



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 AM GMT

PDB ID : 2J6L
Title : Structure of aminoadipate-semialdehyde dehydrogenase
Authors : Bunkoczi, G.; Guo, K.; Debreczeni, J.E.; Smee, C.; Arrowsmith, C.; Edwards, A.; Sundstrom, M.; Weigelt, J.; von Delft, F.; Oppermann, U.
Deposited on : 2006-09-29
Resolution : 1.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

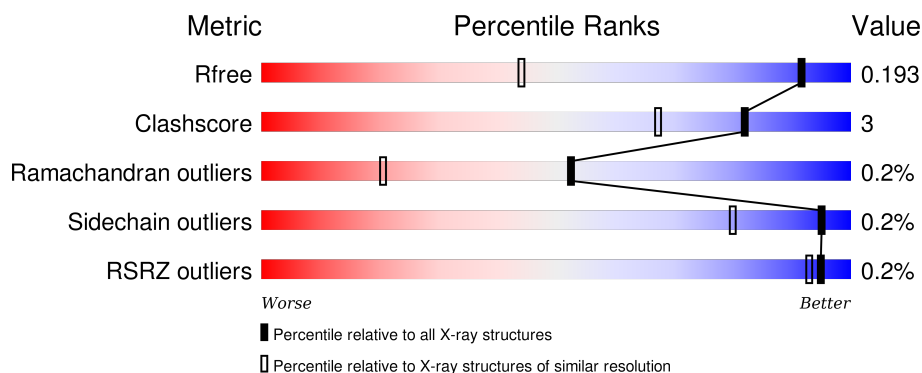
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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.



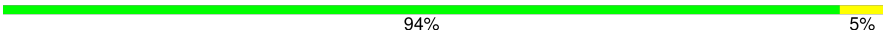

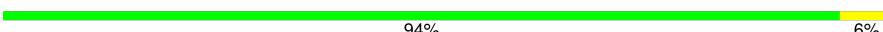
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1475 (1.34-1.26)
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)
RSRZ outliers	91569	1476 (1.34-1.26)

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 $\leq 5\%$. 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	<div> <div>93%</div> <div>6%</div> </div>
1	B	500	<div> <div>95%</div> <div></div> </div>
1	C	500	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
1	D	500	<div> <div>94%</div> <div>6%</div> </div>
1	E	500	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	500	 94% 5%
1	G	500	 93% 6%
1	H	500	 94% 6%

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	NA	A	1504	-	-	-	X
4	NA	D	1503	-	-	-	X
4	NA	E	1505	-	-	-	X
4	NA	G	1503	-	-	-	X
4	NA	H	1503	-	-	-	X

2 Entry composition

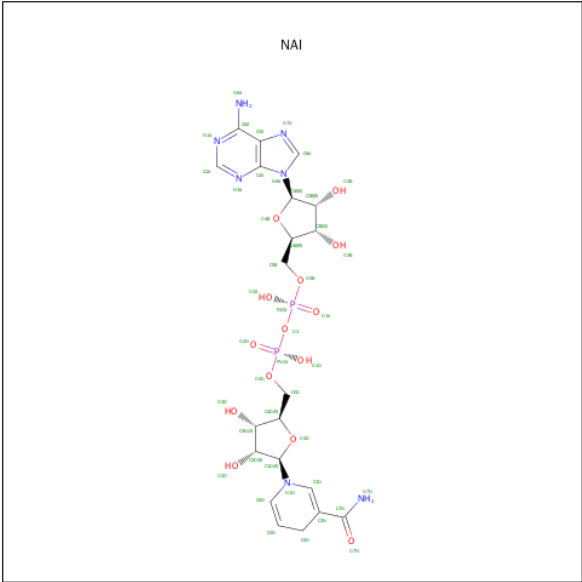
There are 5 unique types of molecules in this entry. The entry contains 36104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FAMILY 7 MEMBER A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	13	0
			3840	2438	664	720	18			
1	B	498	Total	C	N	O	S	0	12	0
			3844	2440	665	720	19			
1	C	497	Total	C	N	O	S	0	9	0
			3807	2417	658	714	18			
1	D	497	Total	C	N	O	S	0	17	0
			3837	2443	660	716	18			
1	E	498	Total	C	N	O	S	0	17	0
			3847	2443	662	724	18			
1	F	498	Total	C	N	O	S	0	16	0
			3851	2445	663	724	19			
1	G	497	Total	C	N	O	S	0	15	0
			3834	2437	660	719	18			
1	H	497	Total	C	N	O	S	0	15	0
			3838	2436	664	720	18			

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Br	0	0
			1	1		
3	D	1	Total	Br	0	0
			1	1		
3	E	3	Total	Br	0	0
			3	3		
3	H	1	Total	Br	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Br 4	0	0
3	C	2	Total 2	Br 2	0	0
3	A	2	Total 2	Br 2	0	0
3	F	1	Total 1	Br 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	646	Total 646	O 646	0	0
5	B	612	Total 612	O 612	0	0
5	C	582	Total 582	O 582	0	0
5	D	627	Total 627	O 627	0	0
5	E	641	Total 641	O 641	0	0

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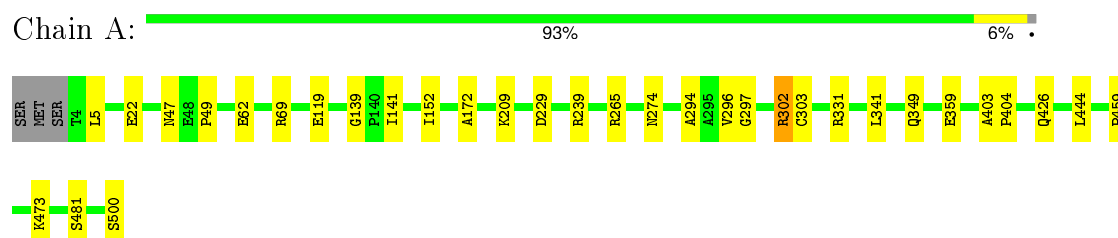
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	631	Total 631	O 631	0	0
5	G	653	Total 653	O 653	0	0
5	H	639	Total 639	O 639	0	0

