Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:08 PM GMT

PDB ID	:	4H80
Title	:	Crystal structure of human ALDH3A1 with its isozyme selective inhibitor - N -[4-(4-methylsulfonyl-2-nitroanilino)phenyl]acetamide
Authors	:	Hurley, T.D.; Parajuli, B.
Deposited on	:	2012-09-21
Resolution	:	2.50 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:

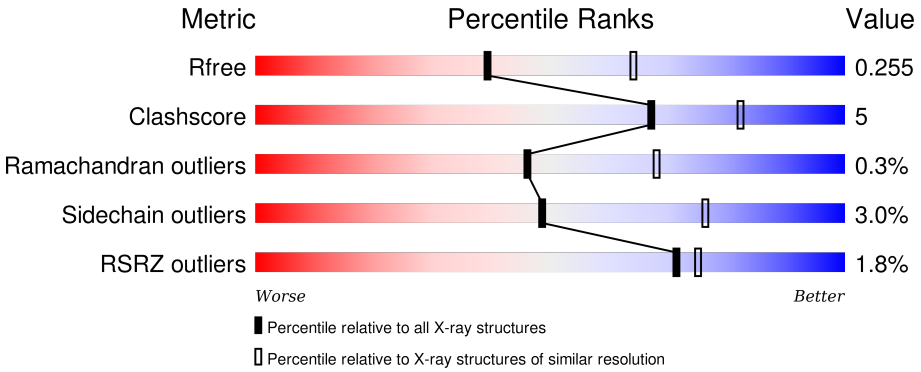
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	469	% 87% 7% • 5%
1	B	469	% 86% 8% • 5%
1	C	469	3% 86% 9% 5%
1	D	469	% 83% 11% • 5%
1	E	469	3% 83% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	469	2% 84% 10% • 5%
1	G	469	2% 85% 9% • 5%
1	H	469	% 86% 9% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	04T	A	501	-	-	X	-
2	04T	B	501	-	-	X	-
2	04T	C	501	-	-	X	X
2	04T	D	501	-	-	-	X
2	04T	E	501	-	-	-	X
2	04T	F	501	-	-	X	-
2	04T	G	501	-	-	-	X
2	04T	H	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28414 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, dimeric NADP-preferring.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	3	0
			3502	2229	598	657	18			
1	B	446	Total	C	N	O	S	0	3	0
			3504	2231	597	658	18			
1	C	447	Total	C	N	O	S	0	1	0
			3495	2225	595	657	18			
1	D	446	Total	C	N	O	S	0	2	0
			3497	2226	596	657	18			
1	E	446	Total	C	N	O	S	0	3	0
			3506	2232	600	656	18			
1	F	446	Total	C	N	O	S	0	0	0
			3483	2217	592	656	18			
1	G	446	Total	C	N	O	S	0	2	0
			3499	2227	598	656	18			
1	H	447	Total	C	N	O	S	0	4	0
			3517	2239	602	658	18			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	EXPRESSION TAG	UNP P30838
A	-15	HIS	-	EXPRESSION TAG	UNP P30838
A	-14	HIS	-	EXPRESSION TAG	UNP P30838
A	-13	HIS	-	EXPRESSION TAG	UNP P30838
A	-12	HIS	-	EXPRESSION TAG	UNP P30838
A	-11	HIS	-	EXPRESSION TAG	UNP P30838
A	-10	SER	-	EXPRESSION TAG	UNP P30838
A	-9	SER	-	EXPRESSION TAG	UNP P30838
A	-8	GLY	-	EXPRESSION TAG	UNP P30838
A	-7	LEU	-	EXPRESSION TAG	UNP P30838
A	-6	VAL	-	EXPRESSION TAG	UNP P30838
A	-5	PRO	-	EXPRESSION TAG	UNP P30838
A	-4	ARG	-	EXPRESSION TAG	UNP P30838

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P30838
A	-2	SER	-	EXPRESSION TAG	UNP P30838
A	-1	HIS	-	EXPRESSION TAG	UNP P30838
A	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
B	-16	HIS	-	EXPRESSION TAG	UNP P30838
B	-15	HIS	-	EXPRESSION TAG	UNP P30838
B	-14	HIS	-	EXPRESSION TAG	UNP P30838
B	-13	HIS	-	EXPRESSION TAG	UNP P30838
B	-12	HIS	-	EXPRESSION TAG	UNP P30838
B	-11	HIS	-	EXPRESSION TAG	UNP P30838
B	-10	SER	-	EXPRESSION TAG	UNP P30838
B	-9	SER	-	EXPRESSION TAG	UNP P30838
B	-8	GLY	-	EXPRESSION TAG	UNP P30838
B	-7	LEU	-	EXPRESSION TAG	UNP P30838
B	-6	VAL	-	EXPRESSION TAG	UNP P30838
B	-5	PRO	-	EXPRESSION TAG	UNP P30838
B	-4	ARG	-	EXPRESSION TAG	UNP P30838
B	-3	GLY	-	EXPRESSION TAG	UNP P30838
B	-2	SER	-	EXPRESSION TAG	UNP P30838
B	-1	HIS	-	EXPRESSION TAG	UNP P30838
B	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
C	-16	HIS	-	EXPRESSION TAG	UNP P30838
C	-15	HIS	-	EXPRESSION TAG	UNP P30838
C	-14	HIS	-	EXPRESSION TAG	UNP P30838
C	-13	HIS	-	EXPRESSION TAG	UNP P30838
C	-12	HIS	-	EXPRESSION TAG	UNP P30838
C	-11	HIS	-	EXPRESSION TAG	UNP P30838
C	-10	SER	-	EXPRESSION TAG	UNP P30838
C	-9	SER	-	EXPRESSION TAG	UNP P30838
C	-8	GLY	-	EXPRESSION TAG	UNP P30838
C	-7	LEU	-	EXPRESSION TAG	UNP P30838
C	-6	VAL	-	EXPRESSION TAG	UNP P30838
C	-5	PRO	-	EXPRESSION TAG	UNP P30838
C	-4	ARG	-	EXPRESSION TAG	UNP P30838
C	-3	GLY	-	EXPRESSION TAG	UNP P30838
C	-2	SER	-	EXPRESSION TAG	UNP P30838
C	-1	HIS	-	EXPRESSION TAG	UNP P30838
C	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
D	-16	HIS	-	EXPRESSION TAG	UNP P30838
D	-15	HIS	-	EXPRESSION TAG	UNP P30838
D	-14	HIS	-	EXPRESSION TAG	UNP P30838
D	-13	HIS	-	EXPRESSION TAG	UNP P30838

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP P30838
D	-11	HIS	-	EXPRESSION TAG	UNP P30838
D	-10	SER	-	EXPRESSION TAG	UNP P30838
D	-9	SER	-	EXPRESSION TAG	UNP P30838
D	-8	GLY	-	EXPRESSION TAG	UNP P30838
D	-7	LEU	-	EXPRESSION TAG	UNP P30838
D	-6	VAL	-	EXPRESSION TAG	UNP P30838
D	-5	PRO	-	EXPRESSION TAG	UNP P30838
D	-4	ARG	-	EXPRESSION TAG	UNP P30838
D	-3	GLY	-	EXPRESSION TAG	UNP P30838
D	-2	SER	-	EXPRESSION TAG	UNP P30838
D	-1	HIS	-	EXPRESSION TAG	UNP P30838
D	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
E	-16	HIS	-	EXPRESSION TAG	UNP P30838
E	-15	HIS	-	EXPRESSION TAG	UNP P30838
E	-14	HIS	-	EXPRESSION TAG	UNP P30838
E	-13	HIS	-	EXPRESSION TAG	UNP P30838
E	-12	HIS	-	EXPRESSION TAG	UNP P30838
E	-11	HIS	-	EXPRESSION TAG	UNP P30838
E	-10	SER	-	EXPRESSION TAG	UNP P30838
E	-9	SER	-	EXPRESSION TAG	UNP P30838
E	-8	GLY	-	EXPRESSION TAG	UNP P30838
E	-7	LEU	-	EXPRESSION TAG	UNP P30838
E	-6	VAL	-	EXPRESSION TAG	UNP P30838
E	-5	PRO	-	EXPRESSION TAG	UNP P30838
E	-4	ARG	-	EXPRESSION TAG	UNP P30838
E	-3	GLY	-	EXPRESSION TAG	UNP P30838
E	-2	SER	-	EXPRESSION TAG	UNP P30838
E	-1	HIS	-	EXPRESSION TAG	UNP P30838
E	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
F	-16	HIS	-	EXPRESSION TAG	UNP P30838
F	-15	HIS	-	EXPRESSION TAG	UNP P30838
F	-14	HIS	-	EXPRESSION TAG	UNP P30838
F	-13	HIS	-	EXPRESSION TAG	UNP P30838
F	-12	HIS	-	EXPRESSION TAG	UNP P30838
F	-11	HIS	-	EXPRESSION TAG	UNP P30838
F	-10	SER	-	EXPRESSION TAG	UNP P30838
F	-9	SER	-	EXPRESSION TAG	UNP P30838
F	-8	GLY	-	EXPRESSION TAG	UNP P30838
F	-7	LEU	-	EXPRESSION TAG	UNP P30838
F	-6	VAL	-	EXPRESSION TAG	UNP P30838
F	-5	PRO	-	EXPRESSION TAG	UNP P30838

