



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1NZW
Title : Cys302Ser mutant of human mitochondrial aldehyde dehydrogenase complexed with NADH and Mg²⁺
Authors : Perez-Miller, S.J.; Hurley, T.D.
Deposited on : 2003-02-20
Resolution : 2.65 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

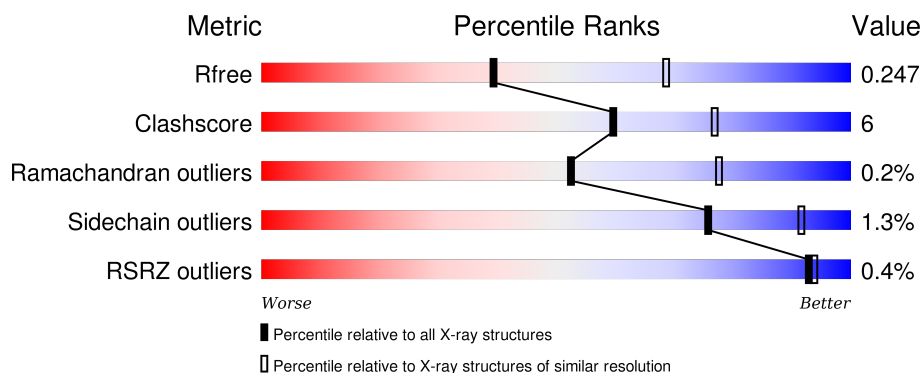
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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>86%</div> <div>13%</div> <div>.</div> </div>
1	B	500	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	500	<div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	D	500	<div> <div>85%</div> <div>14%</div> <div>..</div> </div>
1	E	500	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	500	 85% 14% •
1	G	500	 86% 13% •
1	H	500	 2% 80% 18% ••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31572 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	B	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	C	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	D	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	E	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	F	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	G	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			
1	H	494	Total	C	N	O	S	0	0	0
			3798	2415	648	718	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	SER	CYS	ENGINEERED	UNP P05091
B	302	SER	CYS	ENGINEERED	UNP P05091
C	302	SER	CYS	ENGINEERED	UNP P05091
D	302	SER	CYS	ENGINEERED	UNP P05091
E	302	SER	CYS	ENGINEERED	UNP P05091
F	302	SER	CYS	ENGINEERED	UNP P05091
G	302	SER	CYS	ENGINEERED	UNP P05091
H	302	SER	CYS	ENGINEERED	UNP P05091

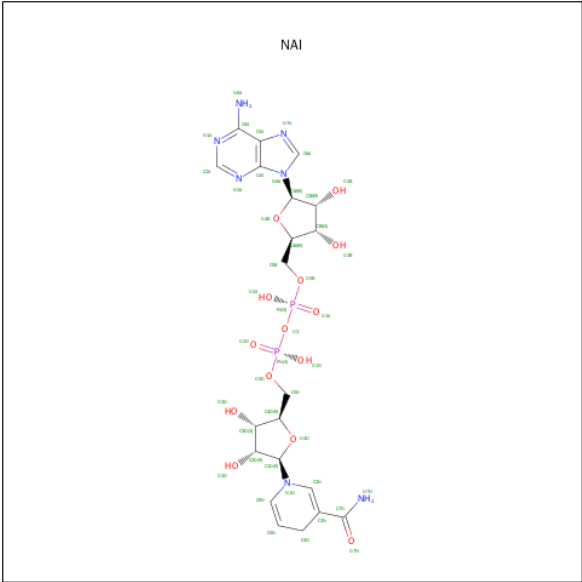
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	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	H	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	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	103	Total	O	0	0
			103	103		
5	C	113	Total	O	0	0
			113	113		
5	D	97	Total	O	0	0
			97	97		

Continued on next page...

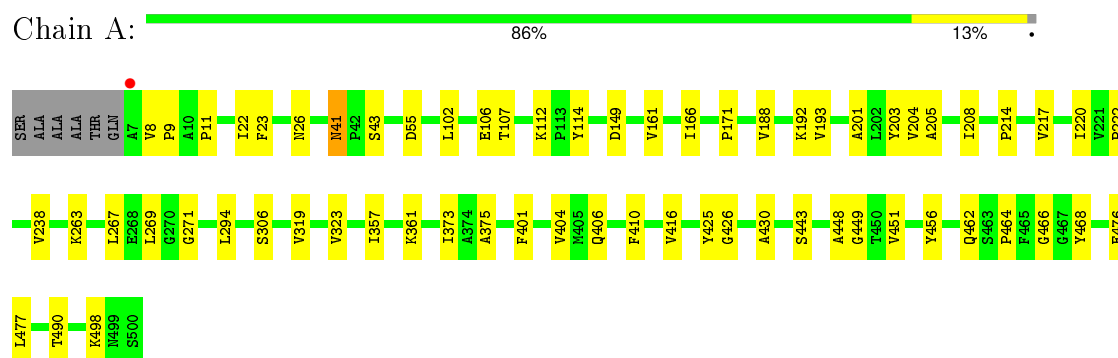
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	84	Total 84	O 84	0	0
5	F	124	Total 124	O 124	0	0
5	G	99	Total 99	O 99	0	0
5	H	81	Total 81	O 81	0	0

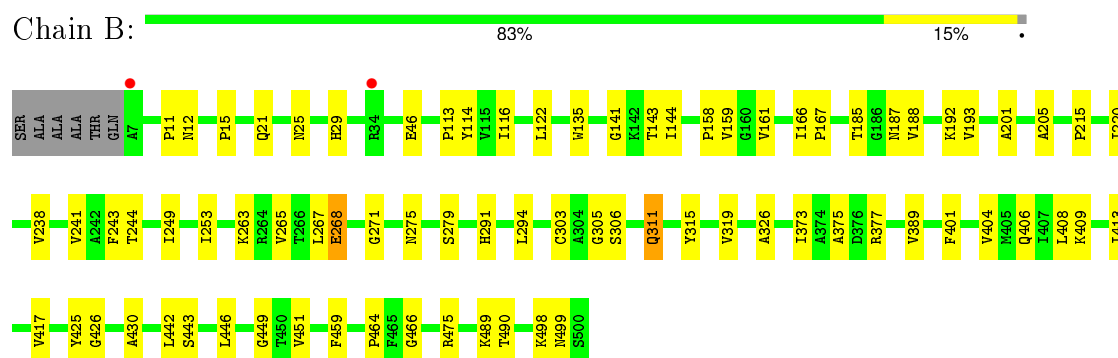
3 Residue-property plots

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.