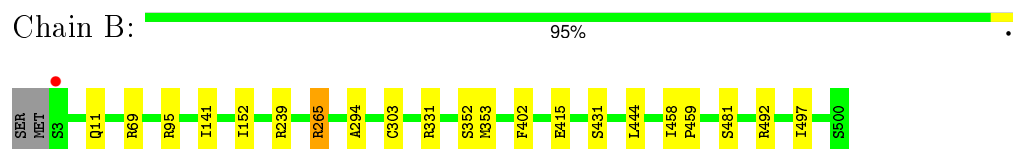
3 Residue-property plots

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.

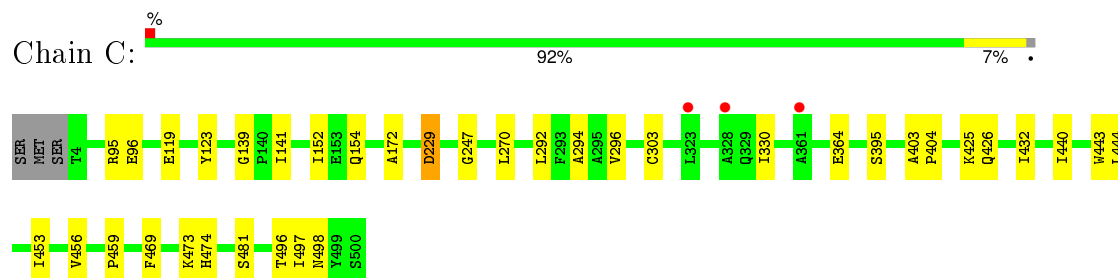
- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1



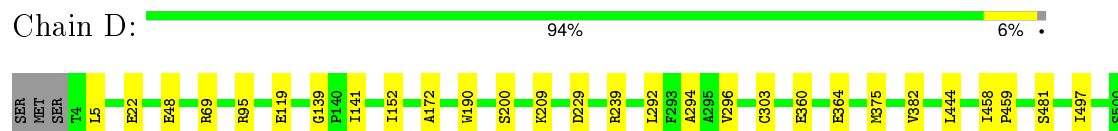
- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1



- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1

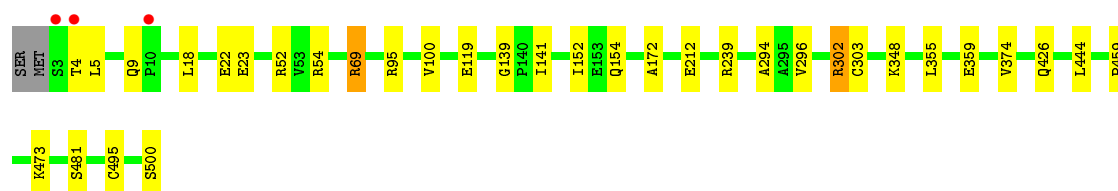


- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1



- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1





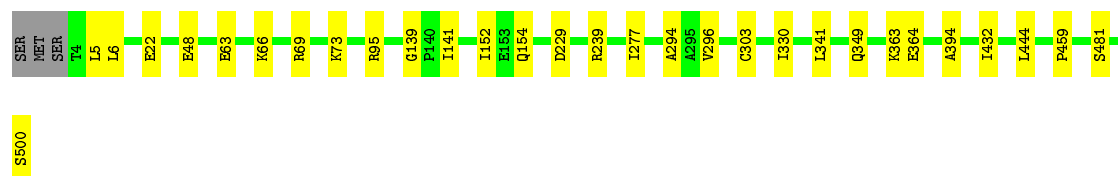
- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1

Chain F: 94% 5%



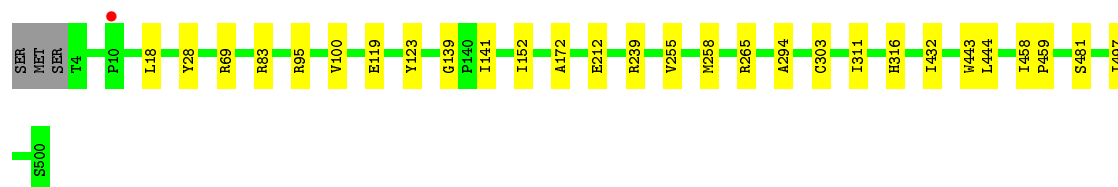
- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1

Chain G: 93% 6%



- Molecule 1: ALDEHYDE DEHYDROGENASE FAMILY 7 MEMBER A1

Chain H: 94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.29Å 162.33Å 159.02Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	50.00 – 1.30 49.20 – 1.30	Depositor EDS
% Data completeness (in resolution range)	85.1 (50.00-1.30) 85.1 (49.20-1.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.137 , 0.189 0.145 , 0.193	Depositor DCC
R_{free} test set	40940 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 816006 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	36104	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, NAI, BR

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	0.70	0/3969	0.77	6/5381 (0.1%)
1	B	0.70	0/3969	0.75	6/5379 (0.1%)
1	C	0.72	0/3921	0.76	4/5318 (0.1%)
1	D	0.65	0/3984	0.74	3/5401 (0.1%)
1	E	0.73	2/3996 (0.1%)	0.80	8/5415 (0.1%)
1	F	0.67	0/3993	0.75	3/5408 (0.1%)
1	G	0.69	0/3975	0.74	2/5385 (0.0%)
1	H	0.69	0/3975	0.74	3/5385 (0.1%)
All	All	0.69	2/31782 (0.0%)	0.76	35/43072 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	359	GLU	CD-OE2	11.77	1.38	1.25
1	E	359	GLU	CD-OE1	7.83	1.34	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ASP	CB-CG-OD1	9.24	126.61	118.30
1	E	302[A]	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	E	302[B]	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	229	ASP	CB-CG-OD1	8.95	126.36	118.30
1	E	302[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	E	302[B]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	D	229	ASP	CB-CG-OD1	7.87	125.38	118.30
1	D	95	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	G	95	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	G	95	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	E	359	GLU	OE1-CD-OE2	7.17	131.91	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	F	95	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	F	95	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	C	95	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	E	95	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	265	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	H	95	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	E	95	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	95	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	C	95	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	H	95	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	302[A]	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	302[B]	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	302[A]	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	H	83	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	331	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	229	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	95	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	E	69	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	492	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	265	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	265[A]	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	B	265[B]	ARG	NE-CZ-NH2	5.07	122.83	120.30

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	3840	0	3831	35	0
1	B	3844	0	3834	24	0
1	C	3807	0	3789	30	0
1	D	3837	0	3828	28	0
1	E	3847	0	3825	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3851	0	3836	30	0
1	G	3834	0	3828	32	0
1	H	3838	0	3833	23	0
2	A	44	0	27	4	0
2	B	44	0	27	3	0
2	C	44	0	27	3	0
2	D	44	0	27	3	0
2	E	44	0	27	3	0
2	F	44	0	27	4	0
2	G	44	0	27	3	0
2	H	44	0	27	3	0
3	A	2	0	0	1	0
3	B	4	0	0	1	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	646	0	0	14	0
5	B	612	0	0	5	0
5	C	582	0	0	5	0
5	D	627	0	0	6	0
5	E	641	0	0	5	0
5	F	631	0	0	4	0
5	G	653	0	0	11	0
5	H	639	0	0	7	0
All	All	36104	0	30820	196	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 3.

All (196) 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:331[A]:ARG:HD3	5:A:2447:HOH:O	1.27	1.33
1:A:331[A]:ARG:CD	5:A:2447:HOH:O	1.75	1.30
1:E:302[B]:ARG:NH1	5:E:2399:HOH:O	1.66	1.25
1:B:265[A]:ARG:HD3	5:B:2591:HOH:O	1.19	1.25
1:F:141[A]:ILE:HG23	5:G:2310:HOH:O	1.36	1.24
1:G:303:CYS:SG	2:G:1501:NAI:H42N	1.84	1.17
1:B:11[A]:GLN:OE1	5:B:2007:HOH:O	1.63	1.16
1:A:303:CYS:SG	2:A:1501:NAI:H42N	1.86	1.15
1:B:141[B]:ILE:HG23	5:C:2272:HOH:O	1.45	1.14
5:A:2294:HOH:O	1:D:141[A]:ILE:HD11	1.47	1.12
1:G:229[A]:ASP:OD1	5:G:2366:HOH:O	1.65	1.11
1:D:303:CYS:SG	2:D:1501:NAI:H42N	1.90	1.11
1:F:303:CYS:SG	2:F:1501:NAI:H42N	1.92	1.09
1:F:70[B]:GLU:OE1	5:F:2149:HOH:O	1.74	1.05
1:C:303:CYS:SG	2:C:1501:NAI:H42N	1.96	1.04
1:H:303:CYS:SG	2:H:1501:NAI:H42N	1.98	1.03
1:F:141[A]:ILE:CG2	5:G:2310:HOH:O	1.98	1.02
3:B:1502:BR:BR	3:B:1506:BR:BR	2.88	1.01
1:B:303:CYS:SG	2:B:1501:NAI:H42N	1.99	1.01
1:E:303:CYS:SG	2:E:1501:NAI:H42N	2.01	1.01
1:H:265[A]:ARG:HD3	5:H:2616:HOH:O	0.82	0.99
1:E:444:LEU:HD13	1:F:152[A]:ILE:HD11	1.45	0.98
1:E:355:LEU:HD21	1:E:374:VAL:HG23	1.49	0.93
1:B:141[B]:ILE:CG2	5:C:2272:HOH:O	2.05	0.91
1:A:141[B]:ILE:HG23	5:D:2302:HOH:O	1.71	0.88
1:B:265[A]:ARG:CD	5:B:2591:HOH:O	1.87	0.88
1:A:141[B]:ILE:CG2	5:D:2302:HOH:O	2.21	0.87
1:G:500[A]:SER:OG	5:G:2642:HOH:O	1.92	0.87
1:A:444:LEU:HD13	1:B:152[B]:ILE:HD11	1.59	0.85
1:F:500[B]:SER:OG	5:F:2623:HOH:O	1.95	0.84
1:C:229:ASP:OD1	5:C:2326:HOH:O	1.95	0.83
1:B:141[B]:ILE:HD13	1:C:154:GLN:OE1	1.77	0.83
1:G:303:CYS:SG	2:G:1501:NAI:C4N	2.65	0.81
1:E:152[A]:ILE:HD11	1:F:444:LEU:HD13	1.61	0.81
1:A:500:SER:OG	5:A:2633:HOH:O	1.99	0.81
1:F:34:GLY:O	1:F:54[B]:ARG:HG2	1.80	0.80
1:A:303:CYS:SG	2:A:1501:NAI:C4N	2.69	0.79
1:F:303:CYS:SG	2:F:1501:NAI:C4N	2.73	0.77
1:G:341:LEU:HD12	5:G:2463:HOH:O	1.86	0.75
1:C:496:THR:HB	1:D:458[A]:ILE:HD11	1.68	0.74
1:D:209:LYS:NZ	5:D:2345:HOH:O	2.19	0.74
1:D:292:LEU:O	1:D:296[B]:VAL:HG22	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:CYS:SG	2:D:1501:NAI:C4N	2.75	0.73
1:A:359[B]:GLU:OE1	5:A:2473:HOH:O	2.06	0.72
1:H:303:CYS:SG	2:H:1501:NAI:C4N	2.78	0.70
1:E:303:CYS:SG	2:E:1501:NAI:C4N	2.79	0.70
1:B:303:CYS:SG	2:B:1501:NAI:C4N	2.78	0.70
1:C:303:CYS:SG	2:C:1501:NAI:C4N	2.79	0.69
1:A:141[A]:ILE:CD1	1:D:152[A]:ILE:HB	2.23	0.69
1:A:209:LYS:HE2	5:A:2335:HOH:O	1.93	0.69
1:C:294:ALA:HB2	1:C:459:PRO:HB2	1.74	0.68
1:F:38:VAL:HG22	1:F:54[B]:ARG:HD2	1.75	0.68
1:C:292:LEU:HD11	1:C:330:ILE:HD11	1.77	0.67
1:A:62:GLU:OE1	5:A:2134:HOH:O	2.13	0.66
1:A:141[A]:ILE:HD11	1:D:152[A]:ILE:HB	1.81	0.63
1:G:444:LEU:HD13	1:H:152[B]:ILE:HD11	1.81	0.62
1:C:444:LEU:HD13	1:D:152[A]:ILE:HD11	1.82	0.61
1:H:212:GLU:HG3	5:H:2050:HOH:O	2.00	0.61
1:C:154:GLN:NE2	5:C:2275:HOH:O	2.34	0.60
1:E:18:LEU:HD21	1:E:100[A]:VAL:HG13	1.83	0.60
1:B:11[A]:GLN:CD	5:B:2007:HOH:O	2.27	0.59
1:E:444:LEU:HD11	1:F:497:ILE:HD11	1.85	0.59
1:H:100[B]:VAL:HG22	5:H:2217:HOH:O	2.03	0.59
1:F:141[B]:ILE:HD11	1:G:152[B]:ILE:HB	1.85	0.58
1:F:141[B]:ILE:CD1	1:G:152[B]:ILE:HB	2.33	0.58
1:E:444:LEU:CD1	1:F:152[A]:ILE:HD11	2.26	0.58
1:F:5:LEU:HD11	1:F:52[A]:ARG:NH1	2.19	0.58
1:A:331[A]:ARG:HD2	5:A:2447:HOH:O	1.70	0.58
1:D:294:ALA:HB2	1:D:459:PRO:HB2	1.86	0.57
1:A:294:ALA:HB2	1:A:459:PRO:HB2	1.87	0.56
1:G:48:GLU:HG2	5:G:2125:HOH:O	2.04	0.56
1:A:303:CYS:HG	2:A:1501:NAI:H42N	1.67	0.56
1:F:38:VAL:CG2	1:F:54[B]:ARG:HD2	2.36	0.56
1:A:349:GLN:NE2	5:A:2468:HOH:O	2.37	0.56
1:C:152:ILE:HD11	1:D:444:LEU:HD13	1.88	0.56
1:G:294:ALA:HB2	1:G:459:PRO:HB2	1.86	0.56
1:D:5:LEU:CD1	1:D:22[B]:GLU:HG3	2.36	0.55
1:E:294:ALA:HB2	1:E:459:PRO:HB2	1.87	0.55
1:A:341:LEU:HD12	5:A:2446:HOH:O	2.05	0.55
1:H:28:TYR:OH	5:H:2050:HOH:O	2.17	0.54
1:C:119:GLU:HG2	1:C:172:ALA:HB2	1.89	0.54
1:B:294:ALA:HB2	1:B:459:PRO:HB2	1.89	0.54
1:D:119:GLU:HG2	1:D:172:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:LEU:HD11	1:D:497:ILE:HD11	1.89	0.54
1:F:154:GLN:NE2	1:G:141[B]:ILE:HD13	2.24	0.53
1:G:141[B]:ILE:HG13	1:G:152[B]:ILE:HG22	1.90	0.53
1:C:498:ASN:HB2	1:D:458[A]:ILE:HG23	1.90	0.53
1:E:119:GLU:HG2	1:E:172:ALA:HB2	1.90	0.52
1:E:4:THR:HG23	1:E:9:GLN:OE1	2.10	0.52
1:G:303:CYS:SG	2:G:1501:NAI:C3N	2.97	0.52
1:E:355:LEU:HD21	1:E:374:VAL:CG2	2.32	0.52
1:A:69:ARG:HD2	1:A:239:ARG:HB3	1.90	0.52
1:G:73[A]:LYS:HD2	5:H:2578:HOH:O	2.09	0.51
1:H:265[A]:ARG:CD	5:H:2616:HOH:O	1.71	0.51
1:E:139:GLY:O	1:H:141[B]:ILE:HG22	2.10	0.51
1:H:119:GLU:HG2	1:H:172:ALA:HB2	1.91	0.51
1:H:294:ALA:HB2	1:H:459:PRO:HB2	1.92	0.51
1:G:63:GLU:HA	1:G:66:LYS:HE3	1.93	0.51
1:D:69:ARG:HD2	1:D:239:ARG:HB3	1.91	0.51
1:G:152[B]:ILE:HD11	1:H:444:LEU:HD13	1.93	0.50
1:B:152[B]:ILE:HB	1:C:141[B]:ILE:CD1	2.42	0.50
1:D:22[A]:GLU:OE2	5:D:2045:HOH:O	2.19	0.50
1:H:18:LEU:HD21	1:H:100[A]:VAL:HG13	1.93	0.50