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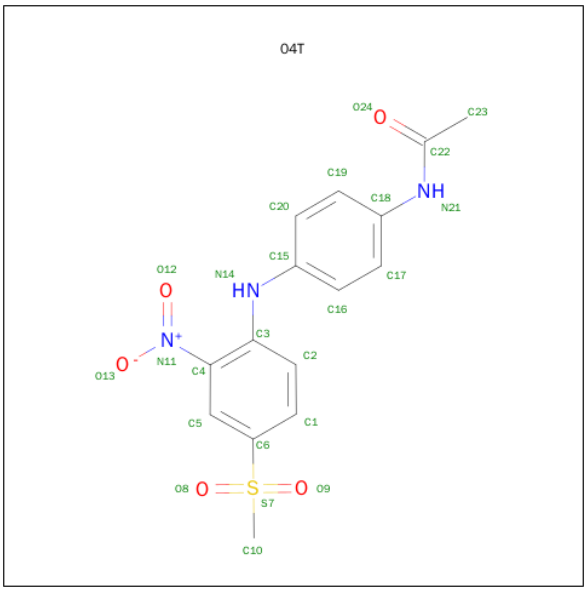
Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ARG	-	EXPRESSION TAG	UNP P30838
F	-3	GLY	-	EXPRESSION TAG	UNP P30838
F	-2	SER	-	EXPRESSION TAG	UNP P30838
F	-1	HIS	-	EXPRESSION TAG	UNP P30838
F	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
G	-16	HIS	-	EXPRESSION TAG	UNP P30838
G	-15	HIS	-	EXPRESSION TAG	UNP P30838
G	-14	HIS	-	EXPRESSION TAG	UNP P30838
G	-13	HIS	-	EXPRESSION TAG	UNP P30838
G	-12	HIS	-	EXPRESSION TAG	UNP P30838
G	-11	HIS	-	EXPRESSION TAG	UNP P30838
G	-10	SER	-	EXPRESSION TAG	UNP P30838
G	-9	SER	-	EXPRESSION TAG	UNP P30838
G	-8	GLY	-	EXPRESSION TAG	UNP P30838
G	-7	LEU	-	EXPRESSION TAG	UNP P30838
G	-6	VAL	-	EXPRESSION TAG	UNP P30838
G	-5	PRO	-	EXPRESSION TAG	UNP P30838
G	-4	ARG	-	EXPRESSION TAG	UNP P30838
G	-3	GLY	-	EXPRESSION TAG	UNP P30838
G	-2	SER	-	EXPRESSION TAG	UNP P30838
G	-1	HIS	-	EXPRESSION TAG	UNP P30838
G	133	ALA	SER	ENGINEERED MUTATION	UNP P30838
H	-16	HIS	-	EXPRESSION TAG	UNP P30838
H	-15	HIS	-	EXPRESSION TAG	UNP P30838
H	-14	HIS	-	EXPRESSION TAG	UNP P30838
H	-13	HIS	-	EXPRESSION TAG	UNP P30838
H	-12	HIS	-	EXPRESSION TAG	UNP P30838
H	-11	HIS	-	EXPRESSION TAG	UNP P30838
H	-10	SER	-	EXPRESSION TAG	UNP P30838
H	-9	SER	-	EXPRESSION TAG	UNP P30838
H	-8	GLY	-	EXPRESSION TAG	UNP P30838
H	-7	LEU	-	EXPRESSION TAG	UNP P30838
H	-6	VAL	-	EXPRESSION TAG	UNP P30838
H	-5	PRO	-	EXPRESSION TAG	UNP P30838
H	-4	ARG	-	EXPRESSION TAG	UNP P30838
H	-3	GLY	-	EXPRESSION TAG	UNP P30838
H	-2	SER	-	EXPRESSION TAG	UNP P30838
H	-1	HIS	-	EXPRESSION TAG	UNP P30838
H	133	ALA	SER	ENGINEERED MUTATION	UNP P30838

- Molecule 2 is N-(4-{[4-(METHYLSULFONYL)-2-NITROPHENYL]AMINO}PHENYL)AC ETAMIDE (three-letter code: 04T) (formula: $C_{15}H_{15}N_3O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	B	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	C	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	D	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	E	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	F	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	G	1	Total	C	N	O	S	0	0
			24	15	3	5	1		
2	H	1	Total	C	N	O	S	0	0
			24	15	3	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	28	Total	O	0	0
			28	28		
3	C	20	Total	O	0	0
			20	20		
3	D	37	Total	O	0	0
			37	37		

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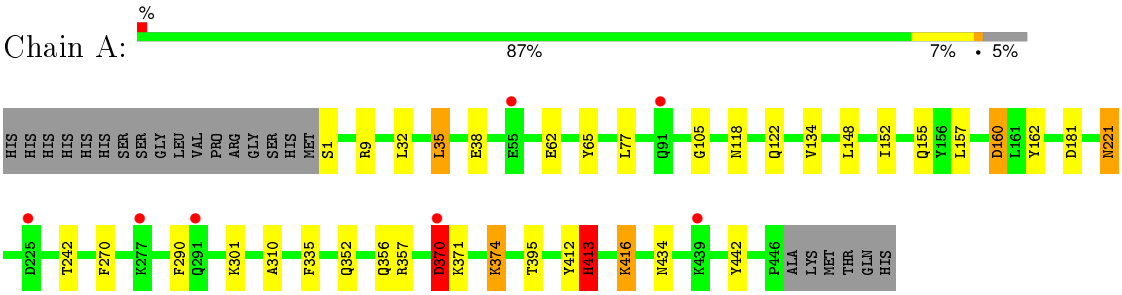
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	32	Total O 32 32	0	0
3	F	16	Total O 16 16	0	0
3	G	17	Total O 17 17	0	0
3	H	19	Total O 19 19	0	0

3 Residue-property plots

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.

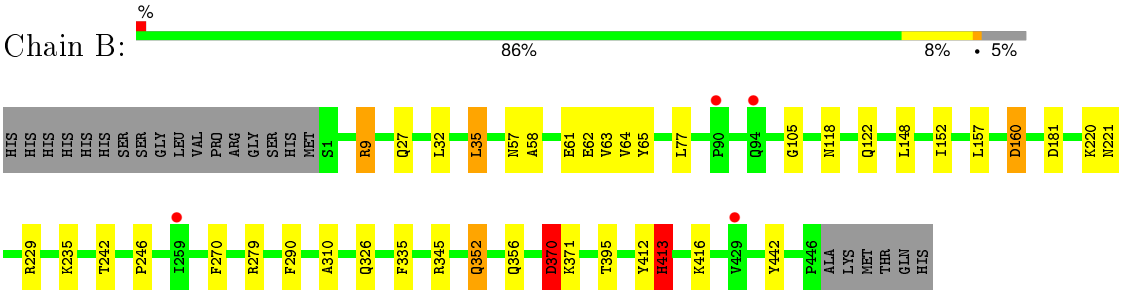
- Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain A:



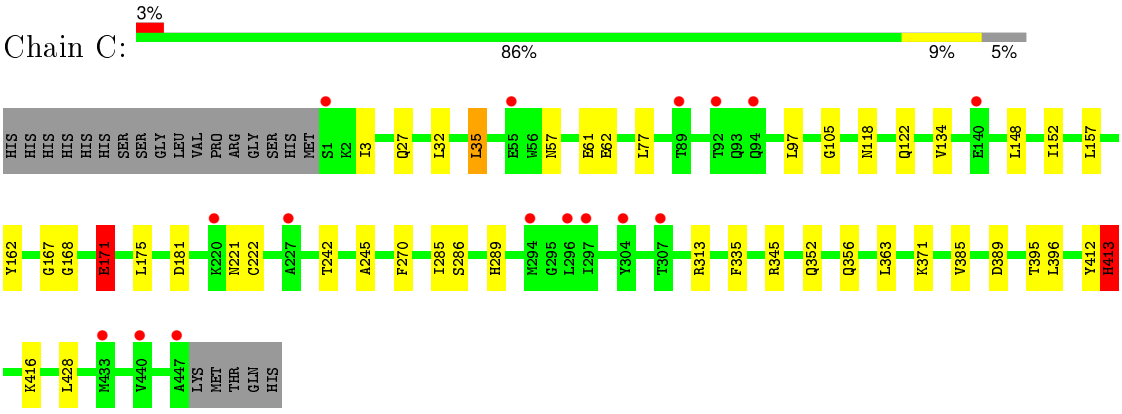
- Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain B:



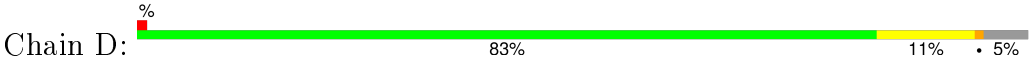
- Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

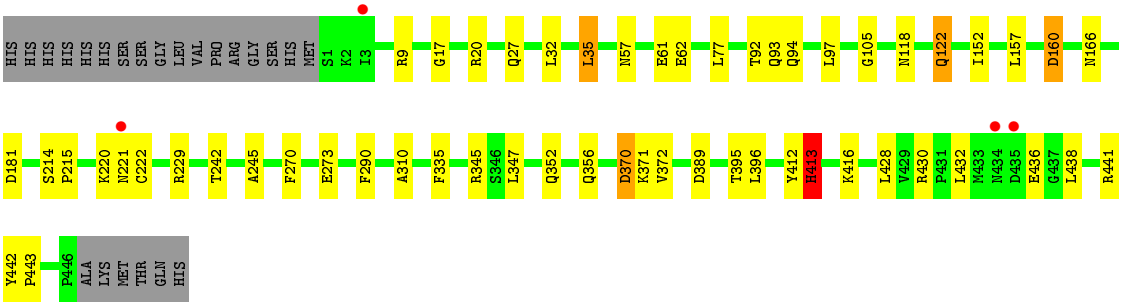
Chain C:



- Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

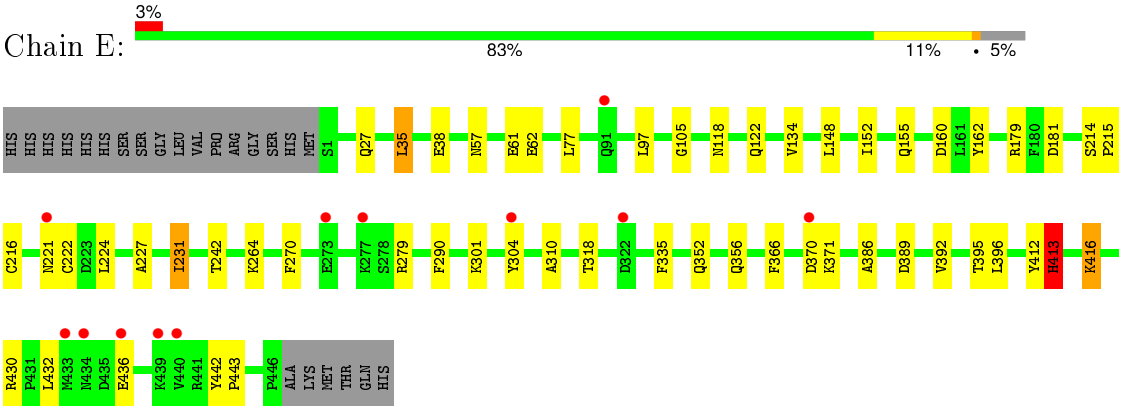
Chain D:





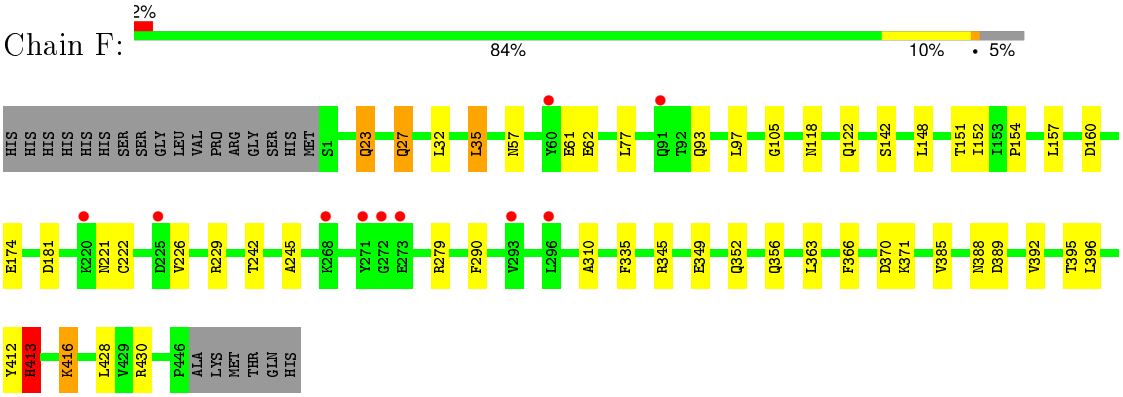
• Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain E:



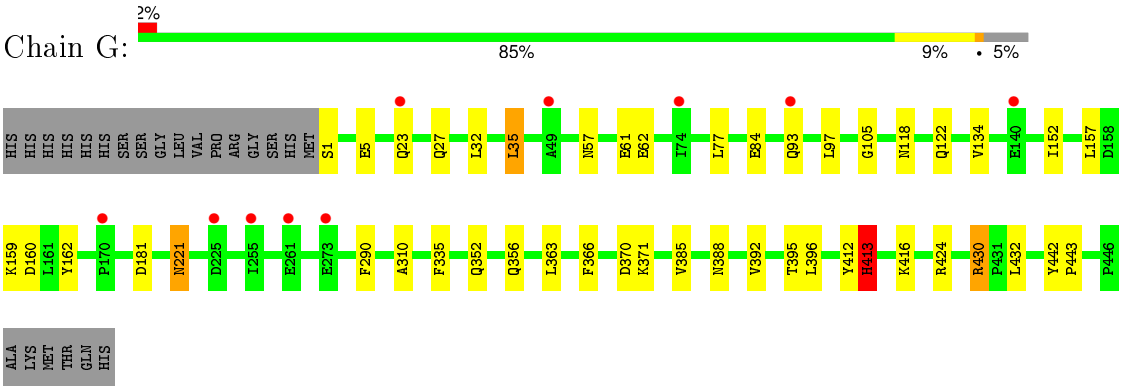
• Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain F:



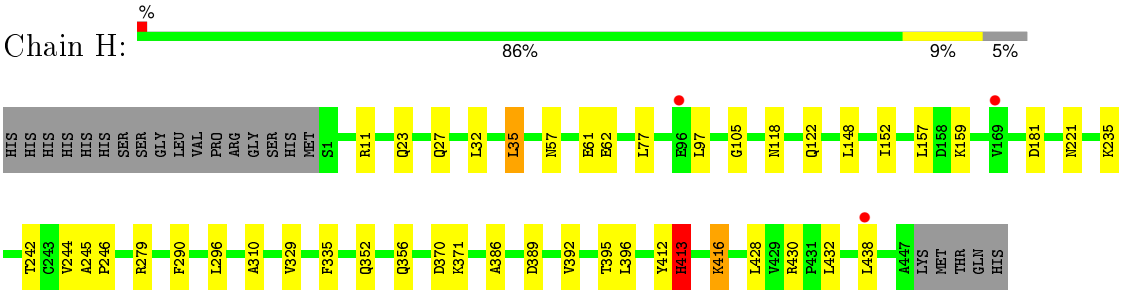
• Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain G:



• Molecule 1: Aldehyde dehydrogenase, dimeric NADP-preferring

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	89.11Å 95.38Å 117.23Å 112.38° 91.68° 90.99°	Depositor
Resolution (Å)	50.00 – 2.50 39.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.00-2.50) 72.9 (39.86-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.234 , 0.255 0.235 , 0.255	Depositor DCC
R_{free} test set	6191 reflections (5.65%)	DCC
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.048 for h,-k,-l 0.014 for -h,k,-k-l 0.007 for -h,-k,k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 115349 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28414	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.88% 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: 04T

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	0.47	0/3584	0.56	3/4857 (0.1%)
1	B	0.43	1/3587 (0.0%)	0.56	3/4862 (0.1%)
1	C	0.54	2/3572 (0.1%)	0.59	4/4843 (0.1%)
1	D	0.45	2/3576 (0.1%)	0.57	2/4848 (0.0%)
1	E	0.41	0/3589	0.56	4/4864 (0.1%)
1	F	0.38	0/3556	0.54	3/4821 (0.1%)
1	G	0.39	0/3578	0.55	3/4849 (0.1%)
1	H	0.43	0/3603	0.54	1/4883 (0.0%)
All	All	0.44	5/28645 (0.0%)	0.56	23/38827 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	GLU	CD-OE1	-19.55	1.04	1.25
1	D	122	GLN	CD-OE1	-5.93	1.10	1.24
1	B	352	GLN	CD-NE2	-5.76	1.18	1.32
1	C	171	GLU	CG-CD	-5.50	1.43	1.51
1	D	122	GLN	CD-NE2	-5.12	1.20	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	171	GLU	CG-CD-OE2	11.14	140.58	118.30
1	D	416	LYS	CD-CE-NZ	8.55	131.36	111.70
1	G	416	LYS	CD-CE-NZ	8.35	130.91	111.70
1	C	171	GLU	CG-CD-OE1	-8.15	101.99	118.30
1	C	416	LYS	CD-CE-NZ	7.75	129.53	111.70
1	B	416	LYS	CD-CE-NZ	5.96	125.42	111.70
1	H	416	LYS	CD-CE-NZ	5.86	125.17	111.70
1	E	416	LYS	CD-CE-NZ	5.45	124.23	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	416	LYS	CD-CE-NZ	5.39	124.09	111.70
1	A	160	ASP	CB-CG-OD2	5.26	123.03	118.30
1	G	370	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	160	ASP	CB-CG-OD2	5.24	123.02	118.30
1	E	370	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	160	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	160	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	160	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	370	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	416	LYS	CD-CE-NZ	5.18	123.62	111.70
1	F	370	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	370	ASP	CB-CG-OD2	5.16	122.95	118.30
1	F	160	ASP	CB-CG-OD2	5.13	122.91	118.30
1	E	231	ILE	CB-CG1-CD1	5.07	128.09	113.90
1	C	171	GLU	OE1-CD-OE2	-5.03	117.27	123.30

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	3502	0	3539	27	0
1	B	3504	0	3534	23	0
1	C	3495	0	3520	40	0
1	D	3497	0	3529	51	1
1	E	3506	0	3541	43	1
1	F	3483	0	3508	44	0
1	G	3499	0	3534	37	0
1	H	3517	0	3554	41	0
2	A	24	0	15	7	0
2	B	24	0	15	8	0
2	C	24	0	15	8	0
2	D	24	0	15	5	0
2	E	24	0	15	5	0
2	F	24	0	15	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	24	0	15	5	0
2	H	24	0	15	10	0
3	A	50	0	0	5	0
3	B	28	0	0	0	0
3	C	20	0	0	2	0
3	D	37	0	0	1	0
3	E	32	0	0	1	0
3	F	16	0	0	2	0
3	G	17	0	0	1	0
3	H	19	0	0	1	0
All	All	28414	0	28379	272	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 (272) 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:167:GLY:HA3	1:C:171:GLU:HG3	1.15	1.09
1:E:179[B]:ARG:HH11	1:E:179[B]:ARG:HG2	1.10	1.07
1:D:20[B]:ARG:HG2	1:D:20[B]:ARG:HH11	1.14	1.06
1:H:279[B]:ARG:HH11	1:H:279[B]:ARG:CG	1.70	1.04
1:H:279[B]:ARG:HH11	1:H:279[B]:ARG:HG2	0.85	1.01
1:E:35:LEU:HD21	1:E:152:ILE:HD12	1.43	1.00
1:H:279[B]:ARG:NH1	1:H:279[B]:ARG:HG2	1.66	0.98
1:E:179[B]:ARG:HH11	1:E:179[B]:ARG:CG	1.76	0.97
1:G:35:LEU:HD21	1:G:152:ILE:HD12	1.47	0.96
1:H:35:LEU:HD21	1:H:152:ILE:HD12	1.47	0.96
1:F:395:THR:HG21	2:F:501:04T:H19	1.45	0.95
1:A:413:HIS:HE1	3:A:626:HOH:O	1.50	0.95
1:D:35:LEU:HD21	1:D:152:ILE:HD12	1.46	0.94
1:F:35:LEU:HD21	1:F:152:ILE:HD12	1.50	0.93
1:C:35:LEU:HD21	1:C:152:ILE:HD12	1.50	0.92
1:A:35:LEU:HD21	1:A:152:ILE:HD12	1.49	0.92
1:B:35:LEU:HD21	1:B:152:ILE:HD12	1.51	0.90
1:C:286:SER:OG	1:C:289:HIS:HB2	1.72	0.88
1:D:20[B]:ARG:CG	1:D:20[B]:ARG:HH11	1.86	0.88
1:G:395:THR:HG21	2:G:501:04T:H19	1.53	0.88
1:F:413:HIS:HE1	3:F:616:HOH:O	1.58	0.87
1:C:242:THR:HG23	2:C:501:04T:H1	1.55	0.87
1:C:167:GLY:CA	1:C:171:GLU:HG3	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HD3	1:B:160:ASP:OD1	1.76	0.85
1:C:413:HIS:HD2	3:C:611:HOH:O	1.60	0.84
1:E:224:LEU:HD21	3:E:631:HOH:O	1.77	0.84
1:D:395:THR:HG21	2:D:501:04T:H19	1.60	0.83
1:B:395:THR:HG21	2:B:501:04T:H19	1.60	0.82
1:D:94:GLN:HG3	1:F:151:THR:HG21	1.62	0.80
1:F:97:LEU:HD21	1:H:396:LEU:HD13	1.65	0.78
1:E:179[B]:ARG:HG2	1:E:179[B]:ARG:NH1	1.92	0.77
2:F:501:04T:C23	2:F:501:04T:H19	2.15	0.75
1:B:58:ALA:O	1:B:63:VAL:HG23	1.87	0.75
2:A:501:04T:H19	2:A:501:04T:C23	2.17	0.74
1:E:264:LYS:HD3	1:E:304:TYR:CD1	2.23	0.73
1:F:396:LEU:HD13	1:H:97:LEU:HD21	1.71	0.72
1:D:17:GLY:HA2	1:D:20[B]:ARG:NH1	2.04	0.72
1:B:370:ASP:N	1:B:370:ASP:OD1	2.19	0.72
2:E:501:04T:C23	2:E:501:04T:H19	2.19	0.72
1:D:94:GLN:NE2	1:F:148:LEU:HD12	2.05	0.72
2:D:501:04T:H23A	2:D:501:04T:H19	1.72	0.71
2:H:501:04T:H19	2:H:501:04T:C23	2.21	0.71
2:G:501:04T:H19	2:G:501:04T:C23	2.20	0.71
1:D:97:LEU:HD21	1:E:396:LEU:HD13	1.72	0.71
1:A:412:TYR:O	1:A:413:HIS:HB2	1.91	0.70
2:H:501:04T:H19	2:H:501:04T:H23B	1.73	0.70
1:H:290:PHE:CE1	1:H:310:ALA:HA	2.27	0.70
2:G:501:04T:H23A	2:G:501:04T:H19	1.73	0.70
2:B:501:04T:H19	2:B:501:04T:C23	2.22	0.70
1:A:413:HIS:CE1	3:A:626:HOH:O	2.33	0.69
1:B:57:ASN:O	1:B:61:GLU:HB2	1.92	0.69
1:F:290:PHE:CE1	1:F:310:ALA:HA	2.28	0.69
1:G:290:PHE:CE1	1:G:310:ALA:HA	2.28	0.69
1:C:62:GLU:HG3	1:C:118:ASN:HB2	1.74	0.68
1:A:370:ASP:OD1	1:A:370:ASP:N	2.13	0.68
1:F:62:GLU:HG3	1:F:118:ASN:HB2	1.76	0.67
1:A:9[A]:ARG:HD3	1:A:160:ASP:OD1	1.94	0.67
1:D:20[B]:ARG:HG2	1:D:20[B]:ARG:NH1	1.96	0.67
1:G:62:GLU:HG3	1:G:118:ASN:HB2	1.75	0.67
1:D:62:GLU:HG3	1:D:118:ASN:HB2	1.76	0.67
1:D:290:PHE:CE1	1:D:310:ALA:HA	2.29	0.66
1:E:62:GLU:HG3	1:E:118:ASN:HB2	1.76	0.66
1:D:412:TYR:O	1:D:413:HIS:HB2	1.94	0.66
1:A:395:THR:HG21	2:A:501:04T:H19	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:LEU:HD23	1:H:392:VAL:HG23	1.77	0.66
2:D:501:04T:H19	2:D:501:04T:C23	2.25	0.66
1:B:290:PHE:CE1	1:B:310:ALA:HA	2.30	0.65
1:E:290:PHE:CE1	1:E:310:ALA:HA	2.30	0.65
1:D:20[B]:ARG:CG	1:D:20[B]:ARG:NH1	2.51	0.65
1:E:395:THR:HG21	2:E:501:04T:H19	1.77	0.65
1:B:62:GLU:HG3	1:B:118:ASN:HB2	1.78	0.65
1:F:389:ASP:OD2	1:H:430:ARG:NH1	2.31	0.64
1:A:290:PHE:CE1	1:A:310:ALA:HA	2.32	0.63
2:E:501:04T:H23B	2:E:501:04T:H19	1.80	0.63
2:F:501:04T:H19	2:F:501:04T:H23A	1.80	0.63
1:B:412:TYR:O	1:B:413:HIS:HB2	1.98	0.63
1:F:412:TYR:O	1:F:413:HIS:HB2	1.99	0.63
1:C:395:THR:HG21	2:C:501:04T:H19	1.81	0.63
1:E:179[B]:ARG:CG	1:E:179[B]:ARG:NH1	2.46	0.62
1:A:242:THR:HG23	2:A:501:04T:H1	1.80	0.62
1:E:412:TYR:O	1:E:413:HIS:HB2	1.99	0.62
1:G:412:TYR:O	1:G:413:HIS:HB2	1.99	0.62
1:D:430:ARG:NH1	1:E:389:ASP:OD2	2.32	0.62
2:C:501:04T:C23	2:C:501:04T:H19	2.30	0.61
1:B:352:GLN:O	1:B:356:GLN:HG3	2.01	0.61
1:B:220:LYS:HE3	1:E:38:GLU:HG2	1.83	0.61
1:F:428:LEU:CD2	1:H:392:VAL:HG23	2.31	0.60
1:D:396:LEU:HD13	1:E:97:LEU:HD21	1.82	0.60
2:A:501:04T:H19	2:A:501:04T:H23A	1.83	0.60
1:G:413:HIS:HE1	3:G:601:HOH:O	1.85	0.60
1:A:270:PHE:HE1	1:B:442:TYR:HB3	1.66	0.60
1:E:227:ALA:O	1:E:231:ILE:HG12	2.01	0.59
1:D:17:GLY:HA2	1:D:20[B]:ARG:HH12	1.65	0.59
1:C:286:SER:O	1:C:313:ARG:HD2	2.03	0.59
1:D:430:ARG:HD2	1:E:389:ASP:HB2	1.84	0.59
1:D:347:LEU:HD22	1:D:372:VAL:HG22	1.84	0.59
1:H:62:GLU:HG3	1:H:118:ASN:HB2	1.84	0.59
1:H:61:GLU:HG2	2:H:501:04T:H17	1.84	0.58
1:F:389:ASP:HB2	1:H:430:ARG:HD2	1.85	0.58
1:D:94:GLN:HE22	1:F:148:LEU:CD1	2.17	0.58
1:E:231:ILE:HD13	1:E:366:PHE:CE1	2.39	0.58
1:C:168:GLY:H	1:C:171:GLU:HG2	1.68	0.57
1:H:412:TYR:O	1:H:413:HIS:HB2	2.05	0.57
1:C:270:PHE:HE1	1:G:442:TYR:HB3	1.69	0.57
1:A:38:GLU:HG2	1:D:220:LYS:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:395:THR:HG21	2:F:501:04T:C19	2.28	0.56
1:C:242:THR:HG23	2:C:501:04T:C1	2.31	0.56
1:C:412:TYR:O	1:C:413:HIS:HB2	2.06	0.56
1:B:65:TYR:OH	2:B:501:04T:H23A	2.05	0.56
2:B:501:04T:H19	2:B:501:04T:H23B	1.87	0.55
1:D:389:ASP:OD2	1:E:430:ARG:NH1	2.39	0.55
1:D:270:PHE:HE1	1:E:442:TYR:HB3	1.71	0.55
1:G:352:GLN:O	1:G:356:GLN:HG3	2.06	0.55
1:A:270:PHE:CE1	1:B:442:TYR:HB3	2.42	0.55
1:D:222:CYS:HB2	1:E:432:LEU:HD23	1.88	0.55
1:D:432:LEU:HD23	1:E:222:CYS:HB2	1.88	0.55
1:C:97:LEU:HD21	1:G:396:LEU:HD13	1.88	0.55
1:D:166:ASN:HA	3:D:623:HOH:O	2.06	0.55
1:F:352:GLN:O	1:F:356:GLN:HG3	2.06	0.55
1:E:264:LYS:HD3	1:E:304:TYR:HD1	1.70	0.54
1:F:222:CYS:HB2	1:H:432:LEU:HD23	1.89	0.54
1:E:352:GLN:O	1:E:356:GLN:HG3	2.08	0.54
1:E:242:THR:HG23	2:E:501:04T:H1	1.90	0.54
1:H:242:THR:HG23	2:H:501:04T:H1	1.89	0.54
1:H:413:HIS:HE1	3:H:619:HOH:O	1.91	0.54
1:E:105:GLY:HA3	1:E:181:ASP:OD1	2.08	0.54
1:D:94:GLN:HE22	1:F:148:LEU:HD12	1.72	0.54
1:C:352:GLN:O	1:C:356:GLN:HG3	2.07	0.53
1:F:345:ARG:HB2	1:G:159:LYS:NZ	2.23	0.53
1:A:155:GLN:OE1	1:D:345:ARG:CB	2.57	0.53
1:A:352:GLN:O	1:A:356:GLN:HG3	2.09	0.53
1:A:62:GLU:HG3	1:A:118:ASN:HB2	1.91	0.53
1:C:396:LEU:HD13	1:G:97:LEU:HD21	1.90	0.52
1:F:345:ARG:CB	1:G:159:LYS:NZ	2.71	0.52
1:G:105:GLY:HA3	1:G:181:ASP:OD1	2.10	0.52
1:A:65:TYR:OH	2:A:501:04T:H23A	2.10	0.52
1:D:389:ASP:HB2	1:E:430:ARG:HD2	1.92	0.52
1:C:105:GLY:HA3	1:C:181:ASP:OD1	2.10	0.52
1:D:436:GLU:HB2	1:F:154:PRO:HG2	1.91	0.52
1:A:155:GLN:OE1	1:D:345:ARG:HB3	2.09	0.52
1:F:23:GLN:HE22	1:F:27:GLN:HE22	1.56	0.52
1:C:222:CYS:HB2	1:G:432:LEU:HD23	1.91	0.51
1:D:352:GLN:O	1:D:356:GLN:HG3	2.10	0.51
1:H:395:THR:HG21	2:H:501:04T:H19	1.92	0.51
1:C:270:PHE:CD1	1:G:443:PRO:HD2	2.45	0.51
2:A:501:04T:H19	2:A:501:04T:H23B	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424[A]:ARG:HG2	1:G:424[A]:ARG:HH11	1.75	0.51
1:H:279[B]:ARG:CG	1:H:279[B]:ARG:NH1	2.43	0.51
1:D:94:GLN:NE2	1:F:148:LEU:CD1	2.72	0.51
2:C:501:04T:H23B	2:C:501:04T:H19	1.92	0.51
1:A:442:TYR:HB3	1:B:270:PHE:HE1	1.75	0.51
1:H:352:GLN:O	1:H:356:GLN:HG3	2.11	0.51
1:H:57:ASN:O	1:H:61:GLU:HB2	2.10	0.51
1:H:244:VAL:HG22	2:H:501:04T:O9	2.11	0.50
1:F:349:GLU:OE1	1:G:159:LYS:HE2	2.10	0.50
1:H:105:GLY:HA3	1:H:181:ASP:OD1	2.11	0.50
1:D:105:GLY:HA3	1:D:181:ASP:OD1	2.11	0.50
1:B:105:GLY:HA3	1:B:181:ASP:OD1	2.12	0.49
2:D:501:04T:C19	2:D:501:04T:C23	2.91	0.49
1:G:395:THR:HG21	2:G:501:04T:H23A	1.95	0.49
1:C:395:THR:HG21	2:C:501:04T:H23A	1.95	0.49
1:D:395:THR:HG21	2:D:501:04T:H23A	1.95	0.49
1:A:105:GLY:HA3	1:A:181:ASP:OD1	2.13	0.49
1:F:413:HIS:CE1	3:F:616:HOH:O	2.45	0.48
1:A:374:LYS:HG3	3:A:641:HOH:O	2.13	0.48
1:D:442:TYR:HB3	1:E:270:PHE:HE1	1.78	0.48
1:B:345[B]:ARG:HB3	1:E:155:GLN:OE1	2.13	0.48
1:C:242:THR:CG2	2:C:501:04T:H1	2.36	0.48
1:A:357:ARG:HD3	3:A:636:HOH:O	2.13	0.47
1:B:395:THR:HG21	2:B:501:04T:C19	2.38	0.47
2:F:501:04T:H19	2:F:501:04T:H23B	1.92	0.47
1:B:242:THR:HG23	2:B:501:04T:H1	1.97	0.47
1:A:412:TYR:O	1:A:413:HIS:CB	2.62	0.47
1:B:32:LEU:HG	1:B:157:LEU:HD21	1.97	0.47
1:C:389:ASP:OD2	1:G:430:ARG:NH1	2.44	0.47
1:D:443:PRO:HD2	1:E:270:PHE:CD1	2.50	0.46
2:A:501:04T:C19	2:A:501:04T:C23	2.88	0.46
1:F:392:VAL:HG23	1:H:428:LEU:CD2	2.45	0.46
1:D:428:LEU:CD2	1:E:392:VAL:HG23	2.45	0.46
1:C:389:ASP:HB2	1:G:430:ARG:HD2	1.98	0.46
1:D:32:LEU:HG	1:D:157:LEU:HD21	1.98	0.46
1:F:430:ARG:NH1	1:H:389:ASP:OD2	2.46	0.45
1:F:226:VAL:O	1:F:229:ARG:HG2	2.16	0.45
1:F:345:ARG:HB3	1:G:159:LYS:NZ	2.32	0.45
1:F:32:LEU:HG	1:F:157:LEU:HD21	1.98	0.45
2:E:501:04T:H23A	2:E:501:04T:H19	1.98	0.45
1:C:168:GLY:H	1:C:171:GLU:CG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:LEU:O	1:E:152:ILE:HG12	2.16	0.45
1:D:428:LEU:O	1:E:386:ALA:HA	2.17	0.45
1:C:413:HIS:CD2	3:C:611:HOH:O	2.48	0.45
1:C:32:LEU:HG	1:C:157:LEU:HD21	1.98	0.45
1:E:57:ASN:O	1:E:61:GLU:HB2	2.17	0.45
1:G:84:GLU:OE1	1:G:424[B]:ARG:NH2	2.49	0.45
1:C:286:SER:OG	1:C:289:HIS:CB	2.55	0.45
1:D:430:ARG:NH1	1:E:392:VAL:HG21	2.31	0.45
1:E:152:ILE:HA	1:E:155:GLN:HE21	1.82	0.44
1:C:168:GLY:N	1:C:171:GLU:HG2	2.30	0.44
1:H:242:THR:HG23	2:H:501:04T:C1	2.48	0.44
1:C:363:LEU:HB3	1:C:385:VAL:HG22	1.98	0.44
1:G:395:THR:HG21	2:G:501:04T:C23	2.47	0.44
1:A:221:ASN:N	1:A:221:ASN:OD1	2.51	0.44
1:C:222:CYS:HB2	1:G:432:LEU:CD2	2.47	0.44
1:H:235:LYS:HD3	1:H:246:PRO:O	2.18	0.44
1:F:105:GLY:HA3	1:F:181:ASP:OD1	2.18	0.44
1:D:270:PHE:CD1	1:E:443:PRO:HD2	2.52	0.44
1:D:57:ASN:O	1:D:61:GLU:HB2	2.18	0.44
1:G:424[A]:ARG:NH1	1:G:424[A]:ARG:HG2	2.32	0.43
1:F:363:LEU:HB3	1:F:385:VAL:HG22	1.99	0.43
1:G:93:GLN:OE1	1:G:93:GLN:HA	2.18	0.43
1:G:32:LEU:HG	1:G:157:LEU:HD21	2.00	0.43
1:A:32:LEU:HG	1:A:157:LEU:HD21	2.00	0.43
1:G:1:SER:O	1:G:5:GLU:HG2	2.17	0.43
1:F:57:ASN:O	1:F:61:GLU:HB2	2.18	0.43
1:C:345:ARG:CG	1:H:159:LYS:HZ1	2.31	0.43
1:H:11[A]:ARG:HG3	1:H:11[A]:ARG:HH11	1.83	0.43
1:F:242:THR:HB	1:F:245:ALA:HB2	2.01	0.43
1:G:57:ASN:O	1:G:61:GLU:HB2	2.19	0.43
1:G:412:TYR:O	1:G:413:HIS:CB	2.67	0.42
1:D:214:SER:HA	1:D:215:PRO:HD3	1.89	0.42
2:B:501:04T:C19	2:B:501:04T:C23	2.92	0.42
1:D:9:ARG:CZ	1:D:160:ASP:OD1	2.67	0.42
1:F:428:LEU:O	1:H:386:ALA:HA	2.20	0.42
1:C:345:ARG:HB2	1:H:159:LYS:NZ	2.34	0.42
1:B:148:LEU:O	1:B:152:ILE:HG12	2.18	0.42
1:D:438:LEU:O	1:D:441:ARG:HG2	2.19	0.42
2:F:501:04T:C23	2:F:501:04T:C19	2.86	0.42
1:C:285:ILE:HG23	1:C:286:SER:N	2.34	0.42
1:C:57:ASN:O	1:C:61:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:TYR:O	1:D:413:HIS:CB	2.64	0.42
1:C:270:PHE:CE1	1:G:442:TYR:HB3	2.51	0.42
2:C:501:04T:C23	2:C:501:04T:C19	2.97	0.42
1:E:304:TYR:O	1:E:318:THR:HA	2.20	0.42
2:B:501:04T:H19	2:B:501:04T:H23A	1.99	0.42
1:A:148:LEU:O	1:A:152:ILE:HG12	2.20	0.41
1:E:216:CYS:SG	1:E:231:ILE:HD12	2.60	0.41
1:E:134:VAL:O	1:E:162:TYR:HA	2.20	0.41
1:F:392:VAL:HG21	1:H:430:ARG:NH1	2.35	0.41
2:H:501:04T:C19	2:H:501:04T:C23	2.88	0.41
1:H:392:VAL:HG12	2:H:501:04T:H23	2.03	0.41
1:G:363:LEU:HB3	1:G:385:VAL:HG22	2.01	0.41
1:C:148:LEU:O	1:C:152:ILE:HG12	2.21	0.41
1:C:242:THR:HB	1:C:245:ALA:HB2	2.02	0.41
1:E:412:TYR:O	1:E:413:HIS:CB	2.68	0.41
1:F:222:CYS:HB2	1:H:432:LEU:CD2	2.50	0.41
1:C:428:LEU:HD23	1:G:392:VAL:HG23	2.01	0.41
1:H:32:LEU:HG	1:H:157:LEU:HD21	2.02	0.41
1:H:148:LEU:O	1:H:152:ILE:HG12	2.21	0.41
1:C:3:ILE:HG23	1:C:175:LEU:HD13	2.02	0.41
1:F:392:VAL:HG23	1:H:428:LEU:HD23	2.01	0.41
1:D:370:ASP:OD1	1:D:370:ASP:N	2.54	0.41
1:F:148:LEU:O	1:F:152:ILE:HG12	2.20	0.41
1:H:242:THR:HB	1:H:245:ALA:HB2	2.02	0.41
1:F:345:ARG:HB2	1:G:159:LYS:CE	2.50	0.41
1:E:214:SER:HA	1:E:215:PRO:HD3	1.93	0.41
1:G:134:VAL:O	1:G:162:TYR:HA	2.20	0.41
1:H:392:VAL:HG12	2:H:501:04T:C23	2.50	0.41
1:H:296:LEU:HB3	1:H:329:VAL:HG23	2.02	0.41
1:A:134:VAL:O	1:A:162:TYR:HA	2.20	0.41
1:D:9:ARG:NE	1:D:160:ASP:OD1	2.54	0.40
1:F:366:PHE:CD2	1:F:388:ASN:HA	2.56	0.40
1:C:134:VAL:O	1:C:162:TYR:HA	2.21	0.40
1:H:11[A]:ARG:HG3	1:H:11[A]:ARG:NH1	2.37	0.40
1:D:242:THR:HB	1:D:245:ALA:HB2	2.04	0.40
1:F:392:VAL:HG12	2:F:501:04T:C23	2.51	0.40
1:D:92:THR:HB	1:D:97:LEU:HD11	2.04	0.40
1:D:428:LEU:HD23	1:E:392:VAL:HG23	2.02	0.40
1:F:93:GLN:HA	1:F:93:GLN:OE1	2.22	0.40
1:G:221:ASN:N	1:G:221:ASN:OD1	2.54	0.40
1:B:412:TYR:O	1:B:413:HIS:CB	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HB3	3:A:635:HOH:O	2.20	0.40
1:B:235:LYS:HD3	1:B:246:PRO:O	2.22	0.40
1:G:366:PHE:CD2	1:G:388:ASN:HA	2.57	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)
1:D:273:GLU:OE2	1:E:301:LYS:NZ[1_565]	1.60	0.60

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	447/469 (95%)	438 (98%)	7 (2%)	2 (0%)	39	61
1	B	447/469 (95%)	439 (98%)	7 (2%)	1 (0%)	52	75
1	C	446/469 (95%)	434 (97%)	11 (2%)	1 (0%)	52	75
1	D	446/469 (95%)	437 (98%)	8 (2%)	1 (0%)	52	75
1	E	447/469 (95%)	436 (98%)	10 (2%)	1 (0%)	52	75
1	F	444/469 (95%)	434 (98%)	9 (2%)	1 (0%)	52	75
1	G	446/469 (95%)	437 (98%)	8 (2%)	1 (0%)	52	75
1	H	449/469 (96%)	440 (98%)	8 (2%)	1 (0%)	52	75
All	All	3572/3752 (95%)	3495 (98%)	68 (2%)	9 (0%)	46	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	C	413	HIS

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Mol	Chain	Res	Type
1	B	413	HIS
1	D	413	HIS
1	E	413	HIS
1	F	413	HIS
1	G	413	HIS
1	H	413	HIS
1	A	434	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/400 (96%)	371 (97%)	12 (3%)	47	75
1	B	383/400 (96%)	369 (96%)	14 (4%)	41	68
1	C	381/400 (95%)	372 (98%)	9 (2%)	57	82
1	D	382/400 (96%)	371 (97%)	11 (3%)	50	77
1	E	383/400 (96%)	372 (97%)	11 (3%)	50	77
1	F	380/400 (95%)	367 (97%)	13 (3%)	44	72
1	G	382/400 (96%)	372 (97%)	10 (3%)	54	81
1	H	384/400 (96%)	371 (97%)	13 (3%)	44	72
All	All	3058/3200 (96%)	2965 (97%)	93 (3%)	48	76

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	35	LEU
1	A	77	LEU
1	A	122	GLN
1	A	221	ASN
1	A	301	LYS
1	A	335	PHE
1	A	370	ASP

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Mol	Chain	Res	Type
1	A	371	LYS
1	A	374	LYS
1	A	413	HIS
1	A	416	LYS
1	B	9	ARG
1	B	27	GLN
1	B	35	LEU
1	B	64	VAL
1	B	77	LEU
1	B	122	GLN
1	B	221	ASN
1	B	229	ARG
1	B	279	ARG
1	B	326	GLN
1	B	335	PHE
1	B	370	ASP
1	B	371	LYS
1	B	413	HIS
1	C	27	GLN
1	C	35	LEU
1	C	77	LEU
1	C	122	GLN
1	C	171	GLU
1	C	221	ASN
1	C	335	PHE
1	C	371	LYS
1	C	413	HIS
1	D	27	GLN
1	D	35	LEU
1	D	77	LEU
1	D	93	GLN
1	D	122	GLN
1	D	221	ASN
1	D	229	ARG
1	D	335	PHE
1	D	370	ASP
1	D	371	LYS
1	D	413	HIS
1	E	27	GLN
1	E	35	LEU
1	E	77	LEU
1	E	122	GLN

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Mol	Chain	Res	Type
1	E	221	ASN
1	E	279	ARG
1	E	335	PHE
1	E	371	LYS
1	E	413	HIS
1	E	416	LYS
1	E	436	GLU
1	F	23	GLN
1	F	27	GLN
1	F	35	LEU
1	F	77	LEU
1	F	122	GLN
1	F	142	SER
1	F	174	GLU
1	F	221	ASN
1	F	279	ARG
1	F	335	PHE
1	F	371	LYS
1	F	413	HIS
1	F	416	LYS
1	G	23	GLN
1	G	27	GLN
1	G	35	LEU
1	G	77	LEU
1	G	122	GLN
1	G	221	ASN
1	G	335	PHE
1	G	371	LYS
1	G	413	HIS
1	G	430	ARG
1	H	23[A]	GLN
1	H	23[B]	GLN
1	H	27	GLN
1	H	35	LEU
1	H	77	LEU
1	H	122	GLN
1	H	221	ASN
1	H	335	PHE
1	H	370	ASP
1	H	371	LYS
1	H	413	HIS
1	H	416	LYS

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Mol	Chain	Res	Type
1	H	438	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	413	HIS
1	B	144	ASN
1	B	155	GLN
1	C	23	GLN
1	C	155	GLN
1	C	289	HIS
1	C	413	HIS
1	D	155	GLN
1	F	23	GLN
1	F	27	GLN
1	F	413	HIS
1	G	27	GLN
1	G	155	GLN
1	G	413	HIS
1	G	434	ASN
1	H	155	GLN
1	H	413	HIS

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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	04T	A	501	-	23,25,25	3.03	2 (8%)	30,36,36	1.99	7 (23%)
2	04T	B	501	-	23,25,25	3.03	2 (8%)	30,36,36	1.76	5 (16%)
2	04T	C	501	-	23,25,25	2.94	2 (8%)	30,36,36	1.82	5 (16%)
2	04T	D	501	-	23,25,25	3.09	1 (4%)	30,36,36	1.72	4 (13%)
2	04T	E	501	-	23,25,25	2.85	2 (8%)	30,36,36	1.74	4 (13%)
2	04T	F	501	-	23,25,25	2.95	2 (8%)	30,36,36	1.86	6 (20%)
2	04T	G	501	-	23,25,25	3.01	2 (8%)	30,36,36	1.83	7 (23%)
2	04T	H	501	-	23,25,25	2.68	1 (4%)	30,36,36	1.85	8 (26%)

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	04T	A	501	-	-	0/17/18/18	0/2/2/2
2	04T	B	501	-	-	0/17/18/18	0/2/2/2
2	04T	C	501	-	-	0/17/18/18	0/2/2/2
2	04T	D	501	-	-	0/17/18/18	0/2/2/2
2	04T	E	501	-	-	0/17/18/18	0/2/2/2
2	04T	F	501	-	-	0/17/18/18	0/2/2/2
2	04T	G	501	-	-	0/17/18/18	0/2/2/2
2	04T	H	501	-	-	0/17/18/18	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	04T	C6-S7	-14.39	1.59	1.77
2	A	501	04T	C6-S7	-14.02	1.59	1.77
2	G	501	04T	C6-S7	-13.93	1.59	1.77
2	B	501	04T	C6-S7	-13.92	1.59	1.77
2	F	501	04T	C6-S7	-13.58	1.60	1.77
2	C	501	04T	C6-S7	-13.54	1.60	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	04T	C6-S7	-13.16	1.60	1.77
2	H	501	04T	C6-S7	-12.27	1.62	1.77
2	F	501	04T	C15-N14	-2.47	1.35	1.40
2	C	501	04T	C15-N14	-2.44	1.35	1.40
2	B	501	04T	C15-N14	-2.43	1.35	1.40
2	A	501	04T	C15-N14	-2.36	1.35	1.40
2	G	501	04T	C15-N14	-2.20	1.36	1.40
2	E	501	04T	C15-N14	-2.13	1.36	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	04T	O9-S7-O8	-4.65	108.04	117.73
2	G	501	04T	O9-S7-O8	-4.19	108.98	117.73
2	C	501	04T	O9-S7-O8	-4.18	109.00	117.73
2	A	501	04T	O9-S7-O8	-4.08	109.22	117.73
2	H	501	04T	O9-S7-O8	-4.03	109.33	117.73
2	E	501	04T	O9-S7-O8	-3.83	109.74	117.73
2	A	501	04T	O24-C22-N21	-3.81	118.59	123.13
2	B	501	04T	O9-S7-O8	-3.67	110.08	117.73
2	B	501	04T	O24-C22-N21	-3.45	119.02	123.13
2	D	501	04T	O9-S7-O8	-3.39	110.65	117.73
2	C	501	04T	O24-C22-N21	-2.76	119.84	123.13
2	H	501	04T	O24-C22-N21	-2.65	119.98	123.13
2	F	501	04T	O24-C22-N21	-2.64	119.99	123.13
2	A	501	04T	O8-S7-C6	-2.61	106.02	108.31
2	H	501	04T	C1-C6-C5	-2.41	117.72	120.52
2	E	501	04T	O24-C22-N21	-2.37	120.30	123.13
2	G	501	04T	O24-C22-N21	-2.33	120.36	123.13
2	G	501	04T	O24-C22-C23	-2.05	118.31	122.06
2	H	501	04T	O9-S7-C6	2.00	110.06	108.31
2	H	501	04T	C2-C1-C6	2.18	121.88	119.48
2	A	501	04T	O9-S7-C6	2.19	110.22	108.31
2	F	501	04T	O9-S7-C6	2.24	110.27	108.31
2	F	501	04T	C1-C6-S7	2.25	121.81	119.59
2	C	501	04T	C18-N21-C22	2.26	131.53	128.03
2	G	501	04T	O9-S7-C6	2.27	110.29	108.31
2	H	501	04T	C1-C6-S7	2.60	122.15	119.59
2	B	501	04T	C1-C6-S7	2.65	122.20	119.59
2	A	501	04T	C1-C6-S7	2.86	122.41	119.59
2	D	501	04T	C1-C6-S7	3.32	122.86	119.59
2	G	501	04T	C1-C6-S7	3.53	123.06	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	04T	C23-C22-N21	3.72	120.27	114.97
2	E	501	04T	C23-C22-N21	4.11	120.82	114.97
2	H	501	04T	C23-C22-N21	4.11	120.82	114.97
2	F	501	04T	C23-C22-N21	4.28	121.07	114.97
2	C	501	04T	C23-C22-N21	4.32	121.12	114.97
2	H	501	04T	C10-S7-C6	4.34	109.94	104.68
2	B	501	04T	C10-S7-C6	4.40	110.01	104.68
2	G	501	04T	C23-C22-N21	4.47	121.33	114.97
2	G	501	04T	C10-S7-C6	4.64	110.30	104.68
2	A	501	04T	C23-C22-N21	4.64	121.58	114.97
2	B	501	04T	C23-C22-N21	4.88	121.92	114.97
2	C	501	04T	C10-S7-C6	5.06	110.80	104.68
2	D	501	04T	C10-S7-C6	5.18	110.95	104.68
2	E	501	04T	C10-S7-C6	5.38	111.19	104.68
2	F	501	04T	C10-S7-C6	5.39	111.21	104.68
2	A	501	04T	C10-S7-C6	5.77	111.67	104.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	04T	7	0
2	B	501	04T	8	0
2	C	501	04T	8	0
2	D	501	04T	5	0
2	E	501	04T	5	0
2	F	501	04T	7	0
2	G	501	04T	5	0
2	H	501	04T	10	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, 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	446/469 (95%)	0.05	7 (1%)	74	78	26, 56, 90, 118	0
1	B	446/469 (95%)	0.07	4 (0%)	85	88	29, 67, 98, 115	0
1	C	447/469 (95%)	0.07	16 (3%)	46	51	27, 64, 115, 132	0
1	D	446/469 (95%)	-0.11	4 (0%)	85	88	27, 50, 81, 105	0
1	E	446/469 (95%)	0.04	12 (2%)	58	62	28, 59, 89, 98	0
1	F	446/469 (95%)	0.06	10 (2%)	65	69	28, 69, 118, 134	0
1	G	446/469 (95%)	-0.00	10 (2%)	65	69	29, 66, 95, 107	0
1	H	447/469 (95%)	-0.07	3 (0%)	89	90	28, 58, 95, 128	0
All	All	3570/3752 (95%)	0.01	66 (1%)	71	75	26, 60, 102, 134	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	273	GLU	4.9
1	F	296	LEU	4.0
1	C	447	ALA	3.9
1	E	436	GLU	3.7
1	F	225	ASP	3.7
1	C	307	THR	3.6
1	A	225	ASP	3.5
1	C	433	MET	3.4
1	F	91	GLN	3.4
1	A	291	GLN	3.2
1	B	259	ILE	3.2
1	F	293	VAL	3.2
1	F	271	TYR	3.1
1	F	220	LYS	3.0
1	B	90	PRO	3.0
1	G	273	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	434	ASN	2.9
1	A	439	LYS	2.8
1	C	304	TYR	2.8
1	E	322	ASP	2.7
1	C	1	SER	2.7
1	D	3	ILE	2.5
1	F	273	GLU	2.5
1	C	92	THR	2.5
1	H	169	VAL	2.5
1	F	60	TYR	2.5
1	D	221	ASN	2.4
1	G	170	PRO	2.4
1	G	93	GLN	2.4
1	B	94	GLN	2.4
1	E	370	ASP	2.4
1	F	272	GLY	2.3
1	H	96	GLU	2.3
1	E	439	LYS	2.3
1	E	221	ASN	2.3
1	C	297	ILE	2.3
1	G	255	ILE	2.3
1	G	74	ILE	2.2
1	C	220	LYS	2.2
1	A	91	GLN	2.2
1	C	440	VAL	2.2
1	C	294	MET	2.2
1	D	434	ASN	2.2
1	E	277	LYS	2.2
1	D	435	ASP	2.2
1	F	268	LYS	2.2
1	A	370	ASP	2.2
1	A	55	GLU	2.2
1	E	440	VAL	2.1
1	G	49	ALA	2.1
1	C	94	GLN	2.1
1	C	89	THR	2.1
1	C	55	GLU	2.1
1	G	140	GLU	2.1
1	H	438	LEU	2.1
1	A	277	LYS	2.1
1	E	91	GLN	2.1
1	G	225	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	140	GLU	2.1
1	B	429	VAL	2.1
1	G	23	GLN	2.1
1	E	433	MET	2.1
1	E	304	TYR	2.1
1	G	261	GLU	2.0
1	C	296	LEU	2.0
1	C	227	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	04T	E	501	24/24	0.87	0.26	3.77	73,78,80,81	0
2	04T	G	501	24/24	0.91	0.24	3.53	76,77,80,81	0
2	04T	D	501	24/24	0.91	0.20	3.02	64,66,67,67	0
2	04T	C	501	24/24	0.91	0.21	2.56	73,75,77,77	0
2	04T	A	501	24/24	0.91	0.17	1.54	60,66,69,69	0
2	04T	H	501	24/24	0.93	0.16	1.54	62,64,67,68	0
2	04T	F	501	24/24	0.92	0.22	1.52	82,87,90,91	0
2	04T	B	501	24/24	0.91	0.19	1.36	76,78,80,81	0

6.5 Other polymers (i)

There are no such residues in this entry.