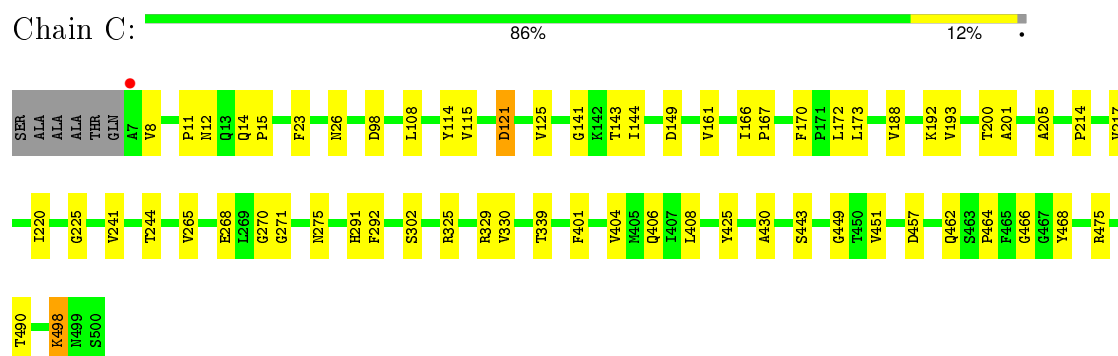
- Molecule 1: Aldehyde dehydrogenase




- Molecule 1: Aldehyde dehydrogenase

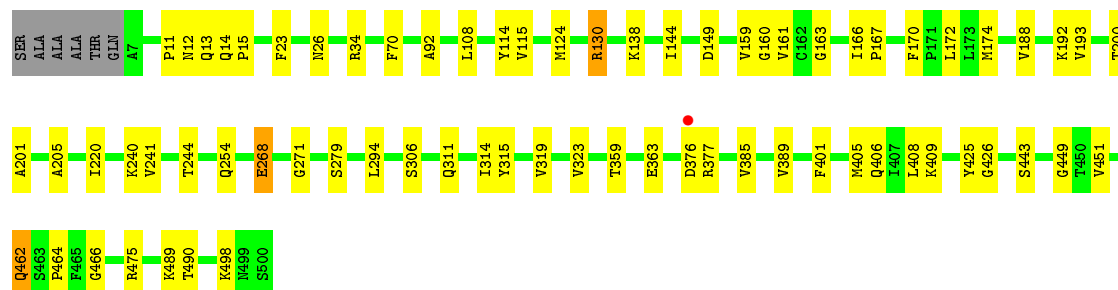


- Molecule 1: Aldehyde dehydrogenase




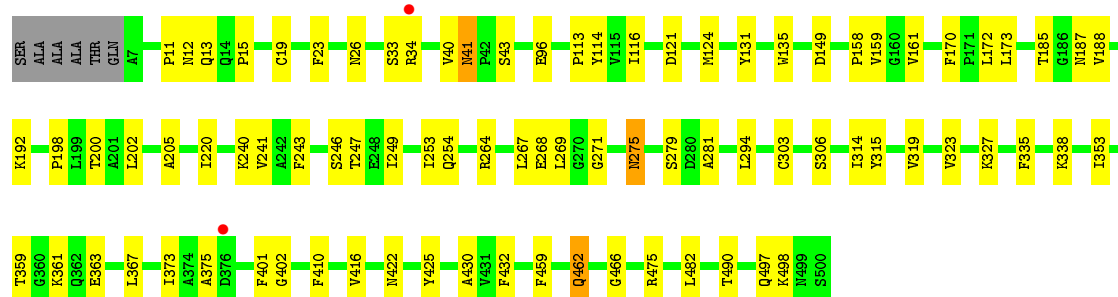
- Molecule 1: Aldehyde dehydrogenase

Chain D:  85% 14% ..




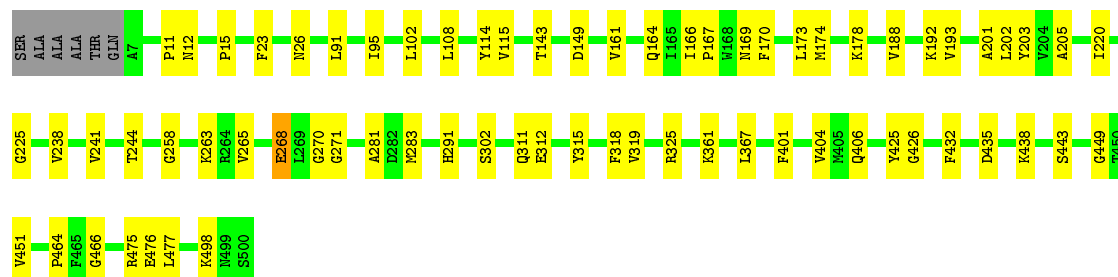
- Molecule 1: Aldehyde dehydrogenase

Chain E:  82% 16% ..




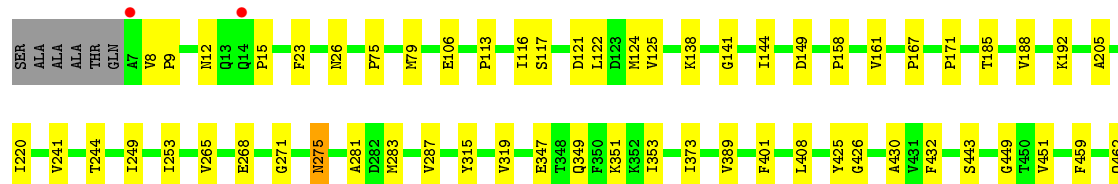
- Molecule 1: Aldehyde dehydrogenase

Chain F:  85% 14% .



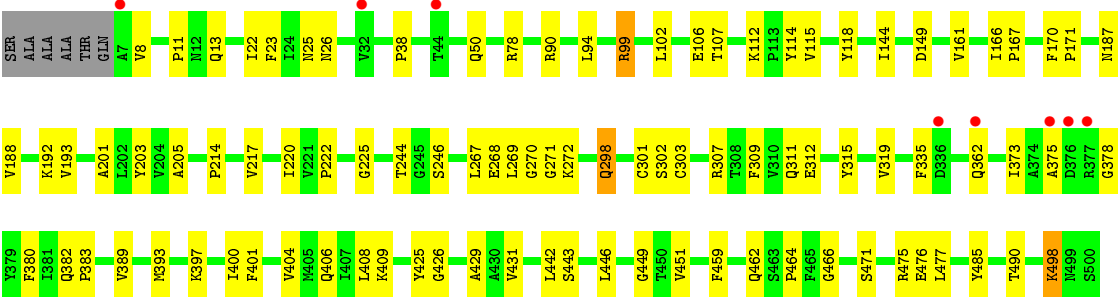
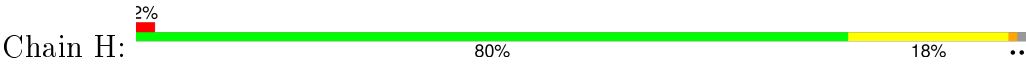
- Molecule 1: Aldehyde dehydrogenase

Chain G:  86% 13% .





● Molecule 1: Aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.36Å 150.49Å 176.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.65 – 2.65 24.64 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.4 (24.65-2.65) 91.5 (24.64-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.252 0.214 , 0.247	Depositor DCC
R_{free} test set	4997 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 100409 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31572	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.05 % 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 3.3341e-06. 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, 0.375 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, MG, NAI

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	0.33	0/3882	0.55	0/5267
1	B	0.31	0/3882	0.55	0/5267
1	C	0.31	0/3882	0.56	0/5267
1	D	0.34	0/3882	0.56	0/5267
1	E	0.32	0/3882	0.56	0/5267
1	F	0.32	0/3882	0.56	0/5267
1	G	0.31	0/3882	0.56	0/5267
1	H	0.33	0/3882	0.55	0/5267
All	All	0.32	0/31056	0.56	0/42136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3798	0	3745	39	0
1	B	3798	0	3745	51	0
1	C	3798	0	3745	44	0
1	D	3798	0	3745	47	0
1	E	3798	0	3745	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3798	0	3745	45	0
1	G	3798	0	3745	38	0
1	H	3798	0	3745	53	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	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	44	0	27	0	0
4	B	44	0	27	0	0
4	C	44	0	27	1	0
4	D	44	0	27	1	0
4	E	44	0	27	0	0
4	F	44	0	27	1	0
4	G	44	0	27	0	0
4	H	44	0	27	2	0
5	A	119	0	0	1	0
5	B	103	0	0	0	0
5	C	113	0	0	2	0
5	D	97	0	0	3	0
5	E	84	0	0	3	0
5	F	124	0	0	1	0
5	G	99	0	0	1	0
5	H	81	0	0	0	0
All	All	31572	0	30176	348	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 6.