1:D:360:GLU:OE2	1:D:364:GLU:OE2	2.30	0.50
1:A:22:GLU:CD	5:A:2044:HOH:O	2.51	0.49
1:D:48[A]:GLU:OE1	5:D:2123:HOH:O	2.19	0.49
1:E:303:CYS:SG	2:E:1501:NAI:C3N	3.01	0.49
1:H:69[B]:ARG:HD2	1:H:239:ARG:HB3	1.95	0.49
1:E:348:LYS:NZ	5:E:2459:HOH:O	2.03	0.49
1:E:296:VAL:O	1:E:296:VAL:HG12	2.13	0.49
1:A:403:ALA:HB1	1:A:404:PRO:HD2	1.95	0.49
1:H:303:CYS:SG	2:H:1501:NAI:C3N	3.01	0.49
1:G:349:GLN:NE2	5:G:2493:HOH:O	2.33	0.49
1:E:212:GLU:OE2	5:E:2320:HOH:O	2.18	0.48
1:A:152[B]:ILE:HB	1:D:141[B]:ILE:CD1	2.43	0.48
1:C:292:LEU:O	1:C:296:VAL:HG22	2.13	0.48
1:A:303:CYS:SG	2:A:1501:NAI:C3N	3.02	0.48
1:A:274:ASN:ND2	5:A:2399:HOH:O	2.45	0.48
1:A:444:LEU:HD11	1:B:497:ILE:HD11	1.95	0.48
1:H:212:GLU:OE1	5:H:2345:HOH:O	2.20	0.48
1:F:303:CYS:SG	2:F:1501:NAI:C3N	3.03	0.47
1:B:141[B]:ILE:HG22	1:C:139:GLY:O	2.15	0.47
1:C:425[A]:LYS:HD2	1:C:474:HIS:CE1	2.49	0.47
1:E:500:SER:HB2	5:E:2624:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152[A]:ILE:HG13	1:E:495:CYS:HB2	1.96	0.47
1:C:496:THR:CB	1:D:458[A]:ILE:HD11	2.41	0.47
1:G:48:GLU:HG2	5:G:2126:HOH:O	2.15	0.46
1:F:63[A]:GLU:HG3	5:F:2133:HOH:O	2.15	0.46
1:G:296:VAL:HG11	1:G:330:ILE:HD13	1.98	0.46
1:D:375:MET:HE3	1:D:382:VAL:O	2.15	0.46
1:E:355:LEU:HD11	1:E:374:VAL:HG21	1.98	0.46
1:F:141[A]:ILE:HG13	1:F:152[A]:ILE:HG22	1.98	0.45
1:B:69:ARG:HD2	1:B:239:ARG:HB3	1.97	0.45
1:G:364:GLU:OE2	1:G:394:ALA:HB1	2.16	0.45
1:F:270:LEU:O	2:F:1501:NAI:H2N	2.16	0.45
1:B:303:CYS:SG	2:B:1501:NAI:C3N	3.05	0.45
1:E:154:GLN:NE2	1:H:141[B]:ILE:HD13	2.31	0.45
1:E:5:LEU:HD11	1:E:52:ARG:NH1	2.31	0.45
1:F:54[A]:ARG:HD2	5:F:2083:HOH:O	2.17	0.45
1:C:96:GLU:HG3	5:C:2195:HOH:O	2.17	0.45
1:H:311:ILE:HG21	1:H:316:HIS:HA	1.99	0.44
1:A:331[B]:ARG:NE	5:A:2445:HOH:O	2.50	0.44
1:B:152[B]:ILE:HB	1:C:141[B]:ILE:HD11	2.00	0.44
1:F:34:GLY:C	1:F:54[B]:ARG:HG2	2.35	0.44
1:F:141[A]:ILE:HD13	1:G:154:GLN:OE1	2.17	0.44
1:B:11[A]:GLN:NE2	5:B:2007:HOH:O	2.47	0.44
1:F:139:GLY:O	1:G:141[B]:ILE:HG22	2.17	0.44
1:E:152[A]:ILE:CG1	1:E:495:CYS:HB2	2.47	0.44
1:G:6:LEU:HD21	1:G:48:GLU:OE1	2.17	0.44
1:A:119:GLU:HG2	1:A:172:ALA:HB2	1.98	0.44
1:A:297:GLY:HA3	1:A:302[A]:ARG:NH1	2.32	0.44
1:C:247:GLY:O	1:C:270:LEU:HA	2.17	0.44
1:A:139:GLY:O	1:D:141[A]:ILE:HG22	2.18	0.44
1:F:152[A]:ILE:HB	1:G:141[A]:ILE:CD1	2.48	0.44
1:C:432:ILE:HG23	1:C:443:TRP:CE2	2.53	0.44
1:G:66:LYS:HG2	5:G:2379:HOH:O	2.18	0.43
1:G:363:LYS:HE2	5:G:2500:HOH:O	2.17	0.43
1:E:348:LYS:NZ	5:E:2460:HOH:O	2.51	0.43
3:A:1502:BR:BR	1:F:353[A]:MET:SD	3.31	0.43
1:H:255:VAL:HA	1:H:258:MET:HE3	1.99	0.43
1:A:426:GLN:O	1:A:473:LYS:HE3	2.17	0.43
1:B:141[A]:ILE:CD1	1:C:152:ILE:HB	2.49	0.43
1:D:303:CYS:SG	2:D:1501:NAI:C3N	3.06	0.43
1:C:497:ILE:HD11	1:D:444:LEU:HD11	1.99	0.43
1:C:364:GLU:OE2	1:C:395:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:277:ILE:HB	1:G:432:ILE:HG22	2.00	0.43
1:A:141[B]:ILE:HG22	1:D:139:GLY:O	2.19	0.43
1:E:23:GLU:OE2	1:E:54:ARG:NE	2.52	0.43
1:A:152[B]:ILE:HD11	1:B:444:LEU:HD13	2.00	0.43
1:E:5:LEU:CD1	1:E:22:GLU:HG3	2.49	0.42
1:E:69:ARG:HD2	1:E:239:ARG:HB3	2.01	0.42
1:G:444:LEU:HD11	1:H:497:ILE:HD11	2.01	0.42
1:B:415:GLU:CD	1:B:415:GLU:H	2.21	0.42
1:C:440:ILE:HG23	1:C:456:VAL:HG21	2.01	0.42
1:D:458[A]:ILE:HG22	5:D:2575:HOH:O	2.18	0.42
1:F:141[A]:ILE:HG22	1:G:139:GLY:O	2.20	0.41
1:G:69:ARG:HD2	1:G:239:ARG:HB3	2.02	0.41
1:C:303:CYS:SG	2:C:1501:NAI:C3N	3.09	0.41
1:E:426:GLN:O	1:E:473:LYS:HE3	2.20	0.41
1:G:48:GLU:CG	5:G:2126:HOH:O	2.68	0.41
1:C:403:ALA:HB1	1:C:404:PRO:HD2	2.02	0.41
1:H:458:ILE:HG13	1:H:459:PRO:HD2	2.02	0.41
1:C:453[A]:ILE:HD11	1:C:469:PHE:CE1	2.56	0.41
1:A:47:ASN:ND2	5:A:2115:HOH:O	2.33	0.41
1:F:364:GLU:OE1	1:F:394:ALA:HB1	2.20	0.41
1:D:190:TRP:CH2	1:D:200:SER:HA	2.56	0.41
1:F:277:ILE:HB	1:F:432:ILE:HG22	2.02	0.41
1:E:141[A]:ILE:HG22	1:H:139:GLY:O	2.21	0.41
1:C:426:GLN:O	1:C:473:LYS:HE3	2.21	0.40
1:B:431[A]:SER:OG	1:B:458:ILE:O	2.32	0.40
1:A:296:VAL:HG12	1:A:296:VAL:O	2.21	0.40
1:H:432:ILE:HG23	1:H:443:TRP:CE2	2.56	0.40
1:G:5:LEU:CD1	1:G:22:GLU:HG3	2.51	0.40
1:B:352:SER:HB2	1:E:355:LEU:HD12	2.04	0.40
1:A:5:LEU:HD23	1:A:49:PRO:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	508/500 (102%)	494 (97%)	13 (3%)	1 (0%)	52	20
1	B	508/500 (102%)	494 (97%)	13 (3%)	1 (0%)	52	20
1	C	504/500 (101%)	489 (97%)	14 (3%)	1 (0%)	52	20
1	D	511/500 (102%)	497 (97%)	13 (2%)	1 (0%)	52	20
1	E	513/500 (103%)	496 (97%)	16 (3%)	1 (0%)	52	20
1	F	511/500 (102%)	497 (97%)	13 (2%)	1 (0%)	52	20
1	G	509/500 (102%)	492 (97%)	16 (3%)	1 (0%)	52	20
1	H	509/500 (102%)	493 (97%)	15 (3%)	1 (0%)	52	20
All	All	4073/4000 (102%)	3952 (97%)	113 (3%)	8 (0%)	52	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	481	SER
1	C	481	SER
1	E	481	SER
1	H	481	SER
1	A	481	SER
1	D	481	SER
1	F	481	SER
1	G	481	SER

