Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 11:59 PM EDT

PDB ID	:	5HSA
Title	:	Alcohol Oxidase AOX1 from Pichia Pastoris
Authors	:	Neumann, P.; Ficner, R.; Feussner, I.; Koch, C.
Deposited on	:	2016-01-25
Resolution	:	2.35 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:

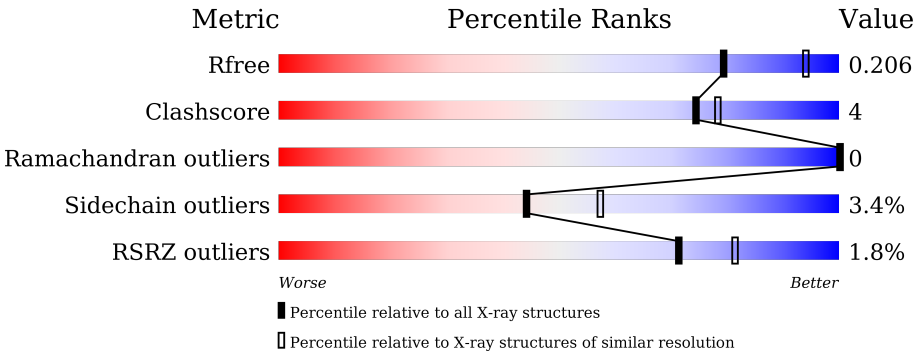
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	663	89% 10%
1	B	663	3% 88% 11%
1	C	663	89% 10%
1	D	663	4% 90% 8%
1	E	663	% 89% 10%
1	F	663	% 89% 9%

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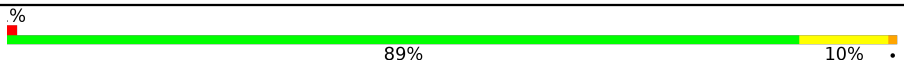
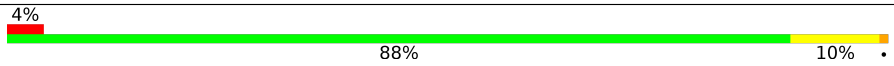
Mol	Chain	Length	Quality of chain
1	G	663	
1	H	663	

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
3	P6G	B	702	-	-	-	X
3	P6G	B	703	-	-	-	X
3	P6G	C	702	-	-	-	X
3	P6G	C	703	-	-	-	X
3	P6G	E	702	-	-	-	X
3	P6G	F	703	-	-	-	X
4	PGE	A	703	-	-	-	X
4	PGE	B	704	-	-	-	X
4	PGE	C	704	-	-	-	X
4	PGE	D	703	-	-	-	X
4	PGE	E	703	-	-	-	X
4	PGE	G	702	-	-	-	X
4	PGE	G	703	-	-	-	X
7	GOL	F	705	-	-	-	X

2 Entry composition (i)

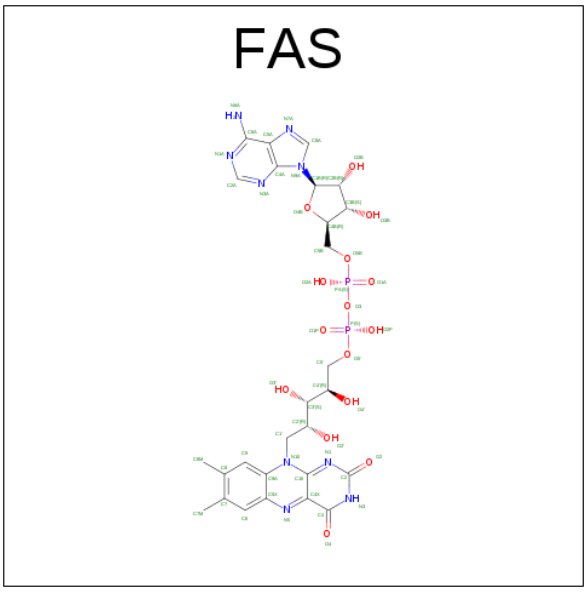
There are 9 unique types of molecules in this entry. The entry contains 44407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol oxidase 1.

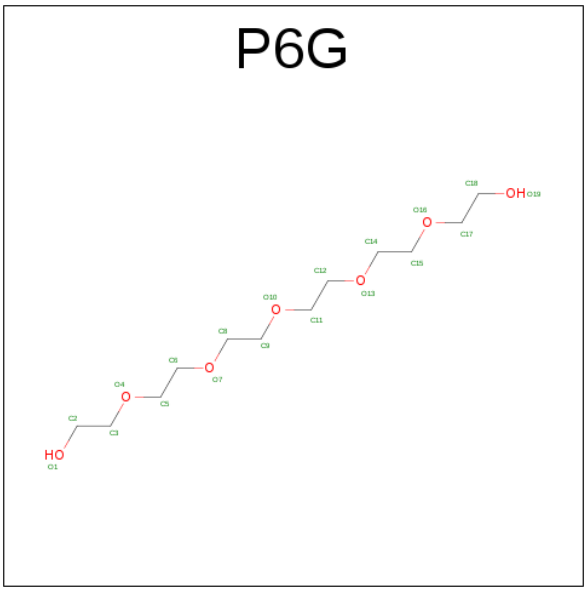
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	B	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	C	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	D	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	E	662	Total	C	N	O	S	0	1	0
			5206	3291	901	988	26			
1	F	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			
1	G	662	Total	C	N	O	S	0	1	0
			5207	3292	901	988	26			
1	H	662	Total	C	N	O	S	0	0	0
			5199	3286	900	987	26			

- Molecule 2 is ARABINO-FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAS) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



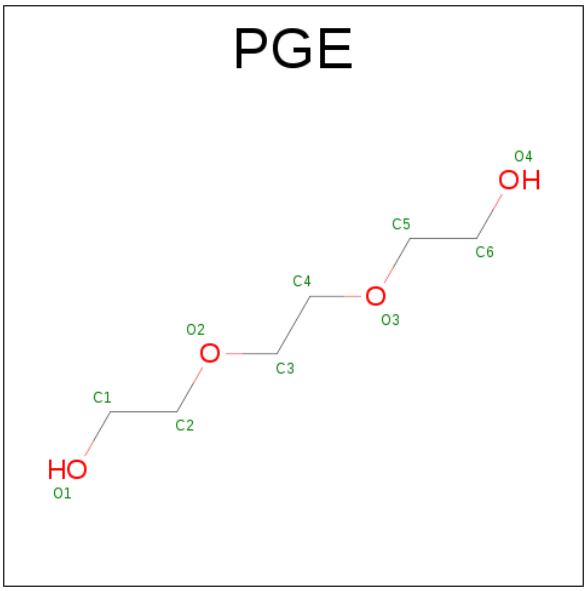
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



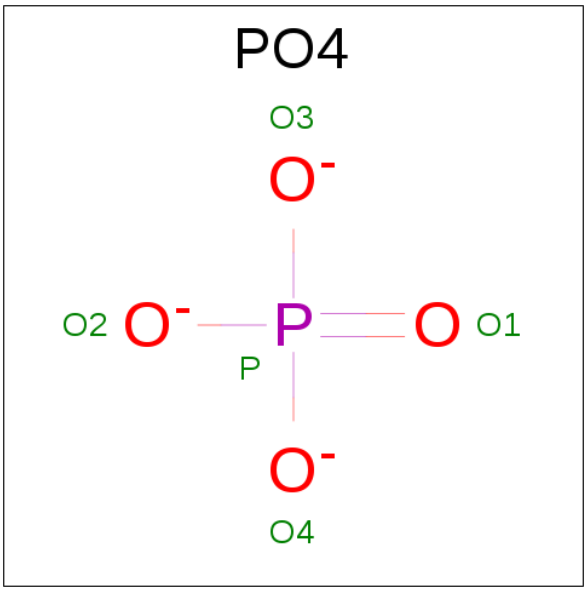
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0
3	B	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0
3	D	1	Total C O 19 12 7	0	0
3	E	1	Total C O 19 12 7	0	0
3	F	1	Total C O 19 12 7	0	0
3	F	1	Total C O 19 12 7	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	G	1	Total C O 10 6 4	0	0
4	G	1	Total C O 10 6 4	0	0
4	H	1	Total C O 10 6 4	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

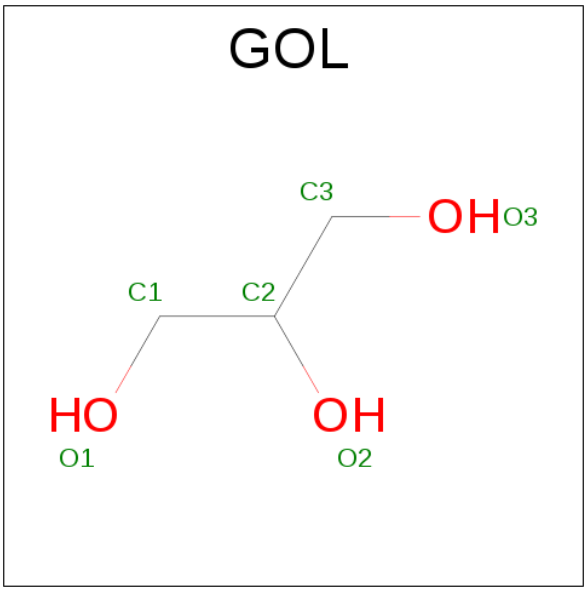


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	1
5	F	1	Total O P 5 4 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	C	2	Total Ca 2 2	0	0
6	A	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	1
7	F	1	Total C O 6 3 3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Cl 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	358	Total O 359 359	0	2
9	B	226	Total O 226 226	0	1
9	C	325	Total O 325 325	0	3
9	D	178	Total O 178 178	0	2
9	E	356	Total O 356 356	0	0
9	F	300	Total O 300 300	0	0

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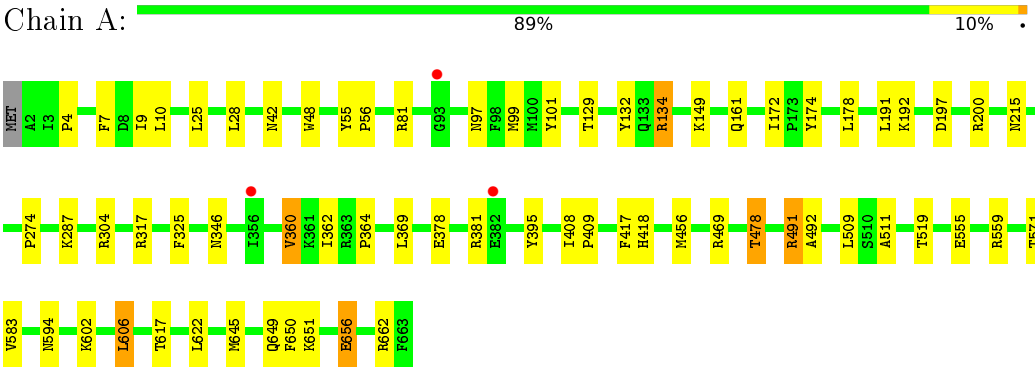
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	211	Total O 211 211	0	0
9	H	129	Total O 129 129	0	0

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.

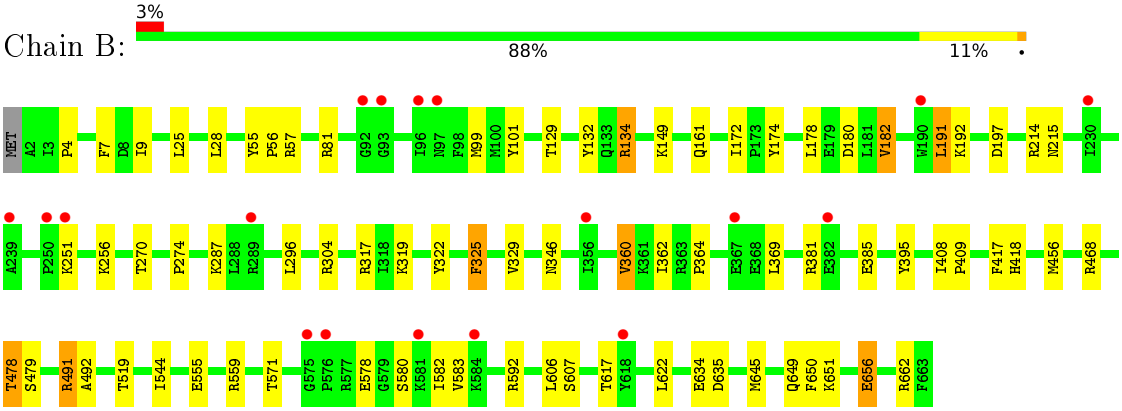
- Molecule 1: Alcohol oxidase 1

Chain A:



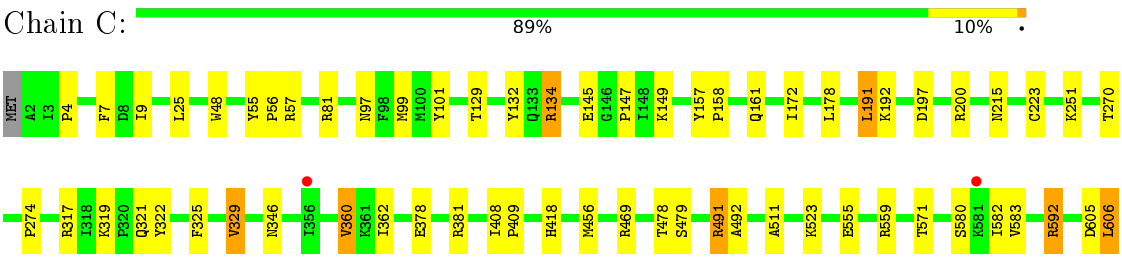
- Molecule 1: Alcohol oxidase 1

Chain B:



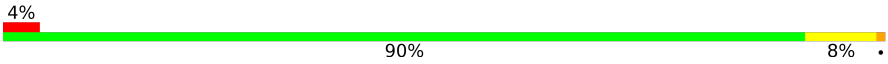
- Molecule 1: Alcohol oxidase 1

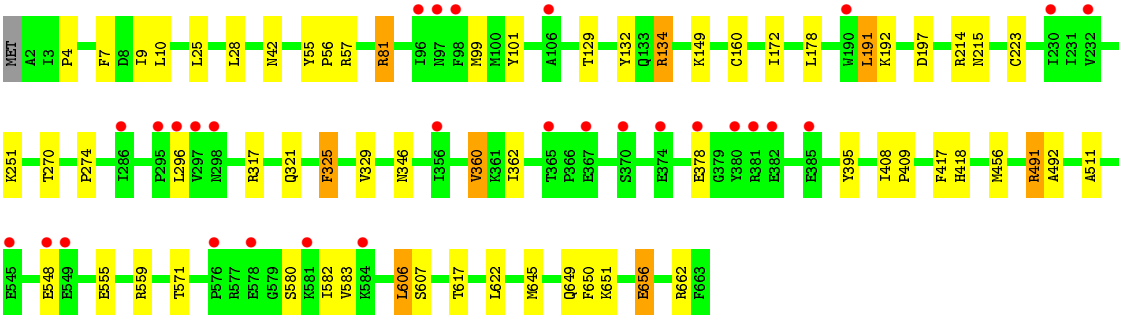
Chain C:



• Molecule 1: Alcohol oxidase 1

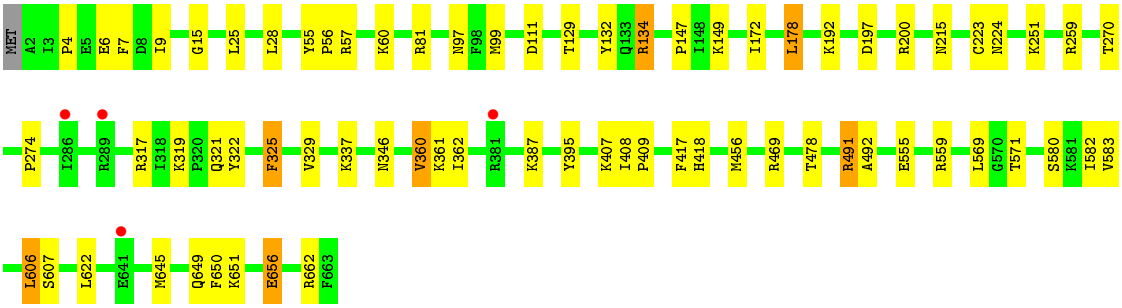
Chain D:





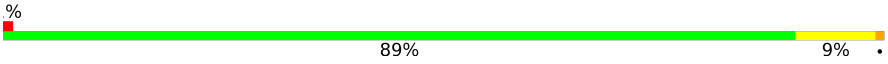
• Molecule 1: Alcohol oxidase 1

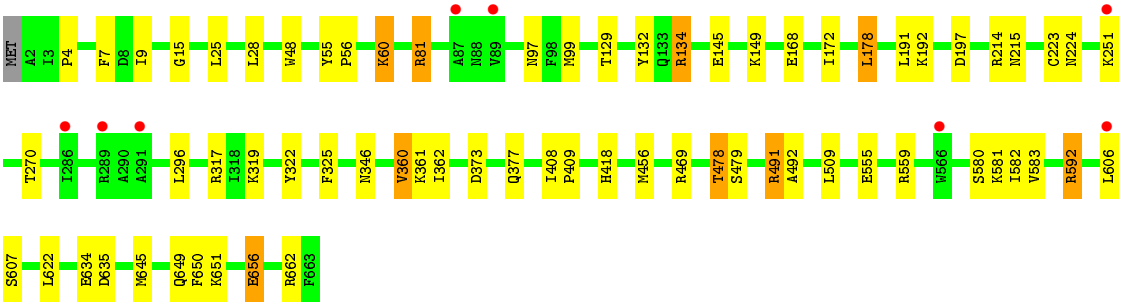
Chain E:



• Molecule 1: Alcohol oxidase 1

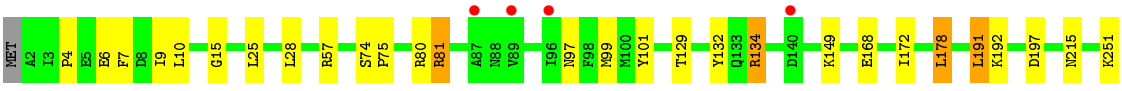
Chain F:



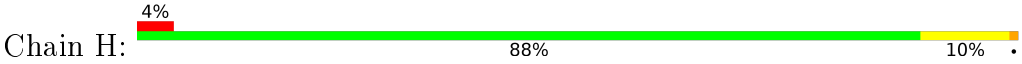


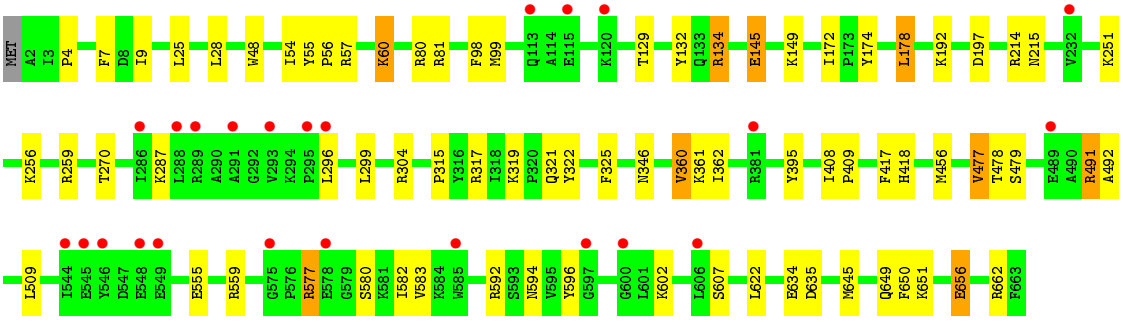
• Molecule 1: Alcohol oxidase 1

Chain G:



• Molecule 1: Alcohol oxidase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.10Å 165.19Å 164.31Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	40.88 – 2.35 45.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.88-2.35) 98.7 (45.67-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.177 , 0.205 0.175 , 0.206	Depositor DCC
R_{free} test set	12268 reflections (4.82%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 254642 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	44407	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 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, FAS, PO4, P6G, CA

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	0.29	0/5341	0.46	0/7245
1	B	0.27	0/5341	0.46	0/7245
1	C	0.29	0/5341	0.47	0/7245
1	D	0.26	0/5341	0.45	0/7245
1	E	0.30	0/5348	0.47	0/7255
1	F	0.28	0/5341	0.46	0/7245
1	G	0.27	0/5349	0.46	0/7256
1	H	0.26	0/5341	0.45	0/7245
All	All	0.28	0/42743	0.46	0/57981

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5199	0	5013	45	0
1	B	5199	0	5013	43	0
1	C	5199	0	5013	50	0
1	D	5199	0	5013	36	0
1	E	5206	0	5021	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5199	0	5013	45	0
1	G	5207	0	5023	45	0
1	H	5199	0	5013	47	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
2	E	53	0	31	3	0
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	H	53	0	31	1	0
3	A	19	0	26	1	0
3	B	38	0	52	10	0
3	C	38	0	52	13	0
3	D	19	0	26	1	0
3	E	19	0	26	4	0
3	F	38	0	52	8	0
4	A	10	0	14	2	0
4	B	20	0	28	1	0
4	C	10	0	14	1	0
4	D	10	0	14	0	0
4	E	10	0	14	0	0
4	G	20	0	28	0	0
4	H	10	0	14	1	0
5	A	5	0	0	1	0
5	F	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
7	C	6	0	8	0	0
7	F	6	0	8	2	0
8	C	1	0	0	0	0
9	A	359	0	0	3	0
9	B	226	0	0	2	0
9	C	325	0	0	4	0
9	D	178	0	0	3	0
9	E	356	0	0	3	0
9	F	300	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	211	0	0	0	0
9	H	129	0	0	1	0
All	All	44407	0	40746	334	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 (334) 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:223:CYS:H	3:B:702:P6G:H62	1.36	0.89
3:C:703:P6G:H111	1:D:42:ASN:HD22	1.48	0.77
1:C:479:SER:HB2	3:F:702:P6G:H62	1.66	0.75
1:C:649:GLN:NE2	1:C:651:LYS:HG2	2.03	0.73
5:F:704:PO4:O3	9:F:801:HOH:O	2.08	0.71
1:C:346:ASN:O	1:C:662:ARG:NH2	2.25	0.70
1:C:592:ARG:NH2	1:C:635:ASP:OD1	2.25	0.69
1:E:649:GLN:NE2	1:E:651:LYS:HG2	2.08	0.68
1:E:346:ASN:O	1:E:662:ARG:NH2	2.26	0.68
1:F:215:ASN:OD1	1:H:656:GLU:HG3	1.93	0.68
1:H:346:ASN:O	1:H:662:ARG:NH2	2.25	0.68
1:B:346:ASN:O	1:B:662:ARG:NH2	2.27	0.68
1:G:346:ASN:O	1:G:662:ARG:NH2	2.26	0.68
1:A:346:ASN:O	1:A:662:ARG:NH2	2.26	0.68
3:C:703:P6G:H141	1:D:223:CYS:HB2	1.75	0.68
1:F:346:ASN:O	1:F:662:ARG:NH2	2.26	0.68
1:D:346:ASN:O	1:D:662:ARG:NH2	2.27	0.67
1:B:214:ARG:C	1:B:215:ASN:HD22	1.97	0.67
1:E:656:GLU:HG3	1:G:215:ASN:OD1	1.95	0.67
5:A:704[B]:PO4:O1	9:A:801:HOH:O	2.12	0.67
1:C:161:GLN:HE21	3:C:703:P6G:H52	1.59	0.67
1:G:656:GLU:HG3	1:H:215:ASN:OD1	1.96	0.66
1:A:215:ASN:OD1	1:B:656:GLU:HG3	1.97	0.65
1:E:215:ASN:OD1	1:F:656:GLU:HG3	1.98	0.64
1:C:147:PRO:HA	1:C:649:GLN:OE1	1.98	0.64
1:H:48:TRP:HH2	4:H:702:PGE:H3	1.62	0.64
1:C:656:GLU:HG3	1:D:215:ASN:OD1	1.97	0.63
1:B:592:ARG:NH2	1:B:635:ASP:OD1	2.32	0.63
1:E:569:LEU:HB3	1:E:606:LEU:HD23	1.81	0.62
1:F:223:CYS:H	3:F:703:P6G:H62	1.65	0.62
1:C:649:GLN:HE21	1:C:651:LYS:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:OE1	1:A:381:ARG:NH1	2.32	0.62
1:E:147:PRO:HA	1:E:649:GLN:OE1	2.00	0.61
1:A:656:GLU:HG3	1:C:215:ASN:OD1	2.00	0.61
1:C:223:CYS:H	3:C:702:P6G:H82	1.65	0.61
1:B:606:LEU:HD21	1:B:617:THR:HB	1.84	0.60
1:A:28:LEU:HB2	1:A:645:MET:HE2	1.82	0.60
1:A:224:ASN:HB2	3:B:702:P6G:H21	1.85	0.59
1:F:478:THR:HG23	3:F:702:P6G:H31	1.83	0.59
1:F:360:VAL:HG13	1:F:362:ILE:HG23	1.86	0.58
1:E:28:LEU:HB2	1:E:645:MET:HE3	1.86	0.58
1:F:28:LEU:HB2	1:F:645:MET:HE3	1.86	0.57
1:H:360:VAL:HG13	1:H:362:ILE:HG23	1.87	0.56
1:C:161:GLN:HE21	3:C:703:P6G:H31	1.69	0.56
1:A:174:TYR:CG	3:C:702:P6G:H51	2.40	0.56
1:C:360:VAL:HG13	1:C:362:ILE:HG23	1.86	0.56
1:D:28:LEU:HB2	1:D:645:MET:HE3	1.86	0.56
1:E:360:VAL:HG13	1:E:362:ILE:HG23	1.86	0.56
1:A:101:TYR:HB3	1:A:191:LEU:HB3	1.87	0.56
1:C:48:TRP:HH2	4:C:704:PGE:H5	1.71	0.56
1:H:28:LEU:HB2	1:H:645:MET:HE3	1.88	0.56
1:A:360:VAL:HG13	1:A:362:ILE:HG23	1.88	0.56
1:D:360:VAL:HG13	1:D:362:ILE:HG23	1.88	0.56
3:C:703:P6G:C14	1:D:223:CYS:H	2.19	0.55
1:C:172:ILE:HG21	1:C:360:VAL:HG22	1.89	0.55
1:E:172:ILE:HG21	1:E:360:VAL:HG22	1.87	0.55
3:B:703:P6G:O19	1:G:478:THR:HG23	2.07	0.55
1:F:48:TRP:HH2	7:F:705:GOL:H2	1.71	0.55
1:G:360:VAL:HG13	1:G:362:ILE:HG23	1.87	0.55
1:H:594:ASN:OD1	1:H:602:LYS:NZ	2.37	0.55
1:G:172:ILE:HG21	1:G:360:VAL:HG22	1.88	0.54
1:H:315:PRO:HG2	1:H:477:VAL:CG1	2.37	0.54
1:B:360:VAL:HG13	1:B:362:ILE:HG23	1.88	0.54
1:D:172:ILE:HG21	1:D:360:VAL:HG22	1.90	0.54
1:H:592:ARG:NH2	1:H:635:ASP:OD1	2.41	0.54
1:H:172:ILE:HG21	1:H:360:VAL:HG22	1.89	0.54
1:A:172:ILE:HG21	1:A:360:VAL:HG22	1.90	0.53
1:C:582:ILE:HG13	1:C:583:VAL:HG23	1.89	0.53
1:H:315:PRO:HG2	1:H:477:VAL:HG11	1.89	0.53
1:B:172:ILE:HG21	1:B:360:VAL:HG22	1.89	0.53
1:F:197:ASP:O	1:F:662:ARG:NH1	2.42	0.53
1:H:197:ASP:O	1:H:662:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HB2	1:B:645:MET:HE3	1.91	0.53
1:G:606[A]:LEU:HD21	1:G:617:THR:HB	1.91	0.53
1:D:197:ASP:O	1:D:662:ARG:NH1	2.42	0.52
1:E:223:CYS:H	3:E:702:P6G:C14	2.22	0.52
1:E:649:GLN:HE21	1:E:651:LYS:HG2	1.72	0.52
4:B:704:PGE:H5	1:G:507:LEU:HA	1.91	0.52
1:F:172:ILE:HG21	1:F:360:VAL:HG22	1.89	0.52
1:G:28:LEU:HB2	1:G:645:MET:HE3	1.90	0.52
1:E:325:PHE:O	1:E:329[A]:VAL:HG22	2.09	0.52
1:E:197:ASP:O	1:E:662:ARG:NH1	2.42	0.52
1:F:223:CYS:N	3:F:703:P6G:H62	2.24	0.52
1:A:197:ASP:O	1:A:662:ARG:NH1	2.42	0.52
1:B:582:ILE:HG13	1:B:583:VAL:HG23	1.92	0.52
1:B:174:TYR:CD2	3:B:702:P6G:H51	2.45	0.51
1:C:408:ILE:HG12	1:C:409:PRO:HD2	1.92	0.51
1:G:592:ARG:NH2	1:G:635:ASP:OD1	2.43	0.51
1:D:329:VAL:HA	1:H:509:LEU:HD12	1.92	0.51
1:F:582:ILE:HG13	1:F:583:VAL:HG23	1.92	0.51
1:G:606[B]:LEU:HD11	1:G:617:THR:HB	1.91	0.51
1:E:337:LYS:NZ	9:E:805:HOH:O	2.43	0.51
1:B:329:VAL:HA	1:G:509:LEU:HD12	1.93	0.51
1:H:319:LYS:HB2	1:H:322:TYR:CD2	2.46	0.51
1:H:582:ILE:HG13	1:H:583:VAL:HG23	1.93	0.51
1:C:197:ASP:O	1:C:662:ARG:NH1	2.44	0.50
1:E:224:ASN:HD22	3:E:702:P6G:H172	1.77	0.50
1:H:408:ILE:HG12	1:H:409:PRO:HD2	1.93	0.50
1:E:582:ILE:HG13	1:E:583:VAL:HG23	1.92	0.50
1:F:48:TRP:CH2	7:F:705:GOL:H2	2.47	0.50
1:G:656:GLU:OE2	1:H:214:ARG:NH1	2.35	0.50
1:E:223:CYS:H	3:E:702:P6G:H141	1.77	0.50
1:B:408:ILE:HG12	1:B:409:PRO:HD2	1.93	0.50
1:D:649:GLN:NE2	1:D:651:LYS:HG2	2.27	0.50
1:B:364:PRO:HB2	1:B:369:LEU:HG	1.94	0.50
1:G:408:ILE:HG12	1:G:409:PRO:HD2	1.93	0.49
1:H:592:ARG:NH1	1:H:634:GLU:OE1	2.45	0.49
1:G:582:ILE:HG13	1:G:583:VAL:HG23	1.93	0.49
1:A:469:ARG:HD2	9:A:820:HOH:O	2.10	0.49
3:D:702:P6G:H111	1:H:479:SER:HA	1.94	0.49
1:E:319:LYS:HB2	1:E:322:TYR:CD2	2.47	0.49
1:D:408:ILE:HG12	1:D:409:PRO:HD2	1.94	0.49
1:H:649:GLN:NE2	1:H:651:LYS:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:SER:HB3	3:B:703:P6G:H32	1.95	0.49
1:F:592:ARG:NH2	1:F:635:ASP:OD1	2.46	0.49
1:A:511:ALA:O	1:E:60:LYS:HE2	2.12	0.49
1:F:408:ILE:HG12	1:F:409:PRO:HD2	1.94	0.49
1:B:478:THR:HG23	3:B:703:P6G:H31	1.95	0.49
1:F:479:SER:HA	3:F:702:P6G:H82	1.94	0.49
1:G:197:ASP:O	1:G:662:ARG:NH1	2.46	0.49
1:A:132:TYR:CE2	1:A:134:ARG:HD2	2.48	0.48
1:F:649:GLN:NE2	1:F:651:LYS:HG2	2.28	0.48
1:C:469:ARG:HD2	9:C:837:HOH:O	2.12	0.48
1:C:629:ALA:HB1	1:C:645:MET:HE1	1.95	0.48
1:A:408:ILE:HG12	1:A:409:PRO:HD2	1.95	0.48
1:A:582:ILE:HG13	1:A:583:VAL:HG23	1.95	0.48
1:E:408:ILE:HG12	1:E:409:PRO:HD2	1.95	0.48
1:E:650:PHE:HB2	1:F:656:GLU:HA	1.95	0.48
1:F:319:LYS:HB2	1:F:322:TYR:CD2	2.48	0.48
3:F:703:P6G:H51	1:H:174:TYR:CG	2.48	0.48
1:A:48:TRP:HH2	4:A:703:PGE:H42	1.79	0.48
1:B:197:ASP:O	1:B:662:ARG:NH1	2.46	0.48
1:H:577:ARG:HG2	1:H:596:TYR:CZ	2.48	0.48
3:C:703:P6G:H142	1:D:223:CYS:H	1.77	0.48
1:C:511:ALA:O	1:F:60:LYS:HE2	2.14	0.48
1:E:555:GLU:O	1:E:559:ARG:HG3	2.14	0.48
1:B:650:PHE:HB2	1:D:656:GLU:HA	1.95	0.48
1:C:134:ARG:NH1	9:C:810:HOH:O	2.47	0.47
1:E:223:CYS:HB2	3:E:702:P6G:H141	1.94	0.47
1:F:469:ARG:HD2	9:F:806:HOH:O	2.14	0.47
1:D:101:TYR:HB3	1:D:191:LEU:HB3	1.96	0.47
1:B:592:ARG:NH1	1:B:634:GLU:OE1	2.46	0.47
1:G:129:THR:HG21	1:G:622:LEU:HD13	1.96	0.47
1:A:287:LYS:HE3	1:A:304:ARG:NH2	2.29	0.47
1:D:9:ILE:HG21	1:D:25:LEU:HD13	1.97	0.47
1:G:168:GLU:OE2	1:H:256:LYS:NZ	2.48	0.47
1:B:256:LYS:NZ	9:B:805:HOH:O	2.37	0.47
1:F:168:GLU:OE1	9:F:802:HOH:O	2.21	0.47
1:H:129:THR:HG21	1:H:622:LEU:HD13	1.96	0.47
1:B:319:LYS:HB2	1:B:322:TYR:CD2	2.50	0.47
1:D:129:THR:HG21	1:D:622:LEU:HD13	1.96	0.47
1:A:129:THR:HG21	1:A:622:LEU:HD13	1.97	0.47
1:B:132:TYR:CE2	1:B:134:ARG:HD2	2.49	0.47
1:B:129:THR:HG21	1:B:622:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TYR:CE2	1:C:134:ARG:HD2	2.50	0.47
1:H:9:ILE:HG21	1:H:25:LEU:HD13	1.97	0.47
1:E:491:ARG:HD3	1:E:492:ALA:O	2.15	0.47
1:H:132:TYR:CE2	1:H:134:ARG:HD2	2.50	0.47
1:C:101:TYR:HB3	1:C:191:LEU:HB3	1.97	0.46
1:A:649:GLN:NE2	1:A:651:LYS:HG2	2.29	0.46
1:C:329:VAL:HA	1:F:509:LEU:HD12	1.97	0.46
1:D:555:GLU:O	1:D:559:ARG:HG3	2.16	0.46
1:E:97:ASN:HA	2:E:701:FAS:C6	2.45	0.46
1:G:491:ARG:HD3	1:G:492:ALA:O	2.15	0.46
1:B:649:GLN:NE2	1:B:651:LYS:HG2	2.30	0.46
1:C:606:LEU:HD21	1:C:617:THR:HB	1.98	0.46
1:B:555:GLU:O	1:B:559:ARG:HG3	2.14	0.46
1:E:319:LYS:HB2	1:E:322:TYR:HD2	1.80	0.46
1:G:9:ILE:HG21	1:G:25:LEU:HD13	1.97	0.46
1:H:491:ARG:HD3	1:H:492:ALA:O	2.16	0.46
1:F:9:ILE:HG21	1:F:25:LEU:HD13	1.97	0.46
1:A:4:PRO:HG2	1:A:7:PHE:CE2	2.51	0.46
1:G:555:GLU:O	1:G:559:ARG:HG3	2.16	0.46
1:H:577:ARG:HG2	1:H:596:TYR:CE1	2.51	0.46
1:A:555:GLU:O	1:A:559:ARG:HG3	2.16	0.46
1:B:9:ILE:HG21	1:B:25:LEU:HD13	1.97	0.46
1:C:9:ILE:HG21	1:C:25:LEU:HD13	1.98	0.46
1:D:99:MET:O	1:D:192:LYS:HA	2.16	0.46
1:A:42:ASN:HB2	3:B:702:P6G:H91	1.97	0.46
1:F:97:ASN:HA	2:F:701:FAS:C6	2.46	0.45
1:H:555:GLU:O	1:H:559:ARG:HG3	2.15	0.45
1:A:656:GLU:HA	1:C:650:PHE:HB2	1.98	0.45
1:E:200:ARG:NH1	9:E:810:HOH:O	2.49	0.45
1:H:99:MET:O	1:H:192:LYS:HA	2.17	0.45
9:D:898:HOH:O	1:H:80:ARG:HD2	2.16	0.45
1:A:161:GLN:HG2	3:C:702:P6G:H121	1.98	0.45
1:H:145:GLU:HG3	1:H:651:LYS:HD3	1.99	0.45
1:B:101:TYR:HB3	1:B:191:LEU:HB3	1.98	0.45
1:B:99:MET:O	1:B:192:LYS:HA	2.16	0.45
1:B:325:PHE:O	1:B:329:VAL:HG13	2.17	0.45
1:E:99:MET:O	1:E:192:LYS:HA	2.16	0.45
1:G:132:TYR:CE2	1:G:134:ARG:HD2	2.51	0.45
1:C:491:ARG:HD3	1:C:492:ALA:O	2.16	0.45
1:E:4:PRO:HG2	1:E:7:PHE:CE2	2.52	0.45
1:E:97:ASN:HB2	2:E:701:FAS:C4X	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:HB2	3:F:703:P6G:H22	1.98	0.45
1:G:97:ASN:HA	2:G:701:FAS:C6	2.47	0.45
1:A:99:MET:O	1:A:192:LYS:HA	2.17	0.45
1:B:270:THR:HA	1:B:607:SER:HB3	1.98	0.45
1:B:4:PRO:HG2	1:B:7:PHE:CE2	2.52	0.45
1:D:132:TYR:CE2	1:D:134:ARG:HD2	2.52	0.45
1:E:656:GLU:HA	1:G:650:PHE:HB2	1.98	0.45
1:B:319:LYS:HB2	1:B:322:TYR:HD2	1.82	0.45
1:C:555:GLU:O	1:C:559:ARG:HG3	2.15	0.45
1:C:129:THR:HG21	1:C:622:LEU:HD13	1.98	0.45
1:A:491:ARG:HD3	1:A:492:ALA:O	2.17	0.45
1:G:319:LYS:HB2	1:G:322:TYR:HD2	1.82	0.45
1:H:270:THR:HA	1:H:607:SER:HB3	1.99	0.45
1:F:555:GLU:O	1:F:559:ARG:HG3	2.17	0.45
1:A:9:ILE:HG21	1:A:25:LEU:HD13	1.99	0.44
1:C:270:THR:HA	1:C:607:SER:HB3	2.00	0.44
1:F:373:ASP:O	1:F:377:GLN:HG3	2.17	0.44
1:B:180:ASP:O	1:B:182:VAL:HG12	2.17	0.44
1:B:287:LYS:HE3	1:B:304:ARG:NH2	2.33	0.44
1:C:319:LYS:HB2	1:C:322:TYR:CD2	2.51	0.44
1:C:99:MET:O	1:C:192:LYS:HA	2.17	0.44
1:F:129:THR:HG21	1:F:622:LEU:HD13	1.99	0.44
1:F:4:PRO:HG2	1:F:7:PHE:CE2	2.53	0.44
1:G:649:GLN:NE2	1:G:651:LYS:HG2	2.31	0.44
9:B:958:HOH:O	1:G:80:ARG:HD2	2.17	0.44
1:A:478:THR:HG21	1:A:519:THR:HG22	1.99	0.44
1:A:48:TRP:CH2	4:A:703:PGE:H5	2.52	0.44
1:F:97:ASN:HB2	2:F:701:FAS:C4X	2.47	0.44
1:G:97:ASN:HB2	2:G:701:FAS:C4X	2.47	0.44
1:G:656:GLU:HA	1:H:650:PHE:HB2	2.00	0.44
3:B:703:P6G:H111	1:G:479:SER:HA	1.99	0.44
1:C:4:PRO:HG2	1:C:7:PHE:CE2	2.52	0.44
1:F:132:TYR:CE2	1:F:134:ARG:HD2	2.53	0.44
1:D:4:PRO:HG2	1:D:7:PHE:CE2	2.53	0.44
1:E:9:ILE:HG21	1:E:25:LEU:HD13	1.99	0.44
1:G:178:LEU:HD22	1:G:361:LYS:HD2	2.00	0.44
1:G:99:MET:O	1:G:192:LYS:HA	2.18	0.44
1:C:319:LYS:HB2	1:C:322:TYR:HD2	1.83	0.44
1:D:606:LEU:HD21	1:D:617:THR:HB	1.98	0.44
1:E:129:THR:HG21	1:E:622:LEU:HD13	1.99	0.44
1:C:223:CYS:N	3:C:702:P6G:H62	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:GLY:HA3	2:E:701:FAS:O5B	2.18	0.44
1:E:178:LEU:HD22	1:E:361:LYS:HD2	2.00	0.43
1:F:99:MET:O	1:F:192:LYS:HA	2.17	0.43
1:H:319:LYS:HB2	1:H:322:TYR:HD2	1.82	0.43
1:H:4:PRO:HG2	1:H:7:PHE:CE2	2.52	0.43
1:C:656:GLU:HA	1:D:650:PHE:HB2	2.00	0.43
1:F:491:ARG:HD3	1:F:492:ALA:O	2.17	0.43
1:E:132:TYR:CE2	1:E:134:ARG:HD2	2.53	0.43
1:G:592:ARG:NH1	1:G:634:GLU:OE1	2.46	0.43
1:A:606:LEU:HD21	1:A:617:THR:HB	2.00	0.43
1:B:161:GLN:HE21	3:B:702:P6G:H172	1.83	0.43
1:G:4:PRO:HG2	1:G:7:PHE:CE2	2.53	0.43
1:F:214:ARG:NH1	1:H:656:GLU:OE2	2.37	0.43
1:D:10:LEU:HD12	1:D:10:LEU:HA	1.89	0.43
1:D:582:ILE:HG13	1:D:583:VAL:HG23	2.01	0.43
1:A:274:PRO:HG3	1:A:571:THR:HB	2.01	0.43
1:C:97:ASN:HA	2:C:701:FAS:C6	2.48	0.43
1:D:160:CYS:HB3	9:D:896:HOH:O	2.18	0.43
1:E:111:ASP:OD2	1:E:387:LYS:NZ	2.51	0.43
1:D:511:ALA:O	1:H:60:LYS:HE2	2.18	0.43
1:A:55:TYR:CD1	1:A:56:PRO:HD3	2.54	0.43
1:C:161:GLN:NE2	3:C:703:P6G:H31	2.32	0.43
1:F:478:THR:HG23	3:F:702:P6G:O1	2.18	0.43
1:F:650:PHE:HB2	1:H:656:GLU:HA	2.00	0.43
1:C:223:CYS:H	3:C:702:P6G:H62	1.84	0.43
1:E:274:PRO:HG3	1:E:571:THR:HB	2.01	0.43
1:G:319:LYS:HB2	1:G:322:TYR:CD2	2.53	0.43
1:G:367:GLU:OE1	1:G:367:GLU:N	2.43	0.43
1:F:15:GLY:HA3	2:F:701:FAS:O5B	2.19	0.42
1:H:54:ILE:H	1:H:54:ILE:HG13	1.75	0.42
1:C:378:GLU:OE1	1:C:381:ARG:NH1	2.52	0.42
1:C:605:ASP:HB2	2:C:701:FAS:O2P	2.19	0.42
3:A:702:P6G:H172	1:E:407:LYS:O	2.18	0.42
1:D:325:PHE:O	1:D:329:VAL:HG22	2.19	0.42
1:A:650:PHE:HB2	1:B:656:GLU:HA	2.00	0.42
1:B:491:ARG:HD3	1:B:492:ALA:O	2.19	0.42
1:F:319:LYS:HB2	1:F:322:TYR:HD2	1.84	0.42
1:A:594:ASN:OD1	1:A:602:LYS:NZ	2.52	0.42
1:C:409:PRO:HD3	9:C:973:HOH:O	2.19	0.42
1:A:364:PRO:HB2	1:A:369:LEU:HG	2.00	0.42
1:B:381:ARG:HG2	1:B:385:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ARG:HD2	9:H:875:HOH:O	2.19	0.42
1:B:478:THR:HG21	1:B:519:THR:HG22	2.00	0.42
1:C:55:TYR:CD1	1:C:56:PRO:HD3	2.55	0.42
1:D:55:TYR:CD1	1:D:56:PRO:HD3	2.54	0.42
1:H:287:LYS:HE3	1:H:304:ARG:NH2	2.35	0.42
1:B:55:TYR:CD1	1:B:56:PRO:HD3	2.54	0.42
1:E:270:THR:HA	1:E:607:SER:HB3	2.02	0.42
1:H:178:LEU:HD22	1:H:361:LYS:HD2	2.01	0.42
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.88	0.41
1:A:97:ASN:HB2	2:A:701:FAS:C4X	2.50	0.41
1:C:200:ARG:HD2	9:C:804:HOH:O	2.19	0.41
1:D:270:THR:HA	1:D:607:SER:HB3	2.02	0.41
1:F:81:ARG:H	1:F:81:ARG:HG2	1.72	0.41
1:G:10:LEU:HA	1:G:10:LEU:HD12	1.91	0.41
1:A:223:CYS:H	3:B:702:P6G:C6	2.18	0.41
1:B:55:TYR:CG	1:B:56:PRO:HD3	2.55	0.41
1:D:55:TYR:CG	1:D:56:PRO:HD3	2.55	0.41
1:E:55:TYR:CD1	1:E:56:PRO:HD3	2.55	0.41
1:F:270:THR:HA	1:F:607:SER:HB3	2.01	0.41
1:F:55:TYR:CD1	1:F:56:PRO:HD3	2.54	0.41
1:C:161:GLN:NE2	3:C:703:P6G:H52	2.32	0.41
1:F:592:ARG:NH1	1:F:634:GLU:OE1	2.47	0.41
1:A:606:LEU:HD13	2:A:701:FAS:H5'2	2.02	0.41
1:C:157:TYR:HA	1:C:158:PRO:HD3	1.90	0.41
1:E:469:ARG:HD2	9:E:1036:HOH:O	2.20	0.41
1:F:178:LEU:HD22	1:F:361:LYS:HD2	2.01	0.41
1:F:581:LYS:HD3	1:F:581:LYS:HA	1.88	0.41
1:G:377:GLN:O	1:G:381:ARG:HG3	2.20	0.41
1:A:200:ARG:HD2	9:A:841:HOH:O	2.20	0.41
1:H:55:TYR:CD1	1:H:56:PRO:HD3	2.55	0.41
1:D:274:PRO:HG3	1:D:571:THR:HB	2.02	0.41
1:B:468:ARG:NE	1:B:544:ILE:HD11	2.35	0.41
1:C:274:PRO:HG3	1:C:571:THR:HB	2.02	0.41
1:D:491:ARG:HD3	1:D:492:ALA:O	2.19	0.41
1:G:6:GLU:HG3	1:G:259:ARG:HB2	2.03	0.41
1:B:274:PRO:HG3	1:B:571:THR:HB	2.03	0.41
1:C:55:TYR:CG	1:C:56:PRO:HD3	2.55	0.41
1:G:101:TYR:HB3	1:G:191:LEU:HB3	2.01	0.41
1:G:81:ARG:H	1:G:81:ARG:HG2	1.70	0.41
1:A:395:TYR:HA	1:A:417:PHE:O	2.21	0.41
1:H:299:LEU:HD23	1:H:299:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:TYR:HA	1:G:417:PHE:O	2.21	0.41
1:E:55:TYR:CG	1:E:56:PRO:HD3	2.56	0.40
1:G:15:GLY:HA3	2:G:701:FAS:O5B	2.21	0.40
1:G:308:ASP:OD1	1:G:309:HIS:N	2.54	0.40
1:G:74:SER:HA	1:G:75:PRO:HD3	1.94	0.40
1:A:509:LEU:HD12	1:E:329[A]:VAL:HA	2.02	0.40
2:D:701:FAS:H51A	9:D:851:HOH:O	2.20	0.40
1:E:395:TYR:HA	1:E:417:PHE:O	2.22	0.40
1:A:55:TYR:CG	1:A:56:PRO:HD3	2.57	0.40
1:D:81:ARG:H	1:D:81:ARG:HG2	1.71	0.40
1:E:6:GLU:HG3	1:E:259:ARG:HB2	2.02	0.40
1:H:395:TYR:HA	1:H:417:PHE:O	2.21	0.40
1:H:98:PHE:HB2	2:H:701:FAS:O4	2.21	0.40
1:C:656:GLU:OE2	1:D:214:ARG:NH1	2.38	0.40
1:D:395:TYR:HA	1:D:417:PHE:O	2.21	0.40
1:B:395:TYR:HA	1:B:417:PHE:O	2.22	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	660/663 (100%)	637 (96%)	23 (4%)	0	100	100
1	B	660/663 (100%)	635 (96%)	25 (4%)	0	100	100
1	C	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	D	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	E	661/663 (100%)	639 (97%)	22 (3%)	0	100	100
1	F	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
1	G	661/663 (100%)	639 (97%)	22 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	660/663 (100%)	638 (97%)	22 (3%)	0	100	100
All	All	5282/5304 (100%)	5102 (97%)	180 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/561 (100%)	545 (97%)	15 (3%)	52	67
1	B	560/561 (100%)	541 (97%)	19 (3%)	44	57
1	C	560/561 (100%)	538 (96%)	22 (4%)	39	51
1	D	560/561 (100%)	540 (96%)	20 (4%)	42	55
1	E	561/561 (100%)	544 (97%)	17 (3%)	48	62
1	F	560/561 (100%)	540 (96%)	20 (4%)	42	55
1	G	561/561 (100%)	544 (97%)	17 (3%)	48	62
1	H	560/561 (100%)	539 (96%)	21 (4%)	40	52
All	All	4482/4488 (100%)	4331 (97%)	151 (3%)	44	57

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	134	ARG
1	A	149	LYS
1	A	178	LEU
1	A	251	LYS
1	A	317	ARG
1	A	325	PHE
1	A	360	VAL
1	A	418	HIS
1	A	456	MET

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Mol	Chain	Res	Type
1	A	478	THR
1	A	491	ARG
1	A	580	SER
1	A	606	LEU
1	A	656	GLU
1	B	57	ARG
1	B	81	ARG
1	B	134	ARG
1	B	149	LYS
1	B	178	LEU
1	B	182	VAL
1	B	191	LEU
1	B	251	LYS
1	B	296	LEU
1	B	317	ARG
1	B	325	PHE
1	B	360	VAL
1	B	418	HIS
1	B	456	MET
1	B	478	THR
1	B	491	ARG
1	B	578	GLU
1	B	580	SER
1	B	656	GLU
1	C	57	ARG
1	C	81	ARG
1	C	134	ARG
1	C	145	GLU
1	C	149	LYS
1	C	178	LEU
1	C	191	LEU
1	C	251	LYS
1	C	317	ARG
1	C	321	GLN
1	C	325	PHE
1	C	329	VAL
1	C	360	VAL
1	C	418	HIS
1	C	456	MET
1	C	478	THR
1	C	491	ARG
1	C	523	LYS

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Mol	Chain	Res	Type
1	C	580	SER
1	C	592	ARG
1	C	606	LEU
1	C	656	GLU
1	D	57	ARG
1	D	81	ARG
1	D	134	ARG
1	D	149	LYS
1	D	178	LEU
1	D	191	LEU
1	D	251	LYS
1	D	296	LEU
1	D	317	ARG
1	D	321	GLN
1	D	325	PHE
1	D	360	VAL
1	D	378	GLU
1	D	418	HIS
1	D	456	MET
1	D	491	ARG
1	D	548	GLU
1	D	580	SER
1	D	606	LEU
1	D	656	GLU
1	E	57	ARG
1	E	81	ARG
1	E	134	ARG
1	E	149	LYS
1	E	178	LEU
1	E	251	LYS
1	E	317	ARG
1	E	321	GLN
1	E	325	PHE
1	E	360	VAL
1	E	418	HIS
1	E	456	MET
1	E	478	THR
1	E	491	ARG
1	E	580	SER
1	E	606	LEU
1	E	656	GLU
1	F	60	LYS

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Mol	Chain	Res	Type
1	F	81	ARG
1	F	134	ARG
1	F	145	GLU
1	F	149	LYS
1	F	178	LEU
1	F	191	LEU
1	F	251	LYS
1	F	296	LEU
1	F	317	ARG
1	F	325	PHE
1	F	360	VAL
1	F	418	HIS
1	F	456	MET
1	F	478	THR
1	F	491	ARG
1	F	580	SER
1	F	592	ARG
1	F	606	LEU
1	F	656	GLU
1	G	57	ARG
1	G	81	ARG
1	G	134	ARG
1	G	149	LYS
1	G	178	LEU
1	G	191	LEU
1	G	251	LYS
1	G	317	ARG
1	G	325	PHE
1	G	360	VAL
1	G	418	HIS
1	G	456	MET
1	G	478	THR
1	G	491	ARG
1	G	515	HIS
1	G	580	SER
1	G	656	GLU
1	H	57	ARG
1	H	60	LYS
1	H	81	ARG
1	H	134	ARG
1	H	145	GLU
1	H	149	LYS

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Mol	Chain	Res	Type
1	H	178	LEU
1	H	251	LYS
1	H	296	LEU
1	H	317	ARG
1	H	321	GLN
1	H	325	PHE
1	H	360	VAL
1	H	418	HIS
1	H	456	MET
1	H	477	VAL
1	H	478	THR
1	H	491	ARG
1	H	577	ARG
1	H	580	SER
1	H	656	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	F	556	ASN
1	G	321	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
2	FAS	A	701	-	52,58,58	1.34	5 (9%)	52,89,89	2.12	10 (19%)
3	P6G	A	702	-	18,18,18	0.47	0	17,17,17	0.40	0
4	PGE	A	703	-	9,9,9	0.33	0	8,8,8	0.36	0
5	PO4	A	704[B]	-	4,4,4	0.79	0	6,6,6	0.24	0
2	FAS	B	701	-	52,58,58	1.34	6 (11%)	52,89,89	2.19	9 (17%)
3	P6G	B	702	-	18,18,18	0.50	0	17,17,17	0.38	0
3	P6G	B	703	-	18,18,18	0.45	0	17,17,17	0.52	0
4	PGE	B	704	-	9,9,9	0.34	0	8,8,8	0.31	0
4	PGE	B	705	-	9,9,9	0.34	0	8,8,8	0.30	0
2	FAS	C	701	-	52,58,58	1.32	5 (9%)	52,89,89	2.11	10 (19%)
3	P6G	C	702	-	18,18,18	0.46	0	17,17,17	0.43	0
3	P6G	C	703	-	18,18,18	0.51	0	17,17,17	0.48	0
4	PGE	C	704	-	9,9,9	0.39	0	8,8,8	0.22	0
7	GOL	C	705[B]	6	5,5,5	0.36	0	5,5,5	0.23	0
2	FAS	D	701	-	52,58,58	1.34	6 (11%)	52,89,89	2.18	8 (15%)
3	P6G	D	702	-	18,18,18	0.48	0	17,17,17	0.32	0
4	PGE	D	703	-	9,9,9	0.34	0	8,8,8	0.31	0
2	FAS	E	701	-	52,58,58	1.38	6 (11%)	52,89,89	2.06	10 (19%)
3	P6G	E	702	-	18,18,18	0.49	0	17,17,17	0.41	0
4	PGE	E	703	-	9,9,9	0.39	0	8,8,8	0.24	0
2	FAS	F	701	-	52,58,58	1.33	5 (9%)	52,89,89	2.26	9 (17%)
3	P6G	F	702	-	18,18,18	0.46	0	17,17,17	0.46	0
3	P6G	F	703	-	18,18,18	0.47	0	17,17,17	0.40	0
5	PO4	F	704	-	4,4,4	0.54	0	6,6,6	0.23	0
7	GOL	F	705	-	5,5,5	0.33	0	5,5,5	0.33	0
2	FAS	G	701	-	52,58,58	1.33	5 (9%)	52,89,89	2.19	11 (21%)
4	PGE	G	702	-	9,9,9	0.35	0	8,8,8	0.24	0
4	PGE	G	703	-	9,9,9	0.35	0	8,8,8	0.27	0
2	FAS	H	701	-	52,58,58	1.34	5 (9%)	52,89,89	2.17	11 (21%)
4	PGE	H	702	-	9,9,9	0.34	0	8,8,8	0.27	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
2	FAS	A	701	-	-	0/30/50/50	0/6/6/6
3	P6G	A	702	-	-	0/16/16/16	0/0/0/0
4	PGE	A	703	-	-	0/7/7/7	0/0/0/0
5	PO4	A	704[B]	-	-	0/0/0/0	0/0/0/0
2	FAS	B	701	-	-	0/30/50/50	0/6/6/6
3	P6G	B	702	-	-	0/16/16/16	0/0/0/0
3	P6G	B	703	-	-	0/16/16/16	0/0/0/0
4	PGE	B	704	-	-	0/7/7/7	0/0/0/0
4	PGE	B	705	-	-	0/7/7/7	0/0/0/0
2	FAS	C	701	-	-	0/30/50/50	0/6/6/6
3	P6G	C	702	-	-	0/16/16/16	0/0/0/0
3	P6G	C	703	-	-	0/16/16/16	0/0/0/0
4	PGE	C	704	-	-	0/7/7/7	0/0/0/0
7	GOL	C	705[B]	6	-	0/4/4/4	0/0/0/0
2	FAS	D	701	-	-	0/30/50/50	0/6/6/6
3	P6G	D	702	-	-	0/16/16/16	0/0/0/0
4	PGE	D	703	-	-	0/7/7/7	0/0/0/0
2	FAS	E	701	-	-	0/30/50/50	0/6/6/6
3	P6G	E	702	-	-	0/16/16/16	0/0/0/0
4	PGE	E	703	-	-	0/7/7/7	0/0/0/0
2	FAS	F	701	-	-	0/30/50/50	0/6/6/6
3	P6G	F	702	-	-	0/16/16/16	0/0/0/0
3	P6G	F	703	-	-	0/16/16/16	0/0/0/0
5	PO4	F	704	-	-	0/0/0/0	0/0/0/0
7	GOL	F	705	-	-	0/4/4/4	0/0/0/0
2	FAS	G	701	-	-	0/30/50/50	0/6/6/6
4	PGE	G	702	-	-	0/7/7/7	0/0/0/0
4	PGE	G	703	-	-	0/7/7/7	0/0/0/0
2	FAS	H	701	-	-	0/30/50/50	0/6/6/6
4	PGE	H	702	-	-	0/7/7/7	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAS	C9A-N10	2.12	1.41	1.38
2	D	701	FAS	C9A-N10	2.26	1.42	1.38
2	E	701	FAS	C10-N10	2.27	1.41	1.39
2	G	701	FAS	C8-C7	2.84	1.48	1.41
2	C	701	FAS	C8-C7	2.84	1.48	1.41
2	D	701	FAS	C8-C7	2.87	1.48	1.41
2	A	701	FAS	C8-C7	2.91	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	FAS	C5A-C4A	2.93	1.47	1.40
2	F	701	FAS	C8-C7	2.93	1.48	1.41
2	B	701	FAS	C8-C7	2.98	1.49	1.41
2	C	701	FAS	C5A-C4A	2.98	1.47	1.40
2	H	701	FAS	C8-C7	3.00	1.49	1.41
2	G	701	FAS	C9A-C5X	3.03	1.49	1.42
2	H	701	FAS	C5A-C4A	3.04	1.47	1.40
2	G	701	FAS	C5A-C4A	3.09	1.47	1.40
2	E	701	FAS	C5A-C4A	3.10	1.47	1.40
2	F	701	FAS	C5A-C4A	3.12	1.47	1.40
2	F	701	FAS	C9A-C5X	3.12	1.49	1.42
2	D	701	FAS	C9A-C5X	3.12	1.49	1.42
2	H	701	FAS	C9A-C5X	3.14	1.49	1.42
2	E	701	FAS	C8-C7	3.14	1.49	1.41
2	A	701	FAS	C5A-C4A	3.15	1.47	1.40
2	B	701	FAS	C9A-C5X	3.16	1.49	1.42
2	C	701	FAS	C9A-C5X	3.16	1.49	1.42
2	B	701	FAS	C5A-C4A	3.19	1.47	1.40
2	E	701	FAS	C9A-C5X	3.19	1.49	1.42
2	A	701	FAS	C9A-C5X	3.33	1.49	1.42
2	H	701	FAS	C4-C4X	3.63	1.48	1.41
2	A	701	FAS	C4-C4X	3.64	1.48	1.41
2	C	701	FAS	C4-C4X	3.66	1.48	1.41
2	B	701	FAS	C4-C4X	3.76	1.48	1.41
2	E	701	FAS	C4-C4X	3.79	1.49	1.41
2	F	701	FAS	C4-C4X	3.81	1.49	1.41
2	G	701	FAS	C4-C4X	3.89	1.49	1.41
2	D	701	FAS	C4-C4X	3.90	1.49	1.41
2	D	701	FAS	C4X-C10	3.92	1.48	1.40
2	B	701	FAS	C4X-C10	3.99	1.48	1.40
2	G	701	FAS	C4X-C10	4.04	1.48	1.40
2	C	701	FAS	C4X-C10	4.11	1.48	1.40
2	A	701	FAS	C4X-C10	4.20	1.48	1.40
2	F	701	FAS	C4X-C10	4.20	1.48	1.40
2	H	701	FAS	C4X-C10	4.27	1.48	1.40
2	E	701	FAS	C4X-C10	4.31	1.48	1.40

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	FAS	N3A-C2A-N1A	-6.91	123.44	128.87
2	G	701	FAS	N3A-C2A-N1A	-6.81	123.52	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	701	FAS	N3A-C2A-N1A	-6.79	123.54	128.87
2	E	701	FAS	N3A-C2A-N1A	-6.76	123.56	128.87
2	H	701	FAS	N3A-C2A-N1A	-6.70	123.61	128.87
2	B	701	FAS	C4-C4X-C10	-6.38	115.86	119.94
2	F	701	FAS	C4-C4X-C10	-6.32	115.90	119.94
2	B	701	FAS	N3A-C2A-N1A	-6.30	123.92	128.87
2	A	701	FAS	N3A-C2A-N1A	-6.14	124.05	128.87
2	G	701	FAS	C4-C4X-C10	-6.05	116.07	119.94
2	C	701	FAS	N3A-C2A-N1A	-5.95	124.20	128.87
2	D	701	FAS	C4-C4X-C10	-5.81	116.22	119.94
2	C	701	FAS	C4-C4X-C10	-5.74	116.27	119.94
2	H	701	FAS	C4-C4X-C10	-5.65	116.32	119.94
2	A	701	FAS	C4-C4X-C10	-5.57	116.38	119.94
2	E	701	FAS	C4-C4X-C10	-5.10	116.68	119.94
2	D	701	FAS	C4X-C4-N3	-4.08	118.19	123.52
2	H	701	FAS	C4X-C4-N3	-4.05	118.22	123.52
2	C	701	FAS	C4X-C4-N3	-3.98	118.33	123.52
2	G	701	FAS	C4X-C4-N3	-3.95	118.36	123.52
2	E	701	FAS	C4X-C4-N3	-3.91	118.41	123.52
2	F	701	FAS	C4X-C4-N3	-3.86	118.47	123.52
2	A	701	FAS	C4X-C4-N3	-3.80	118.56	123.52
2	B	701	FAS	C4X-C4-N3	-3.78	118.58	123.52
2	F	701	FAS	N3-C2-N1	-3.44	121.89	127.69
2	A	701	FAS	N3-C2-N1	-2.99	122.65	127.69
2	B	701	FAS	N3-C2-N1	-2.95	122.73	127.69
2	D	701	FAS	N3-C2-N1	-2.92	122.78	127.69
2	H	701	FAS	N3-C2-N1	-2.88	122.85	127.69
2	H	701	FAS	C4X-C10-N10	-2.82	118.47	120.52
2	C	701	FAS	N3-C2-N1	-2.80	122.98	127.69
2	G	701	FAS	N3-C2-N1	-2.72	123.11	127.69
2	B	701	FAS	C4X-C10-N10	-2.69	118.56	120.52
2	C	701	FAS	C1B-N9A-C4A	-2.63	123.87	126.81
2	F	701	FAS	C1B-N9A-C4A	-2.61	123.89	126.81
2	G	701	FAS	C1B-N9A-C4A	-2.61	123.89	126.81
2	E	701	FAS	N3-C2-N1	-2.57	123.37	127.69
2	E	701	FAS	C1B-N9A-C4A	-2.46	124.06	126.81
2	H	701	FAS	C1'-C2'-C3'	-2.43	102.87	109.82
2	G	701	FAS	C4X-C10-N10	-2.43	118.75	120.52
2	D	701	FAS	C4X-C10-N10	-2.31	118.84	120.52
2	C	701	FAS	C4X-C10-N10	-2.22	118.90	120.52
2	A	701	FAS	C1B-N9A-C4A	-2.16	124.39	126.81
2	H	701	FAS	C1B-N9A-C4A	-2.16	124.39	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAS	C4X-C10-N10	-2.14	118.96	120.52
2	E	701	FAS	C5X-C9A-N10	2.00	119.08	117.58
2	G	701	FAS	C6-C5X-N5	2.03	121.45	118.92
2	E	701	FAS	C2A-N1A-C6A	2.04	122.40	118.77
2	H	701	FAS	C4X-N5-C5X	2.15	119.25	116.72
2	H	701	FAS	C5X-C9A-N10	2.20	119.23	117.58
2	B	701	FAS	C5X-C9A-N10	2.20	119.23	117.58
2	F	701	FAS	C4X-N5-C5X	2.22	119.34	116.72
2	C	701	FAS	C5X-C9A-N10	2.24	119.25	117.58
2	E	701	FAS	C4X-N5-C5X	2.35	119.50	116.72
2	A	701	FAS	C5X-C9A-N10	2.37	119.35	117.58
2	G	701	FAS	C5X-C9A-N10	2.46	119.42	117.58
2	F	701	FAS	C5X-C9A-N10	2.54	119.48	117.58
2	C	701	FAS	C4X-N5-C5X	2.61	119.80	116.72
2	B	701	FAS	C4X-N5-C5X	2.72	119.93	116.72
2	A	701	FAS	C4X-N5-C5X	2.78	120.00	116.72
2	G	701	FAS	C4X-N5-C5X	2.79	120.01	116.72
2	D	701	FAS	C4X-N5-C5X	2.89	120.12	116.72
2	E	701	FAS	C4-C4X-N5	3.27	122.67	118.70
2	A	701	FAS	C4-C4X-N5	3.41	122.85	118.70
2	H	701	FAS	C4-C4X-N5	3.47	122.92	118.70
2	C	701	FAS	C4-C4X-N5	3.80	123.31	118.70
2	G	701	FAS	C4-C4X-N5	3.89	123.43	118.70
2	D	701	FAS	C4-C4X-N5	3.92	123.47	118.70
2	F	701	FAS	C4-C4X-N5	4.00	123.56	118.70
2	B	701	FAS	C4-C4X-N5	4.00	123.56	118.70
2	C	701	FAS	C4-N3-C2	8.37	122.14	115.16
2	E	701	FAS	C4-N3-C2	8.40	122.17	115.16
2	G	701	FAS	C4-N3-C2	8.56	122.30	115.16
2	D	701	FAS	C4-N3-C2	8.64	122.37	115.16
2	A	701	FAS	C4-N3-C2	8.70	122.42	115.16
2	B	701	FAS	C4-N3-C2	8.74	122.45	115.16
2	H	701	FAS	C4-N3-C2	8.89	122.58	115.16
2	F	701	FAS	C4-N3-C2	9.28	122.90	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAS	2	0
3	A	702	P6G	1	0
4	A	703	PGE	2	0
5	A	704[B]	PO4	1	0
3	B	702	P6G	6	0
3	B	703	P6G	4	0
4	B	704	PGE	1	0
2	C	701	FAS	2	0
3	C	702	P6G	5	0
3	C	703	P6G	8	0
4	C	704	PGE	1	0
2	D	701	FAS	1	0
3	D	702	P6G	1	0
2	E	701	FAS	3	0
3	E	702	P6G	4	0
2	F	701	FAS	3	0
3	F	702	P6G	4	0
3	F	703	P6G	4	0
5	F	704	PO4	1	0
7	F	705	GOL	2	0
2	G	701	FAS	3	0
2	H	701	FAS	1	0
4	H	702	PGE	1	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	A	662/663 (99%)	-0.25	3 (0%) 91 96	20, 34, 55, 70	0
1	B	662/663 (99%)	0.05	18 (2%) 58 70	25, 45, 73, 100	0
1	C	662/663 (99%)	-0.25	2 (0%) 94 97	22, 35, 53, 70	0
1	D	662/663 (99%)	0.16	29 (4%) 38 52	30, 52, 76, 102	0
1	E	662/663 (99%)	-0.28	4 (0%) 90 95	21, 34, 54, 91	0
1	F	662/663 (99%)	-0.15	8 (1%) 81 89	22, 41, 66, 86	0
1	G	662/663 (99%)	-0.09	7 (1%) 82 90	26, 44, 63, 87	0
1	H	662/663 (99%)	0.23	24 (3%) 46 60	34, 57, 86, 113	0
All	All	5296/5304 (99%)	-0.07	95 (1%) 71 81	20, 42, 70, 113	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	597	GLY	4.2
1	D	296	LEU	3.4
1	E	641	GLU	3.3
1	H	296	LEU	3.3
1	H	291	ALA	3.3
1	H	293	VAL	3.2
1	D	96	ILE	3.1
1	G	87	ALA	3.0
1	B	575	GLY	3.0
1	D	378	GLU	2.9
1	H	113	GLN	2.9
1	D	581	LYS	2.9
1	F	291	ALA	2.8
1	B	230	ILE	2.8
1	D	232	VAL	2.8
1	H	381	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	365	THR	2.7
1	G	89	VAL	2.7
1	D	548	GLU	2.7
1	H	489	GLU	2.7
1	F	286	ILE	2.6
1	F	87	ALA	2.6
1	H	288	LEU	2.6
1	H	546	TYR	2.6
1	B	96	ILE	2.6
1	H	545	GLU	2.5
1	B	190	TRP	2.5
1	B	584	LYS	2.5
1	H	289	ARG	2.5
1	H	232	VAL	2.5
1	D	382	GLU	2.5
1	H	575	GLY	2.5
1	B	356	ILE	2.5
1	H	286	ILE	2.4
1	D	374	GLU	2.4
1	H	600	GLY	2.4
1	D	549	GLU	2.4
1	D	584	LYS	2.4
1	B	97	ASN	2.4
1	D	381	ARG	2.4
1	D	298	ASN	2.4
1	D	356	ILE	2.4
1	D	106	ALA	2.4
1	G	140	ASP	2.3
1	G	641	GLU	2.3
1	D	385	GLU	2.3
1	D	578	GLU	2.3
1	B	239	ALA	2.3
1	B	289	ARG	2.3
1	F	89	VAL	2.3
1	B	93	GLY	2.3
1	H	585	TRP	2.3
1	D	545	GLU	2.3
1	D	576	PRO	2.3
1	D	370	SER	2.3
1	D	380	TYR	2.3
1	D	190	TRP	2.3
1	A	356	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	230	ILE	2.3
1	H	120	LYS	2.2
1	H	606	LEU	2.2
1	D	97	ASN	2.2
1	B	367	GLU	2.2
1	B	576	PRO	2.2
1	B	251	LYS	2.2
1	G	640	GLY	2.2
1	D	286	ILE	2.2
1	E	289	ARG	2.2
1	B	250	PRO	2.2
1	G	96	ILE	2.1
1	G	381	ARG	2.1
1	A	382	GLU	2.1
1	B	382	GLU	2.1
1	H	115	GLU	2.1
1	H	549	GLU	2.1
1	H	548	GLU	2.1
1	E	286	ILE	2.1
1	H	544	ILE	2.1
1	C	581	LYS	2.1
1	B	618	TYR	2.1
1	F	606	LEU	2.1
1	F	289	ARG	2.1
1	D	367	GLU	2.0
1	H	578	GLU	2.0
1	D	295	PRO	2.0
1	F	566	TRP	2.0
1	E	381	ARG	2.0
1	A	93	GLY	2.0
1	H	295	PRO	2.0
1	B	581	LYS	2.0
1	D	297	VAL	2.0
1	F	251	LYS	2.0
1	D	98	PHE	2.0
1	C	356	ILE	2.0
1	B	92	GLY	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
3	P6G	F	703	19/19	0.81	0.30	13.15	71,74,75,76	0
4	PGE	G	702	10/10	0.86	0.33	11.79	56,59,59,60	0
3	P6G	B	702	19/19	0.76	0.37	10.76	67,68,79,79	0
4	PGE	G	703	10/10	0.82	0.38	9.15	69,69,71,71	0
3	P6G	E	702	19/19	0.78	0.32	8.71	67,69,74,74	0
3	P6G	C	702	19/19	0.87	0.30	8.63	64,67,71,71	0
3	P6G	C	703	19/19	0.80	0.29	7.76	67,75,77,77	0
7	GOL	F	705	6/6	0.68	0.19	4.94	59,61,61,61	0
4	PGE	C	704	10/10	0.76	0.21	4.72	53,61,65,65	0
4	PGE	D	703	10/10	0.83	0.17	4.13	64,67,70,70	0
4	PGE	E	703	10/10	0.87	0.18	3.46	50,54,58,58	0
4	PGE	B	704	10/10	0.83	0.17	3.27	65,67,70,71	0
4	PGE	A	703	10/10	0.90	0.15	2.33	55,56,61,61	0
3	P6G	B	703	19/19	0.95	0.15	2.17	42,47,52,52	0
3	P6G	F	702	19/19	0.95	0.13	1.38	36,38,41,42	0
7	GOL	C	705[B]	6/6	0.90	0.14	1.29	48,50,51,51	6
4	PGE	B	705	10/10	0.92	0.13	1.21	54,55,57,58	0
4	PGE	H	702	10/10	0.87	0.15	1.09	67,68,69,69	0
3	P6G	A	702	19/19	0.96	0.13	0.83	29,34,37,37	0
3	P6G	D	702	19/19	0.94	0.14	0.71	49,52,55,56	0
2	FAS	E	701	53/53	0.98	0.19	0.64	28,29,32,34	0
5	PO4	F	704	5/5	0.90	0.15	0.51	46,50,51,52	0
2	FAS	D	701	53/53	0.95	0.19	0.50	41,45,49,50	0
2	FAS	F	701	53/53	0.97	0.19	0.46	36,40,45,48	0
2	FAS	C	701	53/53	0.98	0.17	0.44	25,28,30,35	0
2	FAS	A	701	53/53	0.98	0.17	0.36	28,30,35,37	0
2	FAS	G	701	53/53	0.97	0.19	0.33	31,33,36,37	0
2	FAS	B	701	53/53	0.95	0.19	0.31	40,43,52,52	0
2	FAS	H	701	53/53	0.95	0.17	0.13	45,48,58,59	0
6	CA	A	705	1/1	0.96	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	CA	F	706	1/1	0.87	0.12	-	89,89,89,89	0
6	CA	B	706	1/1	0.98	0.13	-	76,76,76,76	0
6	CA	C	708	1/1	0.91	0.14	-	97,97,97,97	0
6	CA	E	704	1/1	0.85	0.12	-	98,98,98,98	0
5	PO4	A	704[B]	5/5	0.98	0.15	-	39,41,43,44	5
6	CA	D	704	1/1	0.83	0.11	-	97,97,97,97	0
8	CL	C	706	1/1	0.91	0.08	-	84,84,84,84	0
6	CA	C	707	1/1	0.95	0.16	-	76,76,76,76	0
6	CA	G	704	1/1	0.81	0.22	-	103,103,103,103	0

6.5 Other polymers (i)

There are no such residues in this entry.