All (348) 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:D:15:PRO:HD2	1:D:108:LEU:HD22	1.50	0.90
1:B:279:SER:HB3	1:B:311:GLN:HG2	1.55	0.88
1:E:361:LYS:HE2	1:E:367:LEU:HD22	1.58	0.86
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.60	0.82
1:G:347:GLU:HG2	1:G:351:LYS:HE3	1.64	0.79
1:H:166:ILE:HD11	1:H:193:VAL:HG12	1.65	0.78
1:F:361:LYS:HE2	1:F:367:LEU:HD22	1.70	0.72
1:H:271:GLY:HA2	1:H:425:TYR:CD2	2.24	0.72
1:F:283:MET:HE1	1:F:318:PHE:HD1	1.55	0.72
1:H:311:GLN:HE22	1:H:312:GLU:HG2	1.57	0.70
1:C:161:VAL:HA	1:C:188:VAL:HG23	1.72	0.70
1:D:311:GLN:HG3	5:D:4561:HOH:O	1.91	0.69
1:H:311:GLN:NE2	1:H:312:GLU:HG2	2.08	0.68
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.75	0.68
1:A:166:ILE:HD11	1:A:193:VAL:HG12	1.76	0.68
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.75	0.67
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.76	0.67
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.29	0.66
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.77	0.66
1:G:271:GLY:HA2	1:G:425:TYR:CD2	2.31	0.66
1:C:115:VAL:HG23	5:C:3524:HOH:O	1.96	0.65
1:B:413:ILE:O	1:B:417:VAL:HG23	1.97	0.64
1:B:303:CYS:HG	1:B:459:PHE:HZ	1.45	0.64
1:C:205:ALA:HB2	1:C:220:ILE:HD12	1.79	0.64
1:D:161:VAL:HA	1:D:188:VAL:HG23	1.77	0.64
1:G:117:SER:O	1:G:122:LEU:HD23	1.98	0.64
1:G:121:ASP:O	1:G:125:VAL:HG23	1.98	0.64
1:E:319:VAL:O	1:E:323:VAL:HG23	1.99	0.63
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.81	0.63
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.33	0.63
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.80	0.62
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.34	0.62
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.80	0.62
1:A:161:VAL:HA	1:A:188:VAL:HG23	1.82	0.62
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.81	0.62
1:A:149:ASP:HA	1:A:498:LYS:HB2	1.80	0.62
1:F:271:GLY:HA2	1:F:425:TYR:CD2	2.34	0.62
1:F:225:GLY:HA3	4:F:6502:NAI:C8A	2.29	0.61
1:H:112:LYS:HA	1:H:298:GLN:HE22	1.65	0.61
1:E:113:PRO:HB2	1:E:116:ILE:HG12	1.82	0.61
1:B:271:GLY:HA2	1:B:425:TYR:CD2	2.35	0.61
1:A:102:LEU:HD21	1:A:203:TYR:HD2	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:OH	1:B:489:LYS:HB2	2.01	0.60
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.84	0.60
1:E:161:VAL:HA	1:E:188:VAL:HG23	1.84	0.60
1:E:247:THR:HA	1:E:269:LEU:HD13	1.83	0.60
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.84	0.59
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.84	0.59
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.36	0.59
1:G:149:ASP:HA	1:G:498:LYS:HB2	1.84	0.59
1:A:41:ASN:HD22	1:A:41:ASN:C	2.05	0.59
1:A:22:ILE:HG12	1:A:222:PRO:HD2	1.84	0.59
1:F:283:MET:HE1	1:F:318:PHE:CD1	2.38	0.59
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.37	0.59
1:E:323:VAL:O	1:E:327:LYS:HG3	2.04	0.58
1:E:271:GLY:HA2	1:E:425:TYR:CD2	2.39	0.58
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.39	0.58
1:C:271:GLY:HA2	1:C:425:TYR:CD2	2.38	0.58
1:C:275:ASN:HD22	1:C:430:ALA:HB3	1.69	0.57
1:H:429:ALA:HB1	1:H:446:LEU:HD13	1.85	0.57
1:B:275:ASN:ND2	1:B:430:ALA:HB3	2.18	0.57
1:E:240:LYS:HG2	1:E:241:VAL:N	2.19	0.57
1:B:25:ASN:OD1	1:B:215:PRO:HB2	2.04	0.57
1:E:41:ASN:HD22	1:E:43:SER:H	1.51	0.57
1:F:115:VAL:HG23	5:F:6542:HOH:O	2.03	0.57
1:D:174:MET:HE1	5:D:4552:HOH:O	2.05	0.57
1:E:41:ASN:C	1:E:41:ASN:HD22	2.09	0.56
1:C:167:PRO:HD3	1:C:244:THR:O	2.04	0.56
1:F:166:ILE:HD11	1:F:193:VAL:HG12	1.87	0.56
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.40	0.56
1:B:12:ASN:O	1:B:15:PRO:HD3	2.05	0.56
1:A:41:ASN:ND2	1:A:43:SER:H	2.04	0.55
1:F:102:LEU:HD21	1:F:203:TYR:HD2	1.71	0.55
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.06	0.55
1:B:166:ILE:HD11	1:B:193:VAL:HG12	1.87	0.55
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.42	0.55
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.89	0.54
1:D:92:ALA:HB1	1:D:130:ARG:HH11	1.71	0.54
1:G:249:ILE:O	1:G:253:ILE:HG12	2.08	0.54
1:E:315:TYR:O	1:E:319:VAL:HG23	2.07	0.54
1:H:107:THR:HG23	1:H:112:LYS:O	2.07	0.54
1:D:92:ALA:HB1	1:D:130:ARG:HD2	1.90	0.54
1:F:164:GLN:NE2	1:F:178:LYS:HB3	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.43	0.54
1:D:15:PRO:HD2	1:D:108:LEU:CD2	2.33	0.54
1:B:159:VAL:HG12	1:B:187:ASN:OD1	2.08	0.53
1:F:167:PRO:HD3	1:F:244:THR:O	2.07	0.53
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.08	0.53
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.91	0.53
1:F:15:PRO:HG2	1:F:108:LEU:HD22	1.90	0.53
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.89	0.53
1:H:13:GLN:HA	1:H:335:PHE:CZ	2.44	0.53
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.91	0.53
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.91	0.53
1:E:41:ASN:ND2	1:E:43:SER:H	2.06	0.52
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.90	0.52
1:D:172:LEU:HD21	1:D:200:THR:HB	1.90	0.52
1:F:283:MET:HA	1:F:283:MET:HE2	1.91	0.52
1:H:90:ARG:HH11	1:H:94:LEU:HD21	1.74	0.52
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.32	0.52
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.10	0.52
1:C:225:GLY:HA3	4:C:3502:NAI:C8A	2.39	0.52
1:H:389:VAL:HB	1:H:408:LEU:HG	1.92	0.52
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.92	0.52
1:E:149:ASP:HA	1:E:498:LYS:HB2	1.92	0.51
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.45	0.51
1:E:19:CYS:HA	5:E:5563:HOH:O	2.09	0.51
1:A:41:ASN:HD22	1:A:43:SER:H	1.56	0.51
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.11	0.51
1:F:167:PRO:HD2	1:F:174:MET:HE2	1.92	0.51
1:G:12:ASN:O	1:G:15:PRO:HD3	2.11	0.51
1:E:198:PRO:O	1:E:202:LEU:HG	2.11	0.51
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.46	0.51
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.47	0.50
1:G:443:SER:HA	1:G:451:VAL:HG11	1.93	0.50
1:C:166:ILE:HD11	1:C:193:VAL:HG12	1.93	0.50
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.47	0.50
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.93	0.50
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.47	0.50
1:F:143:THR:OG1	1:G:141:GLY:HA3	2.12	0.50
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.46	0.50
1:E:497:GLN:NE2	1:H:78:ARG:HH11	2.09	0.50
1:H:373:ILE:HG22	1:H:375:ALA:H	1.77	0.50
1:C:270:GLY:HA2	1:C:302:SER:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:GLN:NE2	1:F:312:GLU:HG2	2.26	0.49
1:A:55:ASP:HB3	5:A:1802:HOH:O	2.11	0.49
1:A:443:SER:HA	1:A:451:VAL:HG11	1.93	0.49
1:C:291:HIS:CD2	1:C:325:ARG:HG3	2.47	0.49
1:C:291:HIS:HE1	1:C:329:ARG:HH11	1.59	0.49
1:C:170:PHE:HB3	1:C:173:LEU:HB3	1.95	0.49
1:B:275:ASN:HD22	1:B:430:ALA:HB3	1.76	0.49
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.48	0.49
1:C:11:PRO:HB3	1:C:114:TYR:CE1	2.48	0.49
1:H:307:ARG:HB3	1:H:309:PHE:CE1	2.48	0.49
1:E:353:ILE:HD13	1:E:402:GLY:HA3	1.95	0.49
1:D:306:SER:O	1:D:406:GLN:HB2	2.13	0.49
1:E:264:ARG:HB3	5:E:5574:HOH:O	2.12	0.49
1:G:158:PRO:HG3	1:G:185:THR:O	2.13	0.49
1:H:167:PRO:HD3	1:H:244:THR:O	2.12	0.48
1:H:466:GLY:HA3	1:H:475:ARG:HD3	1.95	0.48
1:D:11:PRO:HB3	1:D:114:TYR:CE1	2.48	0.48
1:D:385:VAL:HG22	1:D:405:MET:HB3	1.95	0.48
1:G:113:PRO:HB2	1:G:116:ILE:HG12	1.94	0.48
1:E:246:SER:O	1:E:269:LEU:HD22	2.13	0.48
1:A:319:VAL:O	1:A:323:VAL:HG23	2.14	0.48
1:A:404:VAL:HG12	1:A:406:GLN:OE1	2.12	0.48
1:C:275:ASN:ND2	1:C:430:ALA:HB3	2.27	0.48
1:F:315:TYR:O	1:F:319:VAL:HG23	2.14	0.48
1:E:170:PHE:HB3	1:E:173:LEU:HB3	1.95	0.48
1:A:448:ALA:O	1:B:489:LYS:HG3	2.14	0.48
1:H:214:PRO:HD2	1:H:217:VAL:HG21	1.94	0.48
1:C:121:ASP:O	1:C:125:VAL:HG23	2.14	0.48
1:H:443:SER:HA	1:H:451:VAL:HG11	1.96	0.48
1:C:292:PHE:HE1	1:C:457:ASP:HB2	1.77	0.48
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.49	0.48
1:E:359:THR:O	1:E:363:GLU:HG2	2.14	0.48
1:B:404:VAL:HG12	1:B:406:GLN:OE1	2.14	0.48
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.13	0.48
1:A:430:ALA:HB2	1:A:456:TYR:CD1	2.49	0.47
1:E:275:ASN:ND2	1:E:430:ALA:HB3	2.28	0.47
1:F:149:ASP:HA	1:F:498:LYS:HB2	1.95	0.47
1:G:171:PRO:HB3	5:G:7514:HOH:O	2.13	0.47
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.36	0.47
1:A:238:VAL:O	1:A:263:LYS:HE3	2.14	0.47
1:H:193:VAL:HG11	1:H:201:ALA:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:ASN:O	1:F:15:PRO:HD3	2.14	0.47
1:H:408:LEU:N	1:H:408:LEU:HD12	2.30	0.47
1:G:347:GLU:HG2	1:G:351:LYS:CE	2.38	0.47
1:A:357:ILE:O	1:A:361:LYS:HG3	2.15	0.47
1:B:244:THR:HG23	1:B:268:GLU:HB3	1.95	0.47
1:D:315:TYR:O	1:D:319:VAL:HG23	2.14	0.47
1:B:46:GLU:HG2	1:B:377:ARG:HH21	1.79	0.47
1:G:349:GLN:O	1:G:353:ILE:HG13	2.14	0.47
1:C:443:SER:HA	1:C:451:VAL:HG11	1.97	0.47
1:B:241:VAL:HG13	1:B:265:VAL:HG13	1.98	0.46
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.45	0.46
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.15	0.46
1:H:270:GLY:HA2	1:H:302:SER:HB2	1.96	0.46
1:B:11:PRO:HB3	1:B:114:TYR:CE1	2.50	0.46
1:G:124:MET:HE3	1:G:459:PHE:HB2	1.95	0.46
1:B:443:SER:HA	1:B:451:VAL:HG11	1.97	0.46
1:F:91:LEU:O	1:F:95:ILE:HG13	2.15	0.46
1:E:279:SER:HA	1:E:314:ILE:HD13	1.98	0.46
1:D:166:ILE:HD11	1:D:193:VAL:HG12	1.98	0.46
1:D:315:TYR:CD1	1:D:409:LYS:HE2	2.51	0.46
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.15	0.46
1:E:361:LYS:HE2	1:E:367:LEU:CD2	2.40	0.46
1:B:238:VAL:O	1:B:263:LYS:HE3	2.16	0.46
1:H:315:TYR:CG	1:H:409:LYS:HE2	2.51	0.45
1:H:149:ASP:HA	1:H:498:LYS:HB2	1.96	0.45
1:H:99:ARG:NH1	1:H:118:TYR:O	2.49	0.45
1:D:294:LEU:HD23	1:D:306:SER:HA	1.97	0.45
1:H:225:GLY:HA3	4:H:8502:NAI:C8A	2.46	0.45
1:H:246:SER:HB3	4:H:8502:NAI:O4D	2.17	0.45
1:F:244:THR:HG23	1:F:268:GLU:HB3	1.98	0.45
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.51	0.45
1:B:449:GLY:HA3	1:B:466:GLY:O	2.15	0.45
1:D:279:SER:HA	1:D:314:ILE:HD13	1.99	0.45
1:C:14:GLN:HE21	1:C:14:GLN:HA	1.81	0.45
1:E:422:ASN:HB3	5:E:5529:HOH:O	2.17	0.45
1:B:389:VAL:HB	1:B:408:LEU:HG	1.97	0.45
1:E:12:ASN:O	1:E:15:PRO:HD3	2.17	0.45
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.51	0.45
1:F:449:GLY:HA3	1:F:466:GLY:O	2.17	0.45
1:C:462:GLN:HB3	1:D:144:ILE:CG2	2.47	0.45
1:A:205:ALA:HA	1:A:208:ILE:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:476:GLU:O	1:H:477:LEU:HB2	2.17	0.45
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.52	0.45
1:F:161:VAL:HA	1:F:188:VAL:CG2	2.45	0.45
1:H:8:VAL:HG21	1:H:115:VAL:HG13	1.98	0.45
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.52	0.44
1:F:443:SER:HA	1:F:451:VAL:HG11	1.98	0.44
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.51	0.44
1:D:115:VAL:HG23	5:D:4507:HOH:O	2.17	0.44
1:G:283:MET:O	1:G:287:VAL:HG23	2.16	0.44
1:B:21:GLN:HB3	1:B:29:HIS:O	2.18	0.44
1:D:167:PRO:HD3	1:D:244:THR:O	2.18	0.44
1:B:498:LYS:HG2	1:B:499:ASN:N	2.33	0.44
1:G:449:GLY:HA3	1:G:466:GLY:O	2.16	0.44
1:H:106:GLU:OE2	1:H:171:PRO:HB2	2.17	0.44
1:D:319:VAL:O	1:D:323:VAL:HG23	2.18	0.44
1:E:172:LEU:HD21	1:E:200:THR:HB	1.99	0.44
1:E:158:PRO:HG3	1:E:185:THR:O	2.17	0.44
1:G:167:PRO:HD3	1:G:244:THR:O	2.18	0.44
1:B:143:THR:OG1	1:C:141:GLY:HA3	2.18	0.44
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.89	0.44
1:D:443:SER:HA	1:D:451:VAL:HG11	1.99	0.44
1:C:214:PRO:HD2	1:C:217:VAL:HG21	2.00	0.44
1:B:141:GLY:HA3	1:C:143:THR:OG1	2.18	0.44
1:A:373:ILE:HG22	1:A:375:ALA:H	1.83	0.44
1:G:144:ILE:CG2	1:H:462:GLN:HB3	2.48	0.44
1:G:315:TYR:O	1:G:319:VAL:HG23	2.18	0.44
1:A:294:LEU:HD23	1:A:306:SER:HA	1.99	0.44
1:B:315:TYR:O	1:B:319:VAL:HG23	2.18	0.44
1:C:291:HIS:HE1	1:C:329:ARG:HD2	1.83	0.43
4:D:4502:NAI:H6N	4:D:4502:NAI:H3D	2.00	0.43
1:B:205:ALA:HB2	1:B:220:ILE:CD1	2.40	0.43
1:H:272:LYS:NZ	1:H:400:ILE:HD12	2.33	0.43
1:A:193:VAL:HG11	1:A:201:ALA:CB	2.49	0.43
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.33	0.43
1:A:107:THR:HG23	1:A:112:LYS:O	2.18	0.43
1:E:373:ILE:HG22	1:E:375:ALA:H	1.84	0.43
1:H:449:GLY:HA3	1:H:466:GLY:O	2.18	0.43
1:E:124:MET:CE	1:E:459:PHE:HB2	2.49	0.43
1:H:378:GLY:HA3	1:H:380:PHE:HE1	1.83	0.43
1:G:75:PRO:O	1:G:79:MET:HB2	2.17	0.43
1:G:373:ILE:HG13	1:G:373:ILE:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:CG2	1:D:462:GLN:HB3	2.49	0.43
1:C:468:TYR:OH	1:D:489:LYS:HB2	2.18	0.43
1:G:462:GLN:HB3	1:H:144:ILE:CG2	2.49	0.43
1:D:359:THR:O	1:D:363:GLU:HG2	2.17	0.43
1:G:389:VAL:HB	1:G:408:LEU:HG	2.00	0.43
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.53	0.43
1:B:442:LEU:O	1:B:446:LEU:HG	2.18	0.43
1:F:169:ASN:N	1:F:169:ASN:OD1	2.52	0.43
1:H:170:PHE:HZ	1:H:301:CYS:HG	1.67	0.43
1:C:12:ASN:O	1:C:15:PRO:HD3	2.19	0.43
1:D:193:VAL:HG11	1:D:201:ALA:CB	2.48	0.43
1:C:404:VAL:HG12	1:C:406:GLN:OE1	2.19	0.43
1:D:170:PHE:O	1:D:174:MET:HG2	2.19	0.43
1:E:303:CYS:SG	1:E:459:PHE:HZ	2.41	0.43
1:D:12:ASN:O	1:D:14:GLN:N	2.52	0.43
1:A:204:VAL:O	1:A:208:ILE:HG13	2.19	0.43
1:F:11:PRO:HB3	1:F:114:TYR:CE2	2.54	0.43
1:E:33:SER:O	1:E:34:ARG:HB2	2.18	0.43
1:C:449:GLY:HA3	1:C:466:GLY:O	2.19	0.42
1:B:167:PRO:HD3	1:B:244:THR:O	2.19	0.42
1:D:149:ASP:HA	1:D:498:LYS:HB2	2.01	0.42
1:E:131:TYR:CE1	1:E:462:GLN:HG3	2.54	0.42
1:D:163:GLY:O	1:D:241:VAL:HA	2.19	0.42
1:E:254:GLN:HG2	1:F:258:GLY:CA	2.48	0.42
1:C:8:VAL:HG21	1:C:115:VAL:HG13	2.01	0.42
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.54	0.42
1:B:249:ILE:O	1:B:253:ILE:HG12	2.19	0.42
1:F:281:ALA:HB2	1:F:432:PHE:O	2.19	0.42
1:A:462:GLN:HB3	1:B:144:ILE:CG2	2.48	0.42
1:A:476:GLU:O	1:A:477:LEU:HB2	2.19	0.42
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.94	0.42
1:D:376:ASP:CG	1:D:377:ARG:N	2.73	0.42
1:E:159:VAL:HG12	1:E:187:ASN:OD1	2.20	0.42
1:F:170:PHE:HB3	1:F:173:LEU:HB3	2.01	0.42
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.53	0.42
1:F:283:MET:CE	1:F:318:PHE:HD1	2.28	0.42
1:G:106:GLU:OE2	1:G:171:PRO:HB2	2.19	0.42
1:F:476:GLU:O	1:F:477:LEU:HB2	2.20	0.42
1:F:238:VAL:O	1:F:263:LYS:HE3	2.18	0.42
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.49	0.42
1:A:410:PHE:CD1	1:A:416:VAL:HB	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLY:HA3	1:A:466:GLY:O	2.20	0.42
1:F:241:VAL:CG1	1:F:265:VAL:HG22	2.50	0.42
1:D:92:ALA:CB	1:D:130:ARG:HD2	2.50	0.42
1:E:185:THR:HG23	1:E:482:LEU:HD22	2.01	0.42
1:A:214:PRO:HD2	1:A:217:VAL:HG21	2.01	0.42
1:E:243:PHE:HB3	1:E:267:LEU:HD23	2.02	0.42
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.84	0.42
1:B:291:HIS:HE1	1:B:326:ALA:HA	1.85	0.42
1:H:431:VAL:HG21	1:H:442:LEU:HB3	2.01	0.42
1:D:34:ARG:HG3	1:D:34:ARG:HH11	1.85	0.42
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.55	0.41
1:H:382:GLN:HA	1:H:383:PRO:HD3	1.93	0.41
1:B:294:LEU:HD23	1:B:305:GLY:O	2.20	0.41
1:A:102:LEU:HD21	1:A:203:TYR:CD2	2.51	0.41
1:G:281:ALA:HB2	1:G:432:PHE:O	2.20	0.41
1:H:187:ASN:ND2	1:H:485:TYR:HB3	2.35	0.41
1:E:13:GLN:HG2	1:E:335:PHE:CG	2.56	0.41
1:H:404:VAL:HG12	1:H:406:GLN:OE1	2.19	0.41
1:G:241:VAL:HG13	1:G:265:VAL:HG13	2.01	0.41
1:C:193:VAL:HG11	1:C:201:ALA:CB	2.50	0.41
1:B:158:PRO:HG3	1:B:185:THR:O	2.21	0.41
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.56	0.41
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.56	0.41
1:C:408:LEU:HD12	1:C:408:LEU:N	2.35	0.41
1:D:315:TYR:CG	1:D:409:LYS:HE2	2.56	0.41
1:F:270:GLY:HA2	1:F:302:SER:HB2	2.02	0.41
1:F:291:HIS:CE1	1:F:325:ARG:HG3	2.56	0.41
1:B:243:PHE:HB3	1:B:267:LEU:HD23	2.03	0.41
1:F:435:ASP:HB3	1:F:438:LYS:HD2	2.03	0.41
1:D:389:VAL:HB	1:D:408:LEU:HG	2.00	0.41
1:B:46:GLU:CG	1:B:377:ARG:HH21	2.33	0.41
1:B:294:LEU:HD23	1:B:306:SER:HA	2.03	0.41
1:C:149:ASP:HA	1:C:498:LYS:HB3	2.02	0.41
1:E:249:ILE:O	1:E:253:ILE:HG12	2.20	0.41
1:E:40:VAL:HG12	1:E:41:ASN:N	2.36	0.41
1:E:294:LEU:HD23	1:E:306:SER:HA	2.01	0.41
1:H:25:ASN:HD22	1:H:25:ASN:HA	1.72	0.41
1:C:149:ASP:HA	1:C:498:LYS:CB	2.51	0.41
1:A:267:LEU:HB3	1:A:269:LEU:HD21	2.02	0.41
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.57	0.40
1:G:408:LEU:HD12	1:G:408:LEU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:VAL:HG12	1:F:406:GLN:OE1	2.20	0.40
1:H:38:PRO:HB3	1:H:50:GLN:HE22	1.86	0.40
1:D:159:VAL:HG11	1:D:240:LYS:HB2	2.03	0.40
1:A:106:GLU:OE2	1:A:171:PRO:HB2	2.21	0.40
1:C:172:LEU:HD21	1:C:200:THR:HB	2.03	0.40
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.52	0.40
1:C:98:ASP:HA	5:C:3539:HOH:O	2.20	0.40
1:D:449:GLY:HA3	1:D:466:GLY:O	2.21	0.40
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.57	0.40
1:E:281:ALA:HB2	1:E:432:PHE:O	2.22	0.40
1:B:373:ILE:HD12	1:B:375:ALA:O	2.22	0.40
1:E:338:LYS:HB3	1:E:338:LYS:HE2	1.88	0.40
1:B:279:SER:CB	1:B:311:GLN:HG2	2.40	0.40
1:D:244:THR:HG23	1:D:268:GLU:HB3	2.03	0.40
1:H:393:MET:O	1:H:397:LYS:HD3	2.21	0.40
1:C:330:VAL:HG12	1:C:339:THR:HA	2.04	0.40
1:H:267:LEU:HB3	1:H:269:LEU:HD21	2.04	0.40
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.57	0.40
1:F:202:LEU:HA	1:F:202:LEU:HD23	1.90	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	492/500 (98%)	473 (96%)	18 (4%)	1 (0%)	52 77
1	B	492/500 (98%)	474 (96%)	17 (4%)	1 (0%)	52 77
1	C	492/500 (98%)	474 (96%)	18 (4%)	0	100 100
1	D	492/500 (98%)	472 (96%)	18 (4%)	2 (0%)	39 65
1	E	492/500 (98%)	473 (96%)	19 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	492/500 (98%)	474 (96%)	17 (4%)	1 (0%)	52	77
1	G	492/500 (98%)	471 (96%)	20 (4%)	1 (0%)	52	77
1	H	492/500 (98%)	471 (96%)	20 (4%)	1 (0%)	52	77
All	All	3936/4000 (98%)	3782 (96%)	147 (4%)	7 (0%)	52	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	13	GLN
1	G	426	GLY
1	B	426	GLY
1	D	426	GLY
1	F	426	GLY
1	A	426	GLY
1	H	426	GLY

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	399/402 (99%)	396 (99%)	3 (1%)	86	95
1	B	399/402 (99%)	394 (99%)	5 (1%)	76	91
1	C	399/402 (99%)	394 (99%)	5 (1%)	76	91
1	D	399/402 (99%)	392 (98%)	7 (2%)	66	88
1	E	399/402 (99%)	391 (98%)	8 (2%)	63	86
1	F	399/402 (99%)	396 (99%)	3 (1%)	86	95
1	G	399/402 (99%)	395 (99%)	4 (1%)	82	94
1	H	399/402 (99%)	391 (98%)	8 (2%)	63	86
All	All	3192/3216 (99%)	3149 (99%)	43 (1%)	76	91

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	192	LYS
1	A	401	PHE
1	B	122	LEU
1	B	192	LYS
1	B	268	GLU
1	B	311	GLN
1	B	401	PHE
1	C	121	ASP
1	C	192	LYS
1	C	268	GLU
1	C	401	PHE
1	C	498	LYS
1	D	124	MET
1	D	130	ARG
1	D	192	LYS
1	D	254	GLN
1	D	268	GLU
1	D	401	PHE
1	D	462	GLN
1	E	41	ASN
1	E	96	GLU
1	E	121	ASP
1	E	192	LYS
1	E	268	GLU
1	E	275	ASN
1	E	401	PHE
1	E	462	GLN
1	F	192	LYS
1	F	268	GLU
1	F	401	PHE
1	G	192	LYS
1	G	268	GLU
1	G	275	ASN
1	G	401	PHE
1	H	99	ARG
1	H	192	LYS
1	H	268	GLU
1	H	298	GLN
1	H	362	GLN
1	H	401	PHE
1	H	471	SER
1	H	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	41	ASN
1	B	83	HIS
1	B	275	ASN
1	C	14	GLN
1	C	275	ASN
1	C	291	HIS
1	D	50	GLN
1	D	390	GLN
1	D	447	GLN
1	D	462	GLN
1	E	14	GLN
1	E	41	ASN
1	E	50	GLN
1	E	175	GLN
1	E	275	ASN
1	E	362	GLN
1	E	462	GLN
1	E	483	GLN
1	F	275	ASN
1	F	349	GLN
1	F	362	GLN
1	G	13	GLN
1	G	50	GLN
1	G	275	ASN
1	G	349	GLN
1	G	362	GLN
1	G	483	GLN
1	H	13	GLN
1	H	25	ASN
1	H	50	GLN
1	H	298	GLN
1	H	362	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 16 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$
4	NAI	A	1502	3	38,48,48	1.84	6 (15%)	48,73,73	1.99	10 (20%)
4	NAI	B	2502	3	38,48,48	1.81	6 (15%)	48,73,73	2.02	12 (25%)
4	NAI	C	3502	3	38,48,48	1.77	5 (13%)	48,73,73	1.81	8 (16%)
4	NAI	D	4502	3	38,48,48	1.78	6 (15%)	48,73,73	1.86	9 (18%)
4	NAI	E	5502	3	38,48,48	1.80	5 (13%)	48,73,73	1.75	8 (16%)
4	NAI	F	6502	3	38,48,48	1.82	5 (13%)	48,73,73	1.83	9 (18%)
4	NAI	G	7502	3	38,48,48	1.74	5 (13%)	48,73,73	1.71	9 (18%)
4	NAI	H	8502	3	38,48,48	1.89	6 (15%)	48,73,73	2.05	8 (16%)

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	NAI	A	1502	3	-	0/25/72/72	0/5/5/5
4	NAI	B	2502	3	-	0/25/72/72	0/5/5/5
4	NAI	C	3502	3	-	0/25/72/72	0/5/5/5
4	NAI	D	4502	3	-	0/25/72/72	0/5/5/5
4	NAI	E	5502	3	-	0/25/72/72	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	F	6502	3	-	0/25/72/72	0/5/5/5
4	NAI	G	7502	3	-	0/25/72/72	0/5/5/5
4	NAI	H	8502	3	-	0/25/72/72	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	8502	NAI	C4N-C5N	-8.02	1.31	1.49
4	F	6502	NAI	C4N-C5N	-7.60	1.32	1.49
4	D	4502	NAI	C4N-C5N	-7.60	1.32	1.49
4	C	3502	NAI	C4N-C5N	-7.57	1.32	1.49
4	A	1502	NAI	C4N-C5N	-7.55	1.32	1.49
4	E	5502	NAI	C4N-C5N	-7.48	1.33	1.49
4	B	2502	NAI	C4N-C5N	-7.37	1.33	1.49
4	G	7502	NAI	C4N-C5N	-7.19	1.33	1.49
4	D	4502	NAI	O4B-C1B	2.24	1.44	1.41
4	D	4502	NAI	C6N-C5N	2.31	1.37	1.33
4	A	1502	NAI	C4A-N3A	2.34	1.39	1.35
4	F	6502	NAI	C8A-N7A	2.52	1.39	1.34
4	C	3502	NAI	C6N-C5N	2.58	1.38	1.33
4	D	4502	NAI	C8A-N7A	2.60	1.39	1.34
4	F	6502	NAI	C6N-C5N	2.62	1.38	1.33
4	B	2502	NAI	C4A-N3A	2.63	1.39	1.35
4	H	8502	NAI	C6N-C5N	2.64	1.38	1.33
4	H	8502	NAI	C4A-N3A	2.67	1.39	1.35
4	E	5502	NAI	C8A-N7A	2.69	1.39	1.34
4	A	1502	NAI	C2A-N1A	2.77	1.39	1.33
4	G	7502	NAI	C6N-C5N	2.79	1.38	1.33
4	A	1502	NAI	C6N-C5N	2.80	1.38	1.33
4	H	8502	NAI	C8A-N7A	2.83	1.40	1.34
4	A	1502	NAI	C8A-N7A	2.84	1.40	1.34
4	C	3502	NAI	C8A-N7A	2.88	1.40	1.34
4	B	2502	NAI	C6N-C5N	2.89	1.38	1.33
4	B	2502	NAI	C8A-N7A	2.94	1.40	1.34
4	E	5502	NAI	C6N-C5N	2.98	1.39	1.33
4	D	4502	NAI	C2A-N1A	3.01	1.39	1.33
4	G	7502	NAI	C8A-N7A	3.02	1.40	1.34
4	C	3502	NAI	C2A-N1A	3.05	1.39	1.33
4	G	7502	NAI	C2A-N1A	3.05	1.39	1.33
4	E	5502	NAI	C2A-N1A	3.06	1.39	1.33
4	B	2502	NAI	C2A-N1A	3.09	1.39	1.33
4	H	8502	NAI	C2A-N1A	3.16	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6502	NAI	C2A-N1A	3.35	1.40	1.33
4	E	5502	NAI	C2A-N3A	4.01	1.39	1.32
4	D	4502	NAI	C2A-N3A	4.02	1.39	1.32
4	C	3502	NAI	C2A-N3A	4.12	1.39	1.32
4	G	7502	NAI	C2A-N3A	4.35	1.39	1.32
4	H	8502	NAI	C2A-N3A	4.39	1.40	1.32
4	B	2502	NAI	C2A-N3A	4.45	1.40	1.32
4	F	6502	NAI	C2A-N3A	4.58	1.40	1.32
4	A	1502	NAI	C2A-N3A	4.78	1.40	1.32

