



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 05:55 PM EDT

PDB ID : 3OET
Title : D-Erythronate-4-Phosphate Dehydrogenase complexed with NAD
Authors : Filippova, E.V.; Wawrzak, Z.; Onopriyenko, O.; Savchenko, A.; Edwards, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : unknown
Resolution : 2.36 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

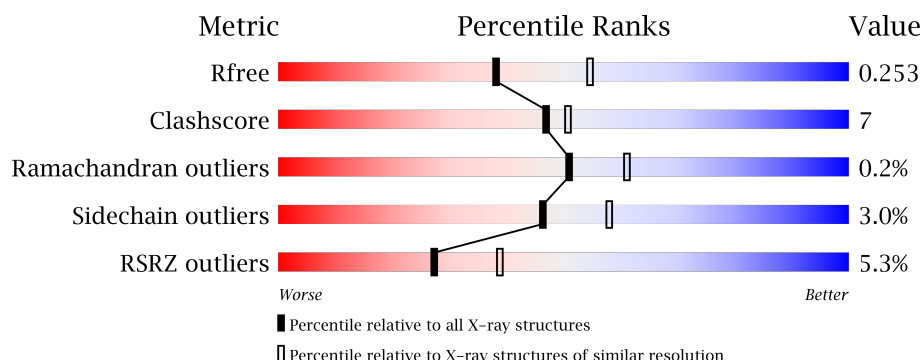
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	381	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	B	381	<div> <div>4%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	381	<div> <div>9%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	D	381	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	E	381	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	381	<div><div></div><div>9%</div><div></div><div>83%</div><div></div><div>12%</div><div></div><div></div></div>
1	G	381	<div><div></div><div>4%</div><div></div><div>75%</div><div></div><div>20%</div><div></div><div></div></div>
1	H	381	<div><div></div><div>7%</div><div></div><div>83%</div><div></div><div>15%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23835 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 Erythronate-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	Se	0	1	0
			2888	1827	514	537	5	5			
1	B	377	Total	C	N	O	S	Se	0	1	0
			2894	1831	511	542	5	5			
1	C	372	Total	C	N	O	S	Se	0	3	0
			2865	1811	506	538	5	5			
1	D	375	Total	C	N	O	S	Se	0	0	0
			2867	1817	506	534	5	5			
1	E	375	Total	C	N	O	S	Se	0	0	0
			2880	1826	507	537	5	5			
1	F	365	Total	C	N	O	S	Se	0	0	0
			2791	1773	489	519	5	5			
1	G	370	Total	C	N	O	S	Se	0	0	0
			2843	1801	501	531	5	5			
1	H	378	Total	C	N	O	S	Se	0	0	0
			2897	1836	516	535	5	5			

There are 24 discrepancies between the modelled and reference sequences:

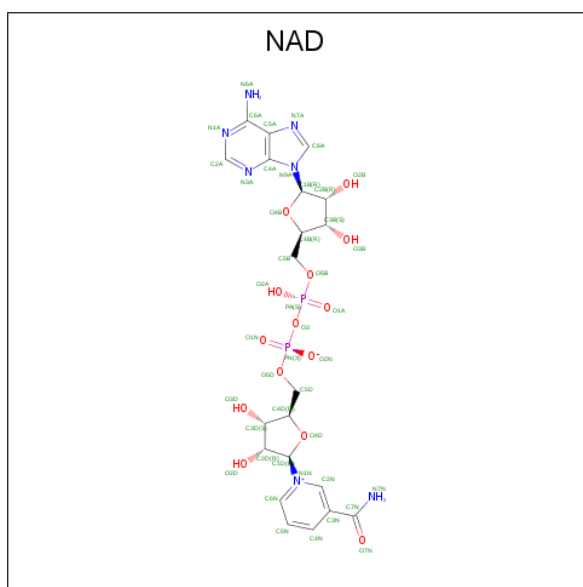
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P60802
A	-1	ASN	-	EXPRESSION TAG	UNP P60802
A	0	ALA	-	EXPRESSION TAG	UNP P60802
B	-2	SER	-	EXPRESSION TAG	UNP P60802
B	-1	ASN	-	EXPRESSION TAG	UNP P60802
B	0	ALA	-	EXPRESSION TAG	UNP P60802
C	-2	SER	-	EXPRESSION TAG	UNP P60802
C	-1	ASN	-	EXPRESSION TAG	UNP P60802
C	0	ALA	-	EXPRESSION TAG	UNP P60802
D	-2	SER	-	EXPRESSION TAG	UNP P60802
D	-1	ASN	-	EXPRESSION TAG	UNP P60802
D	0	ALA	-	EXPRESSION TAG	UNP P60802
E	-2	SER	-	EXPRESSION TAG	UNP P60802

