



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 06:15 AM EDT

PDB ID : 3N81
Title : T244A mutant of Human mitochondrial aldehyde dehydrogenase, apo form
Authors : Gonzalez-Segura, L.; Hurley, T.D.
Deposited on : 2010-05-27
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

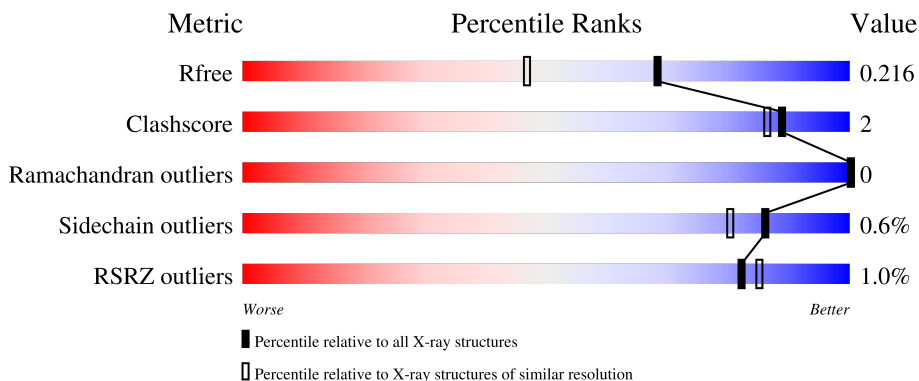
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

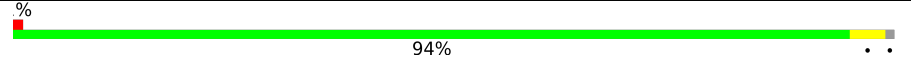
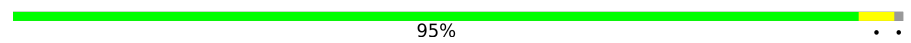
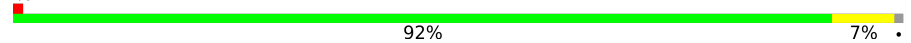

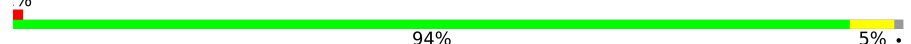
The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



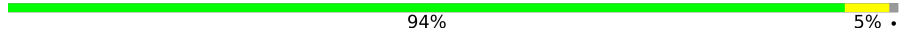
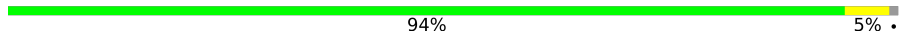
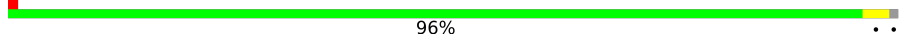
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	500	 94% . .
1	B	500	 95% . .
1	C	500	 92% 7% .
1	D	500	 93% 6% .
1	E	500	 94% 5% .

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Mol	Chain	Length	Quality of chain
1	F	500	 94% 5%
1	G	500	 94% 5%
1	H	500	 % 96% ..

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
4	EDO	F	946	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34624 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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3866	2459	658	727	22	0	11	0
1	B	494	3900	2484	663	732	21	0	16	0
1	C	494	3864	2458	659	725	22	0	11	0
1	D	494	3885	2476	660	728	21	0	14	0
1	E	494	3873	2465	657	730	21	0	12	0
1	F	494	3896	2482	659	734	21	0	16	0
1	G	493	3853	2452	656	722	23	0	10	0
1	H	494	3889	2478	660	729	22	0	15	0

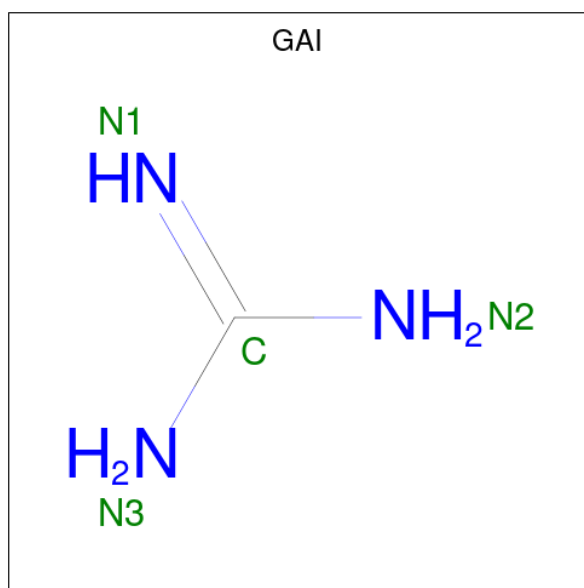
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	THR	engineered mutation	UNP P05091
B	244	ALA	THR	engineered mutation	UNP P05091
C	244	ALA	THR	engineered mutation	UNP P05091
D	244	ALA	THR	engineered mutation	UNP P05091
E	244	ALA	THR	engineered mutation	UNP P05091
F	244	ALA	THR	engineered mutation	UNP P05091
G	244	ALA	THR	engineered mutation	UNP P05091
H	244	ALA	THR	engineered mutation	UNP P05091

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

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

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 4 1 3	0	0
3	A	1	Total C N 4 1 3	0	0
3	B	1	Total C N 4 1 3	0	0
3	B	1	Total C N 4 1 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	C	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	401	Total O 401 401	0	0
5	B	439	Total O 439 439	0	0
5	C	418	Total O 418 418	0	0
5	D	410	Total O 410 410	0	0
5	E	440	Total O 440 440	0	0
5	F	458	Total O 458 458	0	0

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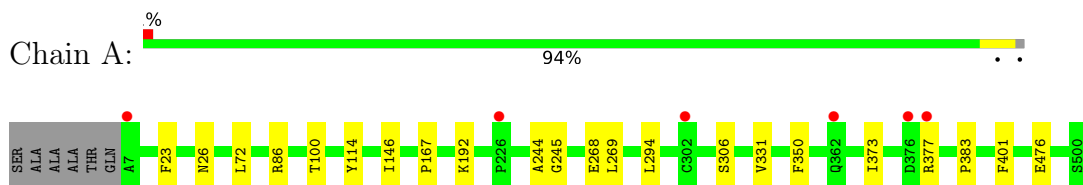
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	415	Total	O	0	0
			415	415		
5	H	417	Total	O	0	0
			417	417		

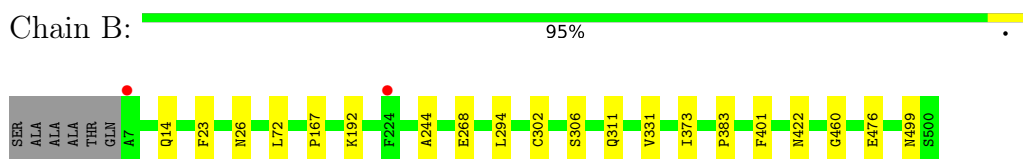
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

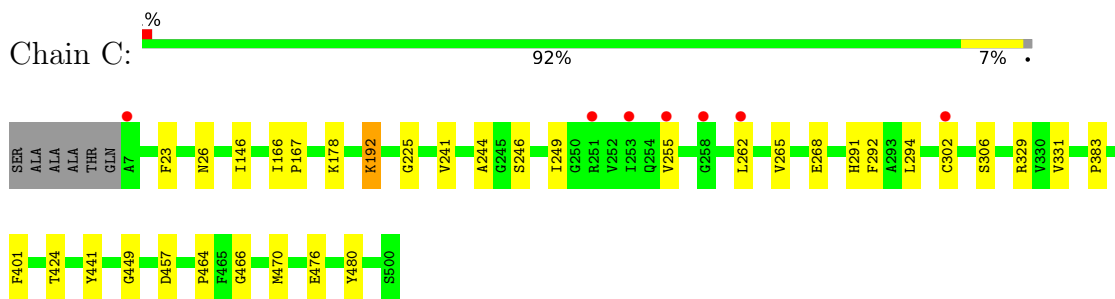
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



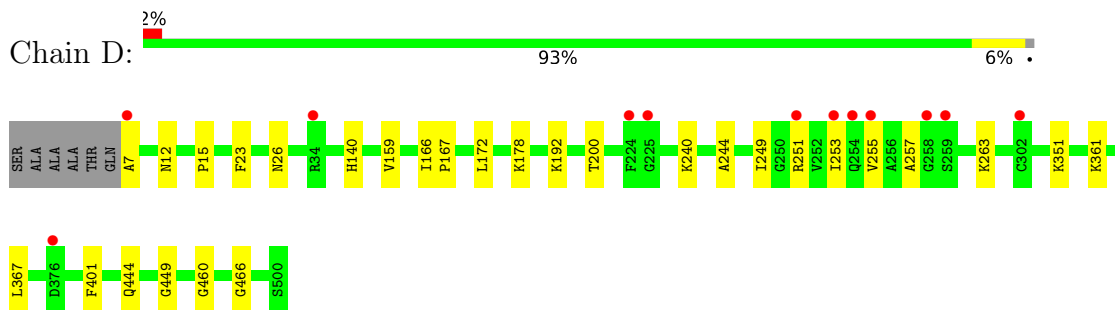
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



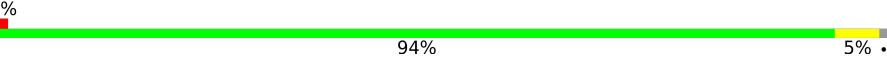
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

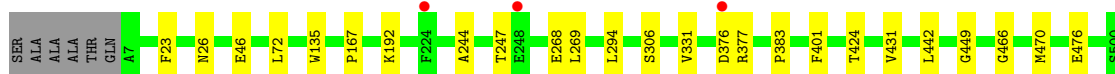


- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E:  94% 5%



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F:  94% 5%



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G:  94% 5%



• Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H:  96% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.75Å 152.19Å 177.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.07 – 1.70 40.76 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.07-1.70) 98.2 (40.76-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.181 , 0.217 0.180 , 0.216	Depositor DCC
R_{free} test set	20681 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtrriage
Anisotropy	0.667	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34624	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9878e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.55	0/3971	0.61	1/5383 (0.0%)
1	B	0.59	0/4018	0.62	0/5446
1	C	0.60	0/3969	0.63	0/5379
1	D	0.59	0/3997	0.61	0/5418
1	E	0.59	0/3982	0.64	0/5400
1	F	0.61	0/4017	0.66	1/5445 (0.0%)
1	G	0.57	0/3958	0.64	0/5364
1	H	0.59	0/4010	0.63	0/5435
All	All	0.59	0/31922	0.63	2/43270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	86	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	86	ARG	NE-CZ-NH1	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3866	0	3829	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3900	0	3871	13	0
1	C	3864	0	3832	24	0
1	D	3885	0	3857	19	0
1	E	3873	0	3829	16	0
1	F	3896	0	3865	15	0
1	G	3853	0	3821	15	0
1	H	3889	0	3862	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	8	0	8	0	0
3	B	8	0	8	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
3	E	8	0	8	0	0
3	F	16	0	16	0	0
3	G	12	0	12	0	0
3	H	8	0	8	0	0
4	A	16	0	24	1	0
4	B	12	0	18	1	0
4	C	16	0	24	1	0
4	D	8	0	12	0	0
4	E	12	0	18	2	0
4	F	20	0	30	5	0
4	G	12	0	18	1	0
4	H	12	0	18	2	0
5	A	401	0	0	1	0
5	B	439	0	0	5	0
5	C	418	0	0	4	0
5	D	410	0	0	2	0
5	E	440	0	0	0	0
5	F	458	0	0	3	0
5	G	415	0	0	0	0
5	H	417	0	0	4	0
All	All	34624	0	31012	115	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 2.

All (115) 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:C:225:GLY:HA2	5:C:2901:HOH:O	1.43	1.19
4:A:941:EDO:H11	1:B:72:LEU:HD21	1.41	0.99
1:G:167:PRO:HD2	1:G:174[B]:MET:HG2	1.46	0.96
1:C:268:GLU:HG2	1:C:476:GLU:OE2	1.74	0.88
1:C:424:THR:HB	1:C:470[A]:MET:HE2	1.59	0.82
1:F:441[B]:TYR:CD1	4:F:946:EDO:H12	2.14	0.81
1:B:268[B]:GLU:HG2	1:B:476:GLU:OE1	1.81	0.81
1:E:268[B]:GLU:HG2	1:E:476:GLU:OE1	1.84	0.77
1:F:441[B]:TYR:CE1	4:F:946:EDO:H12	2.20	0.77
1:G:72:LEU:HD21	4:H:948:EDO:H11	1.69	0.74
1:A:268[B]:GLU:HG2	1:A:476:GLU:OE1	1.87	0.73
1:C:192:LYS:HE2	5:C:2901:HOH:O	1.88	0.73
1:G:268[A]:GLU:HG2	1:G:476:GLU:OE1	1.90	0.72
1:C:291:HIS:HE1	1:C:329:ARG:HH11	1.38	0.71
1:F:268[A]:GLU:HG2	1:F:476:GLU:OE1	1.88	0.71
1:E:46[B]:GLU:OE2	1:E:377:ARG:NH2	2.25	0.69
1:D:361:LYS:HE2	1:D:367:LEU:HD22	1.77	0.68
1:B:14:GLN:NE2	5:B:2850:HOH:O	2.25	0.67
1:E:46[A]:GLU:HB2	4:E:915:EDO:H22	1.78	0.65
1:H:291:HIS:HE1	1:H:329:ARG:HH11	1.46	0.64
1:H:268[A]:GLU:HG2	1:H:476:GLU:OE1	1.99	0.62
1:A:72:LEU:HD21	4:B:942:EDO:H11	1.80	0.62
1:B:311[B]:GLN:OE1	5:B:2809:HOH:O	2.16	0.62
1:E:72:LEU:HD21	4:F:946:EDO:H11	1.83	0.61
1:G:167:PRO:CD	1:G:174[B]:MET:HG2	2.26	0.57
1:C:262:LEU:HD21	1:D:251:ARG:HG2	1.85	0.57
1:H:90:ARG:NH1	5:H:2138:HOH:O	2.36	0.56
1:E:46[A]:GLU:HB2	4:E:915:EDO:C2	2.36	0.56
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.87	0.56
1:G:254:GLN:NE2	1:H:262:LEU:HD23	2.22	0.55
1:E:424:THR:HB	1:E:470:MET:HE2	1.89	0.55
1:A:294:LEU:HD23	1:A:306:SER:HA	1.89	0.54
1:H:291:HIS:HD2	5:H:546:HOH:O	1.90	0.53
1:G:284:ASP:OD1	1:G:321:ARG:NH1	2.42	0.53
1:D:249:ILE:O	1:D:253:ILE:HG12	2.09	0.52
1:B:499:ASN:H	1:D:444:GLN:NE2	2.09	0.51
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.76	0.51
1:E:424:THR:HB	1:E:470:MET:CE	2.40	0.51
1:E:167:PRO:HD3	1:E:244:ALA:HB3	1.93	0.51
1:F:302[A]:CYS:SG	5:F:1722:HOH:O	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1893:HOH:O	1:D:140:HIS:HD2	1.93	0.50
1:C:441:TYR:CD1	4:C:943:EDO:H12	2.46	0.50
1:C:291:HIS:CE1	1:C:329:ARG:HH11	2.25	0.50
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.47	0.50
1:B:499:ASN:H	1:D:444:GLN:HE22	1.59	0.49
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.47	0.49
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.47	0.49
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.48	0.49
1:E:431[B]:VAL:HG21	1:E:442:LEU:HD12	1.95	0.49
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.48	0.48
1:F:167:PRO:HD3	1:F:244:ALA:HB3	1.96	0.48
1:C:246:SER:OG	1:C:249:ILE:HG12	2.13	0.48
1:E:331:VAL:HG21	1:E:383:PRO:HD3	1.95	0.48
1:C:424:THR:HB	1:C:470[A]:MET:CE	2.35	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.48
1:H:311:GLN:HG2	5:H:3158:HOH:O	2.13	0.48
1:C:166:ILE:CG2	1:C:178[A]:LYS:HG3	2.44	0.48
5:B:533:HOH:O	1:D:140:HIS:HE1	1.97	0.47
1:C:302[A]:CYS:SG	5:C:2728:HOH:O	2.54	0.47
1:H:251[B]:ARG:NH2	5:H:2676:HOH:O	2.47	0.47
1:E:247:THR:HA	1:E:269:LEU:HD13	1.97	0.47
1:C:255:VAL:HG13	1:D:255:VAL:HG13	1.96	0.47
1:D:159[A]:VAL:HG11	1:D:240:LYS:HB2	1.97	0.47
1:C:291:HIS:HD2	5:C:528:HOH:O	1.98	0.46
1:F:7:ALA:N	5:F:1038:HOH:O	2.48	0.46
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.51	0.46
1:C:449:GLY:HA3	1:C:466:GLY:O	2.16	0.46
1:B:167:PRO:HD3	1:B:244:ALA:HB3	1.98	0.46
1:H:291:HIS:CE1	1:H:329:ARG:HH11	2.29	0.46
1:D:7:ALA:N	5:D:1932:HOH:O	2.49	0.46
1:D:257:ALA:HB1	1:D:263:LYS:HG3	1.97	0.45
1:F:178:LYS:HD3	5:F:865:HOH:O	2.15	0.45
1:D:172:LEU:HD21	1:D:200:THR:HB	1.99	0.45
1:A:331:VAL:HG21	1:A:383:PRO:HD3	1.99	0.45
1:B:294:LEU:HD23	1:B:306:SER:HA	1.98	0.45
1:A:167:PRO:HD3	1:A:244:ALA:HB3	1.99	0.44
1:F:347:GLU:HG3	4:F:966:EDO:H22	1.99	0.44
1:C:167:PRO:HD3	1:C:244:ALA:HB3	1.99	0.44
1:E:431[B]:VAL:HG21	1:E:442:LEU:CD1	2.48	0.44
1:G:12:ASN:O	1:G:15:PRO:HD3	2.18	0.44
1:H:431[B]:VAL:HG11	1:H:442:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:O	1:A:269:LEU:HA	2.18	0.43
1:D:167:PRO:HD3	1:D:244:ALA:HB3	2.00	0.43
1:F:464:PRO:HG3	1:F:480:TYR:CD1	2.54	0.43
1:C:166:ILE:HG22	1:C:178[A]:LYS:HE2	2.01	0.43
1:F:441[B]:TYR:CE1	4:F:946:EDO:C1	2.98	0.43
1:C:241:VAL:HG13	1:C:265:VAL:HG13	2.01	0.43
1:C:331:VAL:HG21	1:C:383:PRO:HD3	2.00	0.43
1:F:245:GLY:O	1:F:269:LEU:HA	2.19	0.42
1:E:449:GLY:HA3	1:E:466:GLY:O	2.19	0.42
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.54	0.42
1:B:331:VAL:HG21	1:B:383:PRO:HD3	2.02	0.42
1:A:146:ILE:HG13	1:B:460:GLY:HA3	2.02	0.42
1:D:351[A]:LYS:HE3	5:D:2549:HOH:O	2.20	0.41
1:E:294:LEU:HD23	1:E:306:SER:HA	2.02	0.41
1:B:373[B]:ILE:HD11	5:B:1326:HOH:O	2.20	0.41
1:C:464:PRO:HG3	1:C:480:TYR:CD1	2.56	0.41
1:F:449:GLY:HA3	1:F:466:GLY:O	2.20	0.41
1:C:146:ILE:HG13	1:D:460:GLY:HA3	2.03	0.41
1:C:294:LEU:HD23	1:C:306:SER:HA	2.02	0.41
1:G:72:LEU:CD2	4:H:948:EDO:H11	2.43	0.41
1:A:100[A]:THR:HG23	1:A:114:TYR:OH	2.21	0.41
1:G:101:TYR:CG	4:G:927:EDO:H11	2.55	0.41
1:G:106:GLU:O	1:G:110:ASN:HB3	2.20	0.41
1:D:166:ILE:CG2	1:D:178[A]:LYS:HG3	2.50	0.41
1:D:449:GLY:HA3	1:D:466:GLY:O	2.20	0.41
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.56	0.41
1:A:350:PHE:CZ	1:A:373:ILE:HG12	2.56	0.40
1:B:302[A]:CYS:SG	5:B:1112:HOH:O	2.61	0.40
1:D:12:ASN:O	1:D:15:PRO:HD3	2.21	0.40
1:F:352[B]:LYS:HB3	1:F:352[B]:LYS:NZ	2.36	0.40
1:G:301[A]:CYS:SG	1:G:303:CYS:SG	3.18	0.40
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.56	0.40
1:G:449:GLY:HA3	1:G:466:GLY:O	2.20	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	503/500 (101%)	492 (98%)	11 (2%)	0	100	100
1	B	508/500 (102%)	496 (98%)	12 (2%)	0	100	100
1	C	503/500 (101%)	489 (97%)	14 (3%)	0	100	100
1	D	506/500 (101%)	493 (97%)	13 (3%)	0	100	100
1	E	504/500 (101%)	493 (98%)	11 (2%)	0	100	100
1	F	508/500 (102%)	493 (97%)	15 (3%)	0	100	100
1	G	501/500 (100%)	490 (98%)	11 (2%)	0	100	100
1	H	507/500 (101%)	497 (98%)	10 (2%)	0	100	100
All	All	4040/4000 (101%)	3943 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/401 (102%)	406 (99%)	3 (1%)	84	77
1	B	414/401 (103%)	411 (99%)	3 (1%)	84	77
1	C	409/401 (102%)	407 (100%)	2 (0%)	88	83
1	D	412/401 (103%)	410 (100%)	2 (0%)	88	83
1	E	410/401 (102%)	407 (99%)	3 (1%)	84	77
1	F	414/401 (103%)	412 (100%)	2 (0%)	88	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	408/401 (102%)	405 (99%)	3 (1%)	84	77
1	H	413/401 (103%)	411 (100%)	2 (0%)	88	83
All	All	3289/3208 (102%)	3269 (99%)	20 (1%)	86	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	377	ARG
1	A	401	PHE
1	B	192	LYS
1	B	401	PHE
1	B	422	ASN
1	C	192	LYS
1	C	401	PHE
1	D	192	LYS
1	D	401	PHE
1	E	192	LYS
1	E	376	ASP
1	E	401	PHE
1	F	192	LYS
1	F	401	PHE
1	G	192	LYS
1	G	206	ASN
1	G	401	PHE
1	H	192	LYS
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	ASN
1	B	422	ASN
1	B	440	ASN
1	C	291	HIS
1	C	349	GLN
1	D	140	HIS
1	D	390	GLN
1	D	444	GLN
1	E	14	GLN

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Mol	Chain	Res	Type
1	F	358	ASN
1	G	254	GLN
1	G	349	GLN
1	G	358	ASN
1	H	254	GLN
1	H	291	HIS
1	H	362	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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	GAI	E	805	-	3,3,3	1.04	0	3,3,3	0.71	0
4	EDO	E	915	-	3,3,3	0.37	0	2,2,2	0.38	0
4	EDO	F	926	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	E	925	-	3,3,3	0.40	0	2,2,2	0.31	0
4	EDO	C	903	-	3,3,3	0.37	0	2,2,2	0.29	0
4	EDO	A	921	-	3,3,3	0.41	0	2,2,2	0.37	0
4	EDO	D	904	-	3,3,3	0.37	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	G	907	-	3,3,3	0.44	0	2,2,2	0.44	0
4	EDO	F	906	-	3,3,3	0.48	0	2,2,2	0.17	0
3	GAI	F	826	-	3,3,3	1.55	0	3,3,3	0.91	0
4	EDO	E	905	-	3,3,3	0.39	0	2,2,2	0.20	0
4	EDO	C	943	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	H	908	-	3,3,3	0.40	0	2,2,2	0.26	0
3	GAI	A	811	-	3,3,3	1.36	0	3,3,3	0.99	0
4	EDO	B	902	-	3,3,3	0.33	0	2,2,2	0.44	0
3	GAI	C	823	-	3,3,3	1.40	0	3,3,3	1.23	0
4	EDO	F	916	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	C	913	-	3,3,3	0.43	0	2,2,2	0.23	0
4	EDO	H	928	-	3,3,3	0.35	0	2,2,2	0.35	0
4	EDO	A	901	-	3,3,3	0.42	0	2,2,2	0.21	0
4	EDO	F	946	-	3,3,3	0.48	0	2,2,2	0.22	0
3	GAI	F	845	-	3,3,3	1.34	0	3,3,3	0.91	0
4	EDO	G	927	-	3,3,3	0.32	0	2,2,2	0.56	0
3	GAI	D	833	-	3,3,3	1.47	1 (33%)	3,3,3	1.30	0
3	GAI	G	807	-	3,3,3	1.27	0	3,3,3	0.60	0
3	GAI	G	817	-	3,3,3	1.38	0	3,3,3	1.05	0
4	EDO	G	917	-	3,3,3	0.44	0	2,2,2	0.13	0
4	EDO	H	948	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	F	966	-	3,3,3	0.40	0	2,2,2	0.21	0
4	EDO	C	923	-	3,3,3	0.43	0	2,2,2	0.54	0
4	EDO	D	944	-	3,3,3	0.33	0	2,2,2	0.58	0
3	GAI	C	803	-	3,3,3	1.34	0	3,3,3	1.02	0
3	GAI	H	808	-	3,3,3	1.22	0	3,3,3	1.04	0
3	GAI	C	813	-	3,3,3	1.42	0	3,3,3	1.06	0
3	GAI	D	804	-	3,3,3	1.45	0	3,3,3	1.60	1 (33%)
4	EDO	A	911	-	3,3,3	0.40	0	2,2,2	0.29	0
3	GAI	A	801	-	3,3,3	1.54	0	3,3,3	0.76	0
4	EDO	B	942	-	3,3,3	0.50	0	2,2,2	0.33	0
4	EDO	A	941	-	3,3,3	0.45	0	2,2,2	0.28	0
3	GAI	F	806	-	3,3,3	1.44	0	3,3,3	0.46	0
3	GAI	F	816	-	3,3,3	1.59	0	3,3,3	0.84	0
3	GAI	B	812	-	3,3,3	1.53	0	3,3,3	1.06	0
3	GAI	B	802	-	3,3,3	1.50	0	3,3,3	1.36	1 (33%)
3	GAI	H	818	-	3,3,3	1.20	0	3,3,3	0.88	0
3	GAI	E	815	-	3,3,3	1.50	1 (33%)	3,3,3	1.26	0
3	GAI	D	814	-	3,3,3	1.29	0	3,3,3	1.24	0
4	EDO	B	912	-	3,3,3	0.45	0	2,2,2	0.30	0
3	GAI	G	838	-	3,3,3	1.40	0	3,3,3	1.05	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
4	EDO	E	915	-	-	0/1/1/1	-
4	EDO	F	926	-	-	0/1/1/1	-
4	EDO	E	925	-	-	1/1/1/1	-
4	EDO	C	903	-	-	0/1/1/1	-
4	EDO	A	921	-	-	1/1/1/1	-
4	EDO	D	904	-	-	0/1/1/1	-
4	EDO	G	907	-	-	0/1/1/1	-
4	EDO	F	906	-	-	0/1/1/1	-
4	EDO	E	905	-	-	0/1/1/1	-
4	EDO	C	943	-	-	0/1/1/1	-
4	EDO	H	908	-	-	0/1/1/1	-
4	EDO	B	902	-	-	0/1/1/1	-
4	EDO	C	913	-	-	0/1/1/1	-
4	EDO	H	928	-	-	0/1/1/1	-
4	EDO	A	901	-	-	0/1/1/1	-
4	EDO	F	946	-	-	0/1/1/1	-
4	EDO	G	927	-	-	1/1/1/1	-
4	EDO	G	917	-	-	0/1/1/1	-
4	EDO	H	948	-	-	0/1/1/1	-
4	EDO	F	966	-	-	0/1/1/1	-
4	EDO	C	923	-	-	0/1/1/1	-
4	EDO	D	944	-	-	0/1/1/1	-
4	EDO	A	911	-	-	0/1/1/1	-
4	EDO	B	942	-	-	0/1/1/1	-
4	EDO	A	941	-	-	1/1/1/1	-
4	EDO	F	916	-	-	0/1/1/1	-
4	EDO	B	912	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	815	GAI	C-N1	-2.04	1.26	1.30
3	D	833	GAI	C-N1	-2.02	1.26	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	804	GAI	N3-C-N2	2.38	121.80	116.13
3	B	802	GAI	N3-C-N2	2.01	120.92	116.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	925	EDO	O1-C1-C2-O2
4	G	927	EDO	O1-C1-C2-O2
4	A	921	EDO	O1-C1-C2-O2
4	A	941	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	915	EDO	2	0
4	C	943	EDO	1	0
4	F	946	EDO	4	0
4	G	927	EDO	1	0
4	H	948	EDO	2	0
4	F	966	EDO	1	0
4	B	942	EDO	1	0
4	A	941	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/500 (98%)	-0.26	6 (1%) 79 82	11, 18, 29, 39	0
1	B	494/500 (98%)	-0.36	2 (0%) 92 93	10, 16, 26, 40	0
1	C	494/500 (98%)	-0.33	7 (1%) 75 79	10, 16, 25, 45	0
1	D	494/500 (98%)	-0.20	12 (2%) 59 63	10, 16, 29, 48	0
1	E	494/500 (98%)	-0.30	3 (0%) 89 91	10, 15, 25, 37	0
1	F	494/500 (98%)	-0.44	2 (0%) 92 93	10, 15, 23, 34	0
1	G	493/500 (98%)	-0.29	2 (0%) 92 93	10, 17, 27, 34	0
1	H	494/500 (98%)	-0.24	6 (1%) 79 82	10, 16, 26, 38	0
All	All	3951/4000 (98%)	-0.30	40 (1%) 82 85	10, 16, 26, 48	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	224[A]	PHE	6.6
1	A	7	ALA	5.8
1	H	7	ALA	5.6
1	C	255	VAL	4.2
1	B	7	ALA	4.0
1	C	262	LEU	3.9
1	H	377	ARG	3.9
1	C	7	ALA	3.8
1	D	251	ARG	3.8
1	D	255	VAL	3.8
1	E	376	ASP	3.8
1	F	7	ALA	3.8
1	A	376	ASP	3.7
1	H	376	ASP	3.4
1	D	376	ASP	3.2
1	H	302[A]	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	7	ALA	3.1
1	G	14	GLN	3.1
1	D	258	GLY	3.1
1	A	377	ARG	2.9
1	D	253	ILE	2.7
1	A	362	GLN	2.7
1	H	248	GLU	2.6
1	D	302[A]	CYS	2.6
1	B	224[A]	PHE	2.5
1	E	224	PHE	2.5
1	C	251	ARG	2.4
1	C	302[A]	CYS	2.4
1	D	259	SER	2.4
1	E	248	GLU	2.4
1	G	441	TYR	2.3
1	F	302[A]	CYS	2.3
1	H	224[A]	PHE	2.2
1	A	302[A]	CYS	2.1
1	D	225	GLY	2.1
1	A	226	PRO	2.1
1	D	254	GLN	2.1
1	D	34	ARG	2.1
1	C	253	ILE	2.1
1	C	258	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAI	D	814	4/4	0.76	0.18	29,29,29,29	0
4	EDO	E	925	4/4	0.77	0.14	30,31,32,34	0
4	EDO	F	966	4/4	0.81	0.17	36,36,37,39	0
4	EDO	G	927	4/4	0.81	0.18	40,40,40,41	0
3	GAI	H	818	4/4	0.82	0.21	26,27,28,28	0
4	EDO	B	942	4/4	0.82	0.25	19,26,27,28	0
4	EDO	C	923	4/4	0.82	0.14	26,27,28,31	0
4	EDO	A	921	4/4	0.84	0.12	42,43,43,45	0
3	GAI	F	826	4/4	0.84	0.17	40,40,40,40	0
3	GAI	C	813	4/4	0.85	0.15	33,34,34,35	0
4	EDO	C	943	4/4	0.86	0.23	22,27,27,27	0
4	EDO	H	928	4/4	0.86	0.13	31,32,33,35	0
3	GAI	F	816	4/4	0.87	0.19	28,29,29,30	0
3	GAI	G	817	4/4	0.88	0.20	33,34,34,34	0
3	GAI	B	812	4/4	0.88	0.19	22,23,23,25	0
4	EDO	B	912	4/4	0.89	0.11	26,27,28,28	0
4	EDO	A	911	4/4	0.90	0.21	27,28,29,30	0
3	GAI	C	823	4/4	0.91	0.14	38,38,38,38	0
3	GAI	D	833	4/4	0.91	0.11	24,24,24,25	0
4	EDO	D	944	4/4	0.92	0.12	26,29,29,29	0
4	EDO	G	917	4/4	0.92	0.15	28,30,32,33	0
4	EDO	A	941	4/4	0.92	0.20	16,25,25,26	0
4	EDO	F	946	4/4	0.92	0.27	19,26,28,31	0
4	EDO	H	948	4/4	0.92	0.23	17,26,26,29	0
3	GAI	F	845	4/4	0.93	0.11	21,22,22,22	0
4	EDO	F	926	4/4	0.93	0.10	19,19,20,20	0
4	EDO	C	903	4/4	0.94	0.09	22,26,26,27	0
3	GAI	B	802	4/4	0.94	0.08	16,17,18,18	0
3	GAI	G	838	4/4	0.94	0.12	25,26,26,26	0
4	EDO	B	902	4/4	0.94	0.08	20,22,22,26	0
3	GAI	A	811	4/4	0.94	0.13	30,30,30,30	0
3	GAI	E	805	4/4	0.94	0.09	17,18,18,19	0
4	EDO	A	901	4/4	0.95	0.07	18,21,23,24	0
3	GAI	G	807	4/4	0.95	0.09	13,14,15,16	0
4	EDO	G	907	4/4	0.95	0.06	21,24,24,25	0
4	EDO	E	905	4/4	0.95	0.10	23,25,25,26	0
4	EDO	E	915	4/4	0.95	0.18	28,28,29,30	0
4	EDO	C	913	4/4	0.95	0.11	22,23,24,26	0
3	GAI	D	804	4/4	0.95	0.08	17,19,20,21	0
4	EDO	D	904	4/4	0.96	0.07	22,24,24,25	0
4	EDO	F	906	4/4	0.96	0.07	16,21,23,23	0
3	GAI	C	803	4/4	0.96	0.07	15,17,17,19	0
4	EDO	H	908	4/4	0.96	0.07	23,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAI	E	815	4/4	0.96	0.12	22,23,24,24	0
3	GAI	F	806	4/4	0.96	0.09	16,18,18,19	0
2	NA	B	602	1/1	0.97	0.06	15,15,15,15	0
3	GAI	H	808	4/4	0.97	0.05	17,19,19,19	0
4	EDO	F	916	4/4	0.97	0.09	20,21,22,24	0
3	GAI	A	801	4/4	0.98	0.06	18,18,19,20	0
2	NA	A	601	1/1	0.98	0.05	19,19,19,19	0
2	NA	F	606	1/1	0.98	0.05	16,16,16,16	0
2	NA	G	607	1/1	0.98	0.04	18,18,18,18	0
2	NA	E	605	1/1	0.99	0.06	16,16,16,16	0
2	NA	C	603	1/1	0.99	0.05	17,17,17,17	0
2	NA	D	604	1/1	0.99	0.04	14,14,14,14	0
2	NA	H	608	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.