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	407/400 (102%)	407 (100%)	0	100	100
1	B	408/400 (102%)	407 (100%)	1 (0%)	95	80
1	C	401/400 (100%)	400 (100%)	1 (0%)	95	80
1	D	408/400 (102%)	408 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	410/400 (102%)	410 (100%)	0	100	100
1	F	411/400 (103%)	408 (99%)	3 (1%)	88	64
1	G	409/400 (102%)	409 (100%)	0	100	100
1	H	411/400 (103%)	410 (100%)	1 (0%)	95	80
All	All	3265/3200 (102%)	3259 (100%)	6 (0%)	95	80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	402	PHE
1	C	123	TYR
1	F	69	ARG
1	F	123	TYR
1	F	402	PHE
1	H	123	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 23 are monoatomic - leaving 8 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	NAI	A	1501	-	38,48,48	1.36	3 (7%)	48,73,73	1.89	8 (16%)
2	NAI	B	1501	-	38,48,48	1.37	3 (7%)	48,73,73	1.96	9 (18%)
2	NAI	C	1501	-	38,48,48	1.49	4 (10%)	48,73,73	1.68	7 (14%)
2	NAI	D	1501	-	38,48,48	1.53	6 (15%)	48,73,73	1.98	10 (20%)
2	NAI	E	1501	-	38,48,48	1.21	4 (10%)	48,73,73	1.77	5 (10%)
2	NAI	F	1501	-	38,48,48	1.45	7 (18%)	48,73,73	1.83	9 (18%)
2	NAI	G	1501	-	38,48,48	1.44	4 (10%)	48,73,73	1.74	9 (18%)
2	NAI	H	1501	-	38,48,48	1.32	4 (10%)	48,73,73	1.72	6 (12%)

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	NAI	A	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	B	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	C	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	D	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	E	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	F	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	G	1501	-	-	0/25/72/72	0/5/5/5
2	NAI	H	1501	-	-	0/25/72/72	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1501	NAI	C4N-C5N	-5.53	1.37	1.49
2	B	1501	NAI	C4N-C5N	-5.43	1.37	1.49
2	C	1501	NAI	C4N-C5N	-5.07	1.38	1.49
2	H	1501	NAI	C4N-C5N	-5.04	1.38	1.49
2	F	1501	NAI	C4N-C5N	-4.76	1.38	1.49
2	G	1501	NAI	C4N-C5N	-4.73	1.38	1.49
2	A	1501	NAI	C4N-C5N	-4.68	1.39	1.49
2	E	1501	NAI	C4N-C5N	-3.96	1.40	1.49
2	F	1501	NAI	C5A-N7A	-2.27	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1501	NAI	C4A-N3A	-2.20	1.32	1.35
2	E	1501	NAI	C2A-N3A	2.10	1.35	1.32
2	H	1501	NAI	C2A-N3A	2.25	1.36	1.32
2	F	1501	NAI	O4B-C1B	2.39	1.44	1.41
2	D	1501	NAI	C2N-C3N	2.42	1.40	1.34
2	F	1501	NAI	C5A-C4A	2.47	1.46	1.40
2	E	1501	NAI	C5A-C4A	2.54	1.46	1.40
2	E	1501	NAI	C6N-C5N	2.59	1.38	1.33
2	D	1501	NAI	C2A-N3A	2.61	1.36	1.32
2	F	1501	NAI	C2N-C3N	2.64	1.41	1.34
2	C	1501	NAI	C2A-N3A	2.67	1.36	1.32
2	B	1501	NAI	C6N-C5N	2.78	1.38	1.33
2	H	1501	NAI	C6N-C5N	2.83	1.38	1.33
2	D	1501	NAI	C5A-C4A	2.98	1.47	1.40
2	G	1501	NAI	C5A-C4A	3.03	1.47	1.40
2	B	1501	NAI	C2A-N3A	3.10	1.37	1.32
2	G	1501	NAI	C2A-N3A	3.16	1.37	1.32
2	H	1501	NAI	C5A-C4A	3.16	1.47	1.40
2	A	1501	NAI	C6N-C5N	3.17	1.39	1.33
2	C	1501	NAI	C5A-C4A	3.18	1.47	1.40
2	D	1501	NAI	O4B-C1B	3.31	1.45	1.41
2	F	1501	NAI	C6N-C5N	3.40	1.39	1.33
2	D	1501	NAI	C6N-C5N	3.48	1.40	1.33
2	C	1501	NAI	C6N-C5N	3.86	1.40	1.33
2	G	1501	NAI	C6N-C5N	3.95	1.41	1.33
2	A	1501	NAI	C5A-C4A	4.02	1.49	1.40

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1501	NAI	N3A-C2A-N1A	-8.88	122.09	128.89
2	D	1501	NAI	N3A-C2A-N1A	-8.88	122.09	128.89
2	B	1501	NAI	N3A-C2A-N1A	-8.86	122.11	128.89
2	H	1501	NAI	N3A-C2A-N1A	-8.79	122.17	128.89
2	F	1501	NAI	N3A-C2A-N1A	-8.66	122.27	128.89
2	A	1501	NAI	N3A-C2A-N1A	-8.62	122.30	128.89
2	G	1501	NAI	N3A-C2A-N1A	-7.69	123.01	128.89
2	C	1501	NAI	N3A-C2A-N1A	-7.20	123.39	128.89
2	F	1501	NAI	C1B-N9A-C4A	-4.95	119.48	126.94
2	B	1501	NAI	C1B-N9A-C4A	-4.87	119.59	126.94
2	C	1501	NAI	C1B-N9A-C4A	-4.75	119.77	126.94
2	A	1501	NAI	C1B-N9A-C4A	-4.47	120.20	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1501	NAI	C1B-N9A-C4A	-4.43	120.25	126.94
2	D	1501	NAI	C1B-N9A-C4A	-3.96	120.97	126.94
2	E	1501	NAI	C1B-N9A-C4A	-3.70	121.36	126.94
2	B	1501	NAI	C4N-C5N-C6N	-3.37	117.02	122.58
2	B	1501	NAI	C3N-C2N-N1N	-3.24	118.50	123.14
2	D	1501	NAI	C3N-C2N-N1N	-3.23	118.51	123.14
2	D	1501	NAI	C4N-C5N-C6N	-3.09	117.48	122.58
2	H	1501	NAI	C1B-N9A-C4A	-2.98	122.45	126.94
2	B	1501	NAI	O4D-C1D-C2D	-2.71	100.29	106.58
2	A	1501	NAI	C4N-C5N-C6N	-2.51	118.44	122.58
2	C	1501	NAI	C4N-C5N-C6N	-2.45	118.53	122.58
2	C	1501	NAI	C3N-C2N-N1N	-2.37	119.74	123.14
2	D	1501	NAI	O4D-C1D-C2D	-2.33	101.18	106.58
2	H	1501	NAI	C3N-C2N-N1N	-2.31	119.84	123.14
2	H	1501	NAI	C4N-C5N-C6N	-2.26	118.85	122.58
2	G	1501	NAI	C4A-C5A-N7A	-2.24	107.41	109.48
2	F	1501	NAI	O4D-C1D-C2D	-2.24	101.38	106.58
2	C	1501	NAI	C4A-C5A-N7A	-2.23	107.42	109.48
2	F	1501	NAI	C4N-C5N-C6N	-2.19	118.96	122.58
2	F	1501	NAI	C3N-C2N-N1N	-2.15	120.06	123.14
2	G	1501	NAI	C4N-C5N-C6N	-2.12	119.08	122.58
2	A	1501	NAI	C3N-C2N-N1N	-2.12	120.10	123.14
2	D	1501	NAI	C4A-C5A-N7A	-2.11	107.54	109.48
2	E	1501	NAI	C4N-C5N-C6N	-2.09	119.13	122.58
2	B	1501	NAI	O2A-PA-O3	2.01	114.20	105.09
2	G	1501	NAI	O2A-PA-O3	2.01	114.22	105.09
2	E	1501	NAI	O1N-PN-O3	2.07	114.47	105.09
2	G	1501	NAI	O2D-C2D-C1D	2.07	117.17	109.94
2	D	1501	NAI	N6A-C6A-N1A	2.11	123.73	119.20
2	G	1501	NAI	C2A-N1A-C6A	2.12	122.56	118.77
2	F	1501	NAI	O4D-C1D-N1N	2.14	112.58	108.07
2	D	1501	NAI	C4D-O4D-C1D	2.25	114.47	109.52
2	F	1501	NAI	C5N-C4N-C3N	2.49	119.38	112.52
2	B	1501	NAI	O4D-C1D-N1N	2.50	113.34	108.07
2	H	1501	NAI	O4D-C1D-N1N	2.50	113.34	108.07
2	F	1501	NAI	N6A-C6A-N1A	2.52	124.60	119.20
2	A	1501	NAI	O2A-PA-O3	2.65	117.09	105.09
2	H	1501	NAI	C5N-C4N-C3N	2.68	119.90	112.52
2	B	1501	NAI	C5N-C4N-C3N	2.72	120.02	112.52
2	G	1501	NAI	C5N-C4N-C3N	2.73	120.03	112.52
2	F	1501	NAI	O2A-PA-O3	2.73	117.48	105.09
2	G	1501	NAI	N6A-C6A-N1A	2.76	125.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1501	NAI	C5N-C4N-C3N	2.81	120.26	112.52
2	A	1501	NAI	C5N-C4N-C3N	2.87	120.43	112.52
2	C	1501	NAI	C5N-C4N-C3N	2.90	120.50	112.52
2	D	1501	NAI	C5N-C4N-C3N	2.90	120.52	112.52
2	A	1501	NAI	C2A-N1A-C6A	2.99	124.12	118.77
2	C	1501	NAI	N6A-C6A-N1A	3.09	125.83	119.20
2	A	1501	NAI	O4D-C1D-N1N	3.11	114.63	108.07
2	D	1501	NAI	O4D-C1D-N1N	3.56	115.58	108.07
2	B	1501	NAI	N6A-C6A-N1A	3.67	127.08	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	NAI	4	0
2	B	1501	NAI	3	0
2	C	1501	NAI	3	0
2	D	1501	NAI	3	0
2	E	1501	NAI	3	0
2	F	1501	NAI	4	0
2	G	1501	NAI	3	0
2	H	1501	NAI	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	497/500 (99%)	-0.76	0 100 100	8, 13, 22, 35	0
1	B	498/500 (99%)	-0.74	1 (0%) 95 93	9, 13, 22, 37	0
1	C	497/500 (99%)	-0.58	3 (0%) 90 89	8, 14, 27, 39	0
1	D	497/500 (99%)	-0.67	0 100 100	9, 15, 27, 35	1 (0%)
1	E	498/500 (99%)	-0.79	3 (0%) 90 89	8, 12, 22, 36	0
1	F	498/500 (99%)	-0.76	1 (0%) 95 93	9, 13, 22, 36	0
1	G	497/500 (99%)	-0.79	0 100 100	9, 13, 23, 30	0
1	H	497/500 (99%)	-0.71	1 (0%) 95 93	9, 14, 24, 40	0
All	All	3979/4000 (99%)	-0.73	9 (0%) 95 93	8, 13, 24, 40	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	SER	3.0
1	E	3	SER	2.9
1	F	339	ASN	2.6
1	C	361	ALA	2.4
1	E	10	PRO	2.4
1	H	10	PRO	2.4
1	C	328	ALA	2.3
1	E	4	THR	2.2
1	C	323	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	NA	A	1504	1/1	0.98	0.20	22.23	34,34,34,34	0
4	NA	G	1503	1/1	0.99	0.12	15.33	23,23,23,23	0
4	NA	D	1503	1/1	0.91	0.20	10.78	42,42,42,42	0
4	NA	H	1503	1/1	0.88	0.16	8.43	48,48,48,48	0
4	NA	E	1505	1/1	1.00	0.11	5.49	23,23,23,23	0
4	NA	C	1503	1/1	0.95	0.13	1.90	42,42,42,42	0
2	NAI	H	1501	44/44	0.98	0.05	1.31	11,15,19,21	0
4	NA	B	1505	1/1	1.00	0.06	1.14	18,18,18,18	0
4	NA	F	1503	1/1	1.00	0.06	1.10	21,21,21,21	0
2	NAI	D	1501	44/44	0.98	0.05	0.88	10,16,19,23	0
2	NAI	C	1501	44/44	0.98	0.05	0.71	9,14,17,19	0
2	NAI	F	1501	44/44	0.98	0.05	0.59	9,14,17,20	0
2	NAI	G	1501	44/44	0.97	0.05	0.58	11,14,19,21	0
2	NAI	B	1501	44/44	0.97	0.05	0.38	9,14,19,23	0
2	NAI	E	1501	44/44	0.98	0.04	0.05	8,14,17,21	0
3	BR	B	1503	1/1	1.00	0.06	0.05	22,22,22,22	1
3	BR	E	1504	1/1	1.00	0.05	-0.31	20,20,20,20	1
2	NAI	A	1501	44/44	0.98	0.04	-0.35	10,13,16,18	0
3	BR	A	1502	1/1	1.00	0.05	-0.52	19,19,19,19	1
3	BR	A	1503	1/1	0.99	0.03	-2.09	26,26,26,26	1
3	BR	E	1502	1/1	1.00	0.03	-2.34	27,27,27,27	1
3	BR	B	1504	1/1	0.99	0.03	-2.39	29,29,29,29	1
3	BR	G	1502	1/1	1.00	0.03	-2.72	24,24,24,24	1
3	BR	F	1502	1/1	0.99	0.02	-3.13	32,32,32,32	1
3	BR	C	1504	1/1	1.00	0.02	-3.63	17,17,17,17	1
3	BR	H	1502	1/1	1.00	0.01	-4.41	28,28,28,28	1
3	BR	C	1502	1/1	1.00	0.02	-4.45	29,29,29,29	1
3	BR	E	1503	1/1	0.99	0.01	-	28,28,28,28	1
3	BR	B	1506	1/1	0.98	0.16	-	38,38,38,38	1
3	BR	B	1502	1/1	0.99	0.03	-	34,34,34,34	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BR	D	1502	1/1	0.99	0.02	-	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.