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP P60802
E	0	ALA	-	EXPRESSION TAG	UNP P60802
F	-2	SER	-	EXPRESSION TAG	UNP P60802
F	-1	ASN	-	EXPRESSION TAG	UNP P60802
F	0	ALA	-	EXPRESSION TAG	UNP P60802
G	-2	SER	-	EXPRESSION TAG	UNP P60802
G	-1	ASN	-	EXPRESSION TAG	UNP P60802
G	0	ALA	-	EXPRESSION TAG	UNP P60802
H	-2	SER	-	EXPRESSION TAG	UNP P60802
H	-1	ASN	-	EXPRESSION TAG	UNP P60802
H	0	ALA	-	EXPRESSION TAG	UNP P60802

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

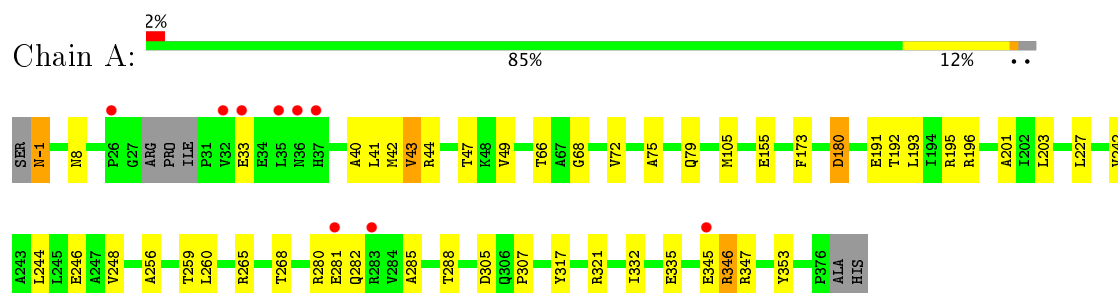
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	79	Total	O	0	3
			79	79		
3	C	78	Total	O	0	0
			78	78		
3	D	62	Total	O	0	0
			62	62		
3	E	91	Total	O	0	1
			91	91		
3	F	84	Total	O	0	1
			85	85		
3	G	47	Total	O	0	1
			48	48		
3	H	36	Total	O	0	0
			36	36		

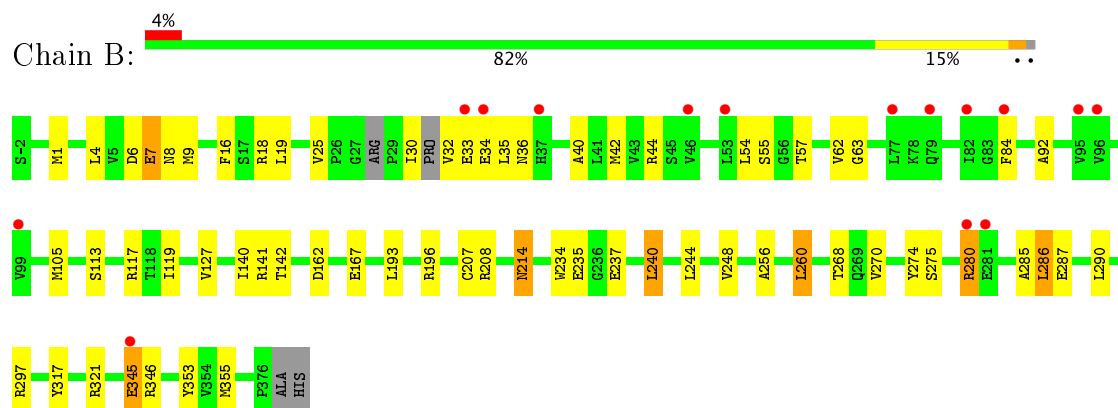
3 Residue-property plots

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

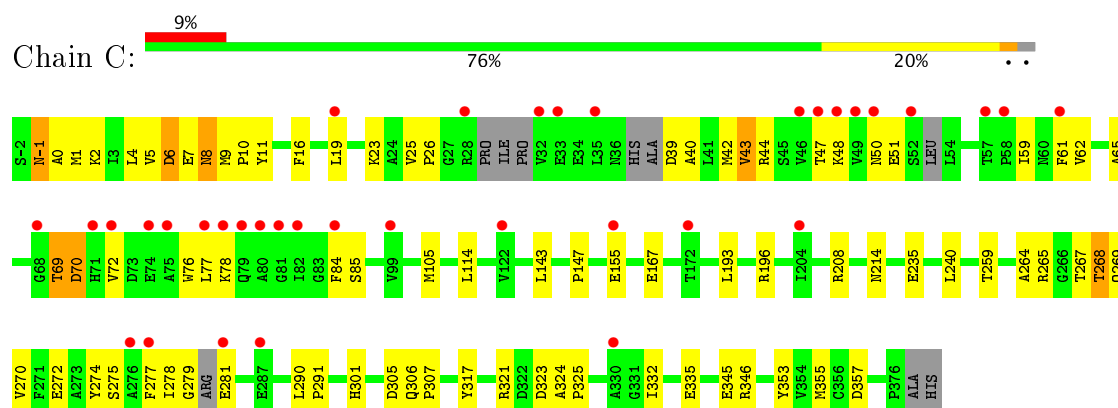
- Molecule 1: Erythronate-4-phosphate dehydrogenase



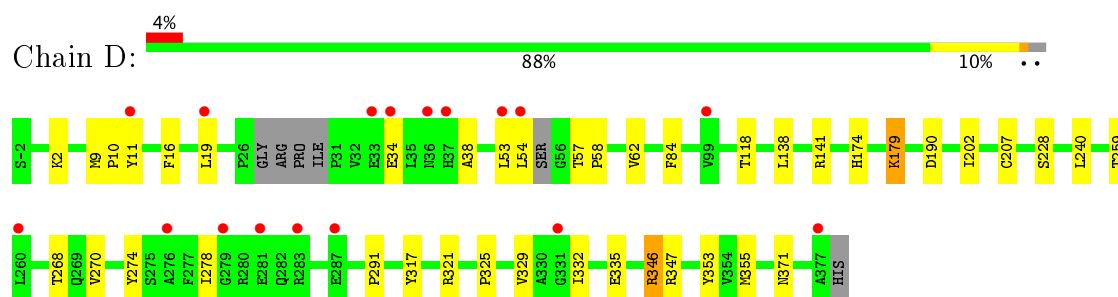
- Molecule 1: Erythronate-4-phosphate dehydrogenase



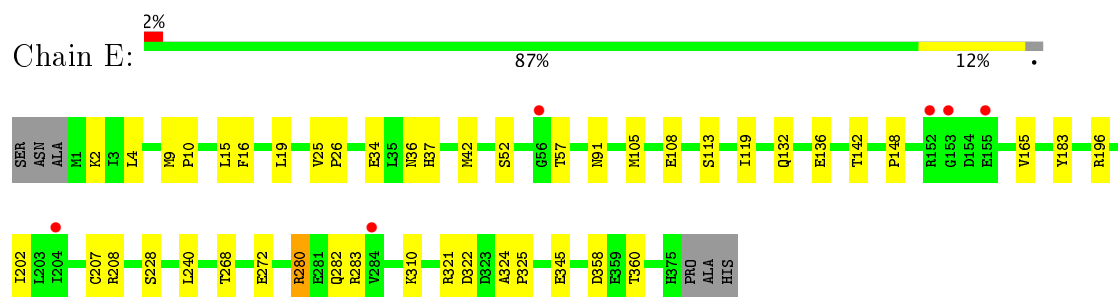
- Molecule 1: Erythronate-4-phosphate dehydrogenase



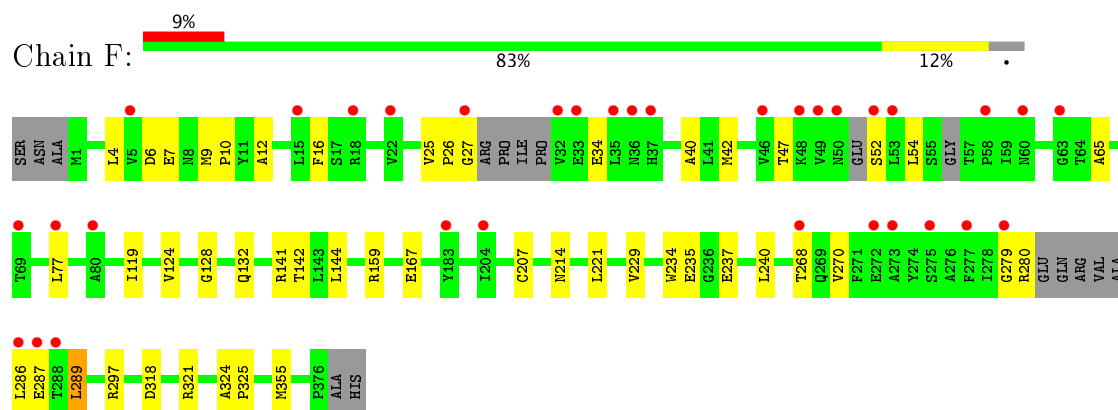
- Molecule 1: Erythronate-4-phosphate dehydrogenase



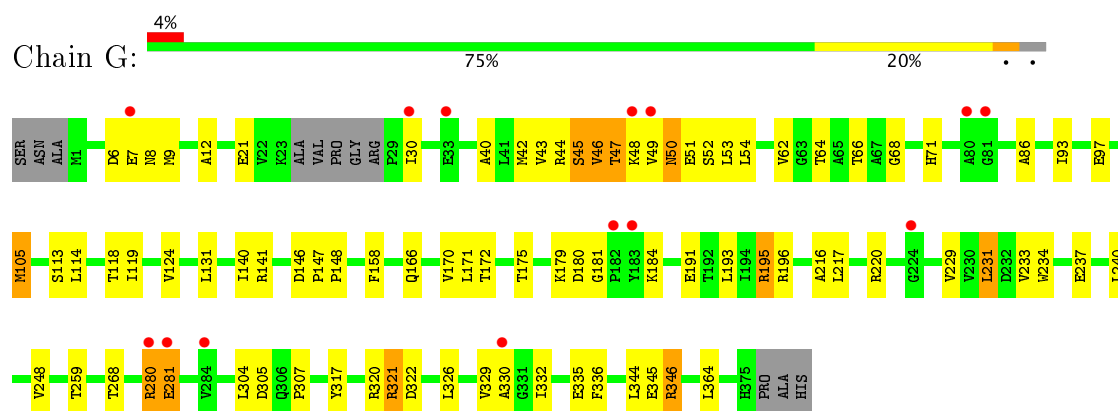
- Molecule 1: Erythronate-4-phosphate dehydrogenase



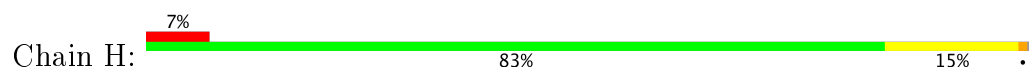
- Molecule 1: Erythronate-4-phosphate dehydrogenase

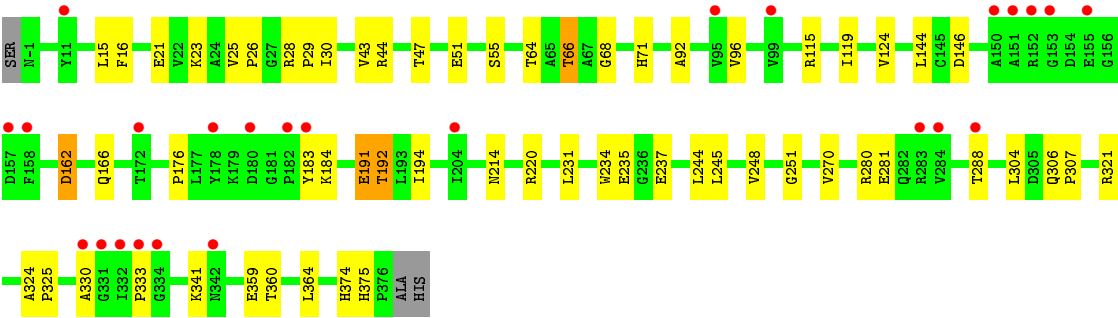


- Molecule 1: Erythronate-4-phosphate dehydrogenase



- Molecule 1: Erythronate-4-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 167.76Å 103.95Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	30.19 – 2.36 30.19 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.19-2.36) 98.7 (30.19-2.36)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.253 0.189 , 0.253	Depositor DCC
R_{free} test set	6469 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23835	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
NAD

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	0.61	0/2937	0.72	0/3981
1	B	0.64	0/2942	0.74	0/3989
1	C	0.63	0/2910	0.72	0/3942
1	D	0.64	0/2915	0.71	0/3953
1	E	0.66	1/2931 (0.0%)	0.71	0/3977
1	F	0.63	0/2837	0.69	0/3846
1	G	0.57	0/2891	0.67	0/3919
1	H	0.54	0/2948	0.64	0/4000
All	All	0.61	1/23311 (0.0%)	0.70	0/31607

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	345	GLU	CG-CD	5.42	1.60	1.51

There are no bond angle outliers.

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	2888	0	2914	40	0
1	B	2894	0	2904	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2865	0	2863	67	0
1	D	2867	0	2883	23	0
1	E	2880	0	2906	26	0
1	F	2791	0	2803	31	0
1	G	2843	0	2864	63	0
1	H	2897	0	2929	41	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	3	0
2	F	44	0	26	1	0
2	G	44	0	26	2	0
2	H	44	0	26	2	0
3	A	79	0	0	1	0
3	B	79	0	0	2	0
3	C	78	0	0	5	0
3	D	62	0	0	2	0
3	E	91	0	0	1	0
3	F	85	0	0	3	0
3	G	48	0	0	1	0
3	H	36	0	0	1	0
All	All	23835	0	23274	329	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 7.

All (329) 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:43:VAL:HG22	1:C:44:ARG:H	1.07	1.17
1:H:43:VAL:HG21	1:H:47:THR:HB	1.28	1.15
1:C:4:LEU:HD22	1:C:23:LYS:HB3	1.40	1.02
1:C:9:MSE:HE3	1:C:65:ALA:HB2	1.44	0.97
1:C:265:ARG:HG2	1:C:269:GLN:HE21	1.33	0.92
1:A:43:VAL:HG21	1:A:47:THR:HB	1.52	0.90
1:G:64:THR:OG1	1:G:66:THR:HG22	1.73	0.89
1:G:43:VAL:HG22	1:G:44:ARG:O	1.72	0.88
1:F:16:PHE:HZ	1:F:270:VAL:HG12	1.38	0.88
1:C:43:VAL:HG22	1:C:44:ARG:N	1.89	0.87
1:B:32:VAL:HA	1:B:35:LEU:HD12	1.62	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:344:LEU:HG	1:G:345:GLU:N	1.94	0.81
1:A:259:THR:HG22	1:A:346[A]:ARG:HG2	1.64	0.79
1:G:118:THR:HG23	1:G:141:ARG:HG2	1.63	0.78
1:H:25:VAL:HG11	1:H:30:ILE:HG23	1.67	0.77
1:A:66:THR:HG22	1:A:68:GLY:H	1.48	0.76
1:D:274:TYR:CZ	1:D:278:ILE:HD11	2.20	0.76
1:B:140:ILE:O	1:B:142:THR:HG23	1.85	0.76
1:G:43:VAL:HG23	1:G:47:THR:HG23	1.66	0.75
1:B:280:ARG:HG3	1:B:280:ARG:HH21	1.52	0.74
1:A:43:VAL:HG21	1:A:47:THR:CB	2.18	0.74
1:B:317:TYR:CD1	1:B:346[B]:ARG:HD2	2.23	0.73
1:C:43:VAL:CG2	1:C:44:ARG:H	1.88	0.73
1:C:2:LYS:O	1:C:39:ASP:HB3	1.88	0.73
1:H:43:VAL:CG2	1:H:47:THR:HB	2.13	0.73
1:H:43:VAL:HG22	1:H:44:ARG:O	1.89	0.73
1:A:256:ALA:O	1:A:346[B]:ARG:NH2	2.20	0.73
1:B:285:ALA:HB1	1:B:287:GLU:OE2	1.88	0.72
1:C:259:THR:HG22	1:C:346:ARG:HG2	1.70	0.72
1:C:9:MSE:HE2	1:C:267:THR:HG23	1.69	0.72
1:H:43:VAL:HG21	1:H:47:THR:CB	2.15	0.71
1:G:259:THR:HG22	1:G:346:ARG:HG2	1.74	0.70
1:C:9:MSE:HE3	1:C:65:ALA:CB	2.20	0.69
1:A:317:TYR:CD1	1:A:346[A]:ARG:HD3	2.28	0.69
1:E:105:MSE:HE2	3:E:425:HOH:O	1.91	0.68
1:G:317:TYR:CD1	1:G:346:ARG:HD3	2.28	0.68
1:C:240:LEU:HD12	1:C:240:LEU:C	2.15	0.67
1:B:317:TYR:CD1	1:B:346[A]:ARG:HD3	2.30	0.67
1:F:324:ALA:HB3	1:F:325:PRO:HD3	1.77	0.66
1:D:291:PRO:O	1:D:347:ARG:NH2	2.29	0.65
1:B:280:ARG:NH2	1:B:280:ARG:HG3	2.11	0.65
1:C:306:GLN:HB3	1:C:307:PRO:HD3	1.78	0.65
3:C:398:HOH:O	1:F:318:ASP:HB3	1.97	0.65
1:H:43:VAL:HG22	1:H:44:ARG:N	2.12	0.65
1:C:4:LEU:CD2	1:C:23:LYS:HB3	2.21	0.65
1:G:43:VAL:CG2	1:G:47:THR:HG23	2.27	0.65
1:C:301:HIS:ND1	1:C:357:ASP:OD2	2.22	0.64
1:F:4:LEU:HD11	1:F:34:GLU:HB3	1.79	0.64
1:G:240:LEU:O	1:G:240:LEU:HD12	1.98	0.64
1:G:93:ILE:O	1:G:97:GLU:HG3	1.98	0.64
1:C:317:TYR:CG	1:C:346:ARG:HD2	2.33	0.64
1:A:75:ALA:O	1:A:79:GLN:HG3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:THR:HG22	1:D:346:ARG:HG2	1.80	0.63
1:B:162:ASP:OD1	1:B:196:ARG:NH1	2.31	0.63
1:A:285:ALA:HB3	1:A:288:THR:HG23	1.81	0.62
1:A:180:ASP:HB3	3:A:418:HOH:O	1.98	0.62
1:E:202:ILE:HG12	1:E:228:SER:HB2	1.82	0.62
1:A:201:ALA:O	1:A:227:LEU:HD12	2.00	0.62
1:B:141:ARG:NH2	1:B:167:GLU:OE1	2.27	0.62
1:G:240:LEU:C	1:G:240:LEU:HD12	2.21	0.61
1:C:43:VAL:HG21	1:C:47:THR:OG1	2.00	0.61
1:G:64:THR:OG1	1:G:66:THR:CG2	2.47	0.61
1:A:191:GLU:OE2	1:A:195:ARG:NH2	2.23	0.61
1:A:353:TYR:HH	1:B:353:TYR:HH	1.49	0.61
1:C:69[B]:THR:O	1:C:70[B]:ASP:C	2.38	0.60
1:A:244:LEU:O	1:A:248:VAL:HG13	2.01	0.60
1:E:280:ARG:O	1:E:282:GLN:HG3	2.03	0.59
1:G:50:ASN:HD22	1:G:50:ASN:N	2.00	0.59
1:G:9:MSE:HG3	1:G:12:ALA:HB2	1.84	0.58
1:F:9:MSE:HB3	1:F:12:ALA:HB2	1.85	0.58
1:C:39:ASP:O	1:C:59:ILE:HA	2.03	0.58
1:A:49:VAL:HB	1:A:72:VAL:HG13	1.85	0.58
1:H:234:TRP:O	1:H:237:GLU:HG3	2.04	0.58
1:C:275:SER:O	1:C:281:GLU:N	2.37	0.58
1:C:51:GLU:HG3	1:C:76:TRP:CE2	2.39	0.58
1:B:42:MSE:HA	1:B:63:GLY:O	2.05	0.57
1:G:326:LEU:O	1:G:330:ALA:HB2	2.04	0.57
1:C:61:PHE:HB3	1:C:274:TYR:HE1	1.69	0.57
1:D:16:PHE:HZ	1:D:270:VAL:HG12	1.68	0.57
1:E:4:LEU:HD21	1:E:34:GLU:HG3	1.87	0.57
1:G:217:LEU:HD21	1:G:229:VAL:HG11	1.85	0.57
1:F:279:GLY:O	1:F:280:ARG:HG3	2.05	0.56
1:G:6:ASP:OD2	1:G:8:ASN:HB2	2.05	0.56
1:C:290:LEU:HB3	1:C:291:PRO:HD2	1.87	0.56
1:G:234:TRP:O	1:G:237:GLU:HG3	2.06	0.56
1:A:317:TYR:CD1	1:A:346[B]:ARG:HD2	2.41	0.56
1:G:166:GLN:HE21	1:G:196:ARG:HH22	1.53	0.56
1:C:7:GLU:N	1:C:25:VAL:O	2.37	0.56
1:G:21:GLU:OE2	1:H:23:LYS:HD3	2.06	0.56
1:B:16:PHE:HZ	1:B:270:VAL:HG12	1.71	0.55
1:H:16:PHE:HZ	1:H:270:VAL:HG12	1.72	0.55
1:H:306:GLN:HB3	1:H:307:PRO:HD3	1.89	0.55
1:E:16:PHE:CE1	1:E:42:MSE:HE3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:ALA:O	1:H:96:VAL:HG23	2.07	0.55
1:F:287:GLU:HG2	1:F:287:GLU:O	2.07	0.55
1:G:166:GLN:HE21	1:G:196:ARG:NH2	2.04	0.55
1:G:231:LEU:HD22	1:G:248:VAL:HG11	1.89	0.55
1:F:286:LEU:HD23	1:F:289:LEU:HD12	1.87	0.55
1:C:9:MSE:CE	1:C:65:ALA:HB2	2.28	0.55
1:F:6:ASP:OD2	1:F:27:GLY:HA3	2.08	0.54
1:C:196:ARG:HD3	3:C:428:HOH:O	2.06	0.54
1:F:9:MSE:HE2	1:F:65:ALA:HB3	1.90	0.54
1:F:40:ALA:HB1	1:F:42:MSE:HE2	1.89	0.54
1:C:72:VAL:HG11	1:C:84:PHE:CE1	2.43	0.54
1:E:165:VAL:HG11	1:E:196:ARG:NH1	2.23	0.54
1:A:317:TYR:CE1	1:A:346[B]:ARG:HD2	2.43	0.54
1:A:242:VAL:O	1:A:246:GLU:HG2	2.07	0.53
1:B:62:VAL:O	1:B:84:PHE:HA	2.08	0.53
1:C:193:LEU:HD23	1:C:193:LEU:C	2.29	0.53
1:D:53:LEU:O	1:D:54:LEU:HG	2.08	0.53
1:B:287:GLU:CD	1:B:287:GLU:H	2.12	0.53
1:C:332:ILE:HB	1:C:335:GLU:HG3	1.90	0.53
1:G:332:ILE:HG22	1:G:335:GLU:HG2	1.91	0.53
1:G:66:THR:HG23	1:G:68:GLY:O	2.09	0.53
1:E:240:LEU:C	1:E:240:LEU:HD12	2.29	0.53
1:B:286:LEU:HD13	1:B:290:LEU:HD11	1.90	0.52
1:G:119:ILE:HG12	1:G:170:VAL:HB	1.91	0.52
1:C:48:LYS:HG3	3:C:419:HOH:O	2.08	0.52
1:H:304:LEU:HD23	1:H:364:LEU:HD23	1.91	0.52
1:F:4:LEU:CD1	1:F:34:GLU:HB3	2.39	0.52
1:C:277:PHE:C	1:C:277:PHE:CD2	2.83	0.52
1:C:51:GLU:HG3	1:C:76:TRP:NE1	2.24	0.52
1:E:240:LEU:HD12	1:E:240:LEU:O	2.10	0.52
1:G:48:LYS:O	1:G:50:ASN:ND2	2.42	0.52
1:H:25:VAL:HG12	1:H:26:PRO:O	2.09	0.52
1:A:285:ALA:CB	1:A:288:THR:HG23	2.40	0.52
1:G:105:MSE:HE2	1:G:320:ARG:HD3	1.91	0.52
1:B:260:LEU:HD13	1:B:345:GLU:HB2	1.92	0.52
1:C:77:LEU:HD23	1:C:84:PHE:HB2	1.92	0.52
1:E:324:ALA:HB3	1:E:325:PRO:HD3	1.92	0.52
1:B:4:LEU:HD21	1:B:34:GLU:CG	2.40	0.51
1:B:40:ALA:HB2	1:B:274:TYR:OH	2.09	0.51
1:G:43:VAL:HG22	1:G:44:ARG:N	2.24	0.51
1:E:108:GLU:OE2	1:E:310:LYS:HE3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:GLU:HG3	1:H:192:THR:N	2.25	0.51
1:B:297:ARG:HB3	1:B:355:MSE:HE2	1.91	0.51
1:B:260:LEU:HD13	1:B:345:GLU:CB	2.40	0.51
1:D:2:LYS:HB3	1:D:38:ALA:HA	1.92	0.51
1:C:143:LEU:HD23	1:H:333:PRO:HG2	1.92	0.51
1:G:166:GLN:NE2	1:G:196:ARG:HH22	2.09	0.51
1:F:16:PHE:CZ	1:F:270:VAL:HG12	2.30	0.50
1:B:7:GLU:HB3	1:B:25:VAL:O	2.11	0.50
1:G:54:LEU:HD11	1:G:62:VAL:HG21	1.94	0.50
1:H:244:LEU:O	1:H:248:VAL:HG13	2.12	0.50
1:G:49:VAL:HG21	1:G:62:VAL:HG11	1.93	0.50
1:D:57:THR:HB	1:D:58:PRO:CD	2.42	0.49
1:B:244:LEU:O	1:B:248:VAL:HG13	2.12	0.49
1:C:40:ALA:HB2	1:C:274:TYR:OH	2.12	0.49
1:E:19:LEU:C	1:E:19:LEU:HD12	2.33	0.49
1:H:162:ASP:O	1:H:166:GLN:HG3	2.12	0.49
1:G:216:ALA:O	1:G:220:ARG:HG2	2.12	0.49
1:H:25:VAL:HG13	1:H:26:PRO:HD2	1.94	0.49
1:H:146:ASP:OD2	2:H:379:NAD:H1B	2.13	0.49
1:C:240:LEU:O	1:C:240:LEU:HD12	2.12	0.49
1:G:45:SER:HA	1:G:71:HIS:CE1	2.48	0.49
1:H:183:TYR:O	1:H:184:LYS:C	2.51	0.49
1:H:64:THR:HG23	1:H:66:THR:HG22	1.95	0.49
1:C:317:TYR:CD1	1:C:346:ARG:CD	2.96	0.49
1:G:30:ILE:HD11	1:G:47:THR:HG21	1.95	0.49
1:A:8:ASN:HB2	1:A:44:ARG:NH1	2.28	0.48
1:C:-1:ASN:OD1	1:C:-1:ASN:N	2.45	0.48
1:C:355:MSE:HE1	3:F:386:HOH:O	2.13	0.48
1:H:66:THR:HG23	1:H:68:GLY:O	2.13	0.48
1:H:43:VAL:CG2	1:H:44:ARG:N	2.76	0.48
1:A:285:ALA:HB3	1:A:288:THR:CG2	2.43	0.48
1:B:8:ASN:HB2	1:B:44:ARG:NH1	2.29	0.48
1:C:324:ALA:HB3	1:C:325:PRO:HD3	1.95	0.48
1:E:36:ASN:OD1	1:E:57:THR:HG22	2.14	0.48
1:G:124:VAL:HG23	1:G:146:ASP:HB2	1.96	0.48
1:G:147:PRO:HB2	1:G:148:PRO:HD3	1.96	0.48
1:G:51:GLU:C	1:G:53:LEU:H	2.17	0.48
1:B:4:LEU:HD21	1:B:34:GLU:HG3	1.95	0.48
1:C:16:PHE:HZ	1:C:270:VAL:HG12	1.79	0.47
1:C:317:TYR:CD1	1:C:346:ARG:HD3	2.48	0.47
1:C:61:PHE:HD2	1:C:277:PHE:CD1	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ILE:HB	1:D:335:GLU:HG3	1.96	0.47
1:A:43:VAL:CG2	1:A:47:THR:HB	2.36	0.47
1:H:214:ASN:ND2	3:H:385:HOH:O	2.33	0.47
1:A:41:LEU:C	1:A:41:LEