAL	2.2
1	D	134	LEU	2.1
1	H	37	GLN	2.1
2	A	62	LEU	2.1
2	B	62	LEU	2.1
2	G	64	LEU	2.1
1	F	81	ILE	2.1
1	C	134	LEU	2.1
1	D	133	LEU	2.1
1	C	261	ASP	2.1
1	D	21	ASP	2.1
1	H	133	LEU	2.0
2	G	62	LEU	2.0
2	G	143	LEU	2.0
1	F	238	ALA	2.0
1	H	15	ALA	2.0
2	A	99	THR	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
4	GOL	C	405	6/6	0.90	0.27	10.03	44,55,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	B	502	6/6	0.75	0.31	9.27	59,60,66,66	0
8	PGE	B	505	10/10	0.78	0.22	8.78	37,62,64,66	0
5	MPO	C	407	13/13	0.94	0.22	8.01	28,35,60,62	0
4	GOL	B	501	6/6	0.87	0.28	7.42	38,44,51,62	0
3	PO4	E	401	5/5	0.79	0.39	6.26	65,68,93,98	0
3	PO4	A	401	5/5	0.79	0.30	5.64	56,68,78,88	0
3	PO4	H	404	5/5	0.93	0.23	4.96	63,76,90,99	0
4	GOL	C	404	6/6	0.93	0.17	4.76	39,47,49,49	0
4	GOL	B	503	6/6	0.90	0.17	4.28	43,46,48,50	0
5	MPO	H	406	13/13	0.96	0.19	4.00	29,38,63,67	1
4	GOL	D	405	6/6	0.93	0.22	3.49	38,53,56,57	0
6	TRS	C	408	8/8	0.87	0.21	2.71	44,50,54,56	0
9	PEG	D	407	7/7	0.81	0.20	2.46	46,48,56,57	0
10	NA	E	402	1/1	0.99	0.14	2.03	35,35,35,35	0
3	PO4	F	405	5/5	0.96	0.16	2.01	51,51,60,63	0
5	MPO	C	406	13/13	0.91	0.21	1.90	63,68,82,85	0
9	PEG	H	407	7/7	0.85	0.28	1.73	58,60,63,64	0
3	PO4	C	403	5/5	0.96	0.13	1.49	33,34,35,40	0
7	CL	D	409	1/1	0.67	0.16	1.29	47,47,47,47	1
9	PEG	D	408	7/7	0.73	0.18	1.10	58,61,65,66	0
3	PO4	C	402	5/5	0.97	0.12	1.06	42,45,53,55	0
3	PO4	H	405	5/5	0.97	0.14	0.99	41,46,48,51	0
5	MPO	D	406	13/13	0.95	0.13	0.79	44,53,57,59	2
3	PO4	D	401	5/5	0.98	0.11	0.47	34,36,38,43	0
3	PO4	D	404	5/5	0.98	0.12	0.38	27,31,32,33	0
3	PO4	F	401	5/5	0.97	0.11	0.34	45,46,55,58	0
3	PO4	F	406	5/5	0.97	0.13	0.18	41,42,44,46	0
4	GOL	B	504	6/6	0.95	0.11	-0.23	23,26,30,34	0
3	PO4	H	402	5/5	0.99	0.10	-0.41	33,34,36,43	0
3	PO4	F	404	5/5	0.96	0.12	-0.47	47,47,50,59	0
3	PO4	D	403	5/5	0.98	0.10	-0.54	39,41,43,47	0
3	PO4	C	401	5/5	0.97	0.11	-0.56	50,55,65,66	0
3	PO4	F	403	5/5	0.97	0.12	-0.59	33,35,37,43	0
3	PO4	D	402	5/5	0.97	0.13	-0.68	47,51,65,67	0
3	PO4	F	402	5/5	0.96	0.11	-0.88	39,39,41,42	0
7	CL	C	409	1/1	0.93	0.09	-1.05	46,46,46,46	0
3	PO4	H	401	5/5	0.97	0.08	-1.45	42,46,51,52	0
3	PO4	H	403	5/5	0.97	0.09	-2.64	50,50,53,55	0

6.5 Other polymers

There are no such residues in this entry.