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	8502	NAI	N3A-C2A-N1A	-10.01	121.23	128.89
4	A	1502	NAI	N3A-C2A-N1A	-8.36	122.49	128.89
4	E	5502	NAI	N3A-C2A-N1A	-7.98	122.78	128.89
4	F	6502	NAI	N3A-C2A-N1A	-7.86	122.87	128.89
4	B	2502	NAI	N3A-C2A-N1A	-7.66	123.03	128.89
4	C	3502	NAI	N3A-C2A-N1A	-7.39	123.23	128.89
4	D	4502	NAI	N3A-C2A-N1A	-6.91	123.61	128.89
4	G	7502	NAI	N3A-C2A-N1A	-6.12	124.21	128.89
4	B	2502	NAI	O4D-C4D-C3D	-4.63	95.82	105.15
4	G	7502	NAI	PN-O3-PA	-4.53	120.00	132.73
4	A	1502	NAI	C4N-C5N-C6N	-4.20	115.66	122.58
4	D	4502	NAI	C4N-C5N-C6N	-4.18	115.69	122.58
4	H	8502	NAI	C4N-C5N-C6N	-4.16	115.72	122.58
4	D	4502	NAI	C2B-C1B-N9A	-4.10	108.03	114.29
4	B	2502	NAI	PN-O3-PA	-3.89	121.79	132.73
4	C	3502	NAI	C4N-C5N-C6N	-3.79	116.33	122.58
4	E	5502	NAI	PN-O3-PA	-3.74	122.23	132.73
4	F	6502	NAI	C4N-C5N-C6N	-3.66	116.54	122.58
4	C	3502	NAI	PN-O3-PA	-3.66	122.45	132.73
4	B	2502	NAI	C2B-C3B-C4B	-3.61	95.19	102.61
4	A	1502	NAI	C4B-O4B-C1B	-3.61	105.75	109.72
4	H	8502	NAI	C3N-C2N-N1N	-3.50	118.13	123.14
4	F	6502	NAI	PN-O3-PA	-3.47	122.98	132.73
4	B	2502	NAI	C4N-C5N-C6N	-3.44	116.91	122.58
4	G	7502	NAI	C4N-C5N-C6N	-3.39	116.99	122.58
4	D	4502	NAI	C3N-C2N-N1N	-3.38	118.30	123.14
4	D	4502	NAI	O4D-C4D-C3D	-3.29	98.52	105.15
4	D	4502	NAI	PN-O3-PA	-3.26	123.58	132.73
4	B	2502	NAI	C3N-C2N-N1N	-3.21	118.55	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3502	NAI	C2B-C3B-C4B	-3.15	96.14	102.61
4	A	1502	NAI	C1D-N1N-C2N	-3.13	115.46	120.91
4	F	6502	NAI	C2B-C3B-C4B	-3.04	96.37	102.61
4	A	1502	NAI	C2B-C1B-N9A	-3.01	109.70	114.29
4	H	8502	NAI	C2B-C3B-C4B	-3.00	96.45	102.61
4	C	3502	NAI	C1D-N1N-C2N	-2.99	115.70	120.91
4	G	7502	NAI	C2B-C3B-C4B	-2.99	96.47	102.61
4	E	5502	NAI	C4N-C5N-C6N	-2.89	117.81	122.58
4	C	3502	NAI	C2B-C1B-N9A	-2.82	109.98	114.29
4	B	2502	NAI	C2B-C1B-N9A	-2.73	110.13	114.29
4	C	3502	NAI	C3N-C2N-N1N	-2.71	119.25	123.14
4	G	7502	NAI	C2B-C1B-N9A	-2.70	110.17	114.29
4	F	6502	NAI	C3N-C2N-N1N	-2.69	119.29	123.14
4	A	1502	NAI	PN-O3-PA	-2.65	125.30	132.73
4	E	5502	NAI	O4D-C4D-C3D	-2.54	100.02	105.15
4	D	4502	NAI	C2B-C3B-C4B	-2.43	97.61	102.61
4	A	1502	NAI	C3N-C2N-N1N	-2.32	119.81	123.14
4	A	1502	NAI	C2B-C3B-C4B	-2.23	98.03	102.61
4	H	8502	NAI	C4B-O4B-C1B	-2.19	107.31	109.72
4	G	7502	NAI	C3N-C2N-N1N	-2.17	120.02	123.14
4	F	6502	NAI	C1D-N1N-C2N	-2.14	117.17	120.91
4	D	4502	NAI	C2D-C3D-C4D	-2.11	98.27	102.61
4	H	8502	NAI	O4D-C4D-C3D	-2.11	100.89	105.15
4	A	1502	NAI	C3D-C2D-C1D	-2.07	97.24	101.40
4	F	6502	NAI	C3D-C2D-C1D	-2.06	97.26	101.40
4	G	7502	NAI	O4D-C4D-C3D	-2.04	101.04	105.15
4	B	2502	NAI	C2D-C3D-C4D	-2.04	98.42	102.61
4	E	5502	NAI	C2D-C3D-C4D	-2.01	98.47	102.61
4	B	2502	NAI	O3-PA-O5B	2.02	108.30	102.94
4	E	5502	NAI	O3-PA-O5B	2.09	108.49	102.94
4	F	6502	NAI	O5B-C5B-C4B	2.12	116.92	109.12
4	H	8502	NAI	O5D-C5D-C4D	2.26	117.45	109.12
4	G	7502	NAI	O3-PA-O5B	2.27	108.96	102.94
4	E	5502	NAI	O5B-C5B-C4B	2.38	117.89	109.12
4	B	2502	NAI	O5B-C5B-C4B	2.55	118.52	109.12
4	B	2502	NAI	O3-PN-O5D	2.59	109.80	102.94
4	E	5502	NAI	C5N-C4N-C3N	2.86	120.40	112.52
4	B	2502	NAI	C5N-C4N-C3N	3.17	121.25	112.52
4	C	3502	NAI	C5N-C4N-C3N	3.26	121.50	112.52
4	H	8502	NAI	C5N-C4N-C3N	3.32	121.66	112.52
4	A	1502	NAI	C5N-C4N-C3N	3.33	121.70	112.52
4	D	4502	NAI	C5N-C4N-C3N	3.36	121.78	112.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6502	NAI	C5N-C4N-C3N	3.36	121.78	112.52
4	G	7502	NAI	C5N-C4N-C3N	3.41	121.93	112.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3502	NAI	1	0
4	D	4502	NAI	1	0
4	F	6502	NAI	1	0
4	H	8502	NAI	2	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%)	-0.28	1 (0%) 95 96	16, 30, 40, 49	0
1	B	494/500 (98%)	-0.41	2 (0%) 93 94	17, 28, 38, 46	0
1	C	494/500 (98%)	-0.52	1 (0%) 95 96	14, 23, 34, 45	0
1	D	494/500 (98%)	-0.35	1 (0%) 95 96	15, 29, 41, 49	0
1	E	494/500 (98%)	-0.39	2 (0%) 93 94	16, 29, 38, 49	0
1	F	494/500 (98%)	-0.56	0 100 100	13, 23, 32, 43	0
1	G	494/500 (98%)	-0.38	2 (0%) 93 94	16, 28, 39, 49	0
1	H	494/500 (98%)	-0.11	8 (1%) 74 74	15, 32, 43, 54	0
All	All	3952/4000 (98%)	-0.38	17 (0%) 93 94	13, 28, 40, 54	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASP	3.6
1	G	7	ALA	3.1
1	H	377	ARG	2.9
1	B	7	ALA	2.9
1	C	7	ALA	2.9
1	H	362	GLN	2.9
1	H	44	THR	2.8
1	E	34	ARG	2.6
1	H	7	ALA	2.6
1	G	14	GLN	2.5
1	H	32	VAL	2.3
1	H	375	ALA	2.3
1	D	376	ASP	2.3
1	A	7	ALA	2.2
1	E	376	ASP	2.1
1	H	336	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	34	ARG	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, 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
2	NA	B	1602	1/1	0.60	0.22	1.33	41,41,41,41	0
2	NA	F	1606	1/1	0.90	0.13	0.12	27,27,27,27	0
2	NA	E	1605	1/1	0.76	0.15	-0.06	40,40,40,40	0
2	NA	G	1607	1/1	0.75	0.13	-0.46	34,34,34,34	0
4	NAI	G	7502	44/44	0.96	0.12	-0.78	24,26,28,29	0
4	NAI	A	1502	44/44	0.96	0.12	-0.94	24,27,31,32	0
2	NA	D	1604	1/1	0.77	0.13	-1.08	41,41,41,41	0
4	NAI	F	6502	44/44	0.98	0.10	-1.16	11,19,21,23	0
4	NAI	B	2502	44/44	0.96	0.11	-1.22	21,25,28,29	0
4	NAI	C	3502	44/44	0.98	0.10	-1.24	15,19,21,22	0
4	NAI	D	4502	44/44	0.96	0.11	-1.32	21,26,30,32	0
4	NAI	H	8502	44/44	0.96	0.12	-1.49	26,31,34,36	0
2	NA	A	1601	1/1	0.84	0.11	-1.71	31,31,31,31	0
2	NA	H	1608	1/1	0.89	0.11	-1.74	34,34,34,34	0
4	NAI	E	5502	44/44	0.97	0.10	-1.90	21,25,27,27	0
2	NA	C	1603	1/1	0.93	0.06	-3.17	27,27,27,27	0
3	MG	B	1702	1/1	0.92	0.09	-	22,22,22,22	0
3	MG	G	1707	1/1	0.91	0.07	-	28,28,28,28	0
3	MG	F	1706	1/1	0.94	0.13	-	27,27,27,27	0
3	MG	D	1704	1/1	0.95	0.16	-	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	E	1705	1/1	0.92	0.12	-	35,35,35,35	0
3	MG	C	1703	1/1	0.94	0.13	-	26,26,26,26	0
3	MG	H	1708	1/1	0.92	0.11	-	32,32,32,32	0
3	MG	A	1701	1/1	0.92	0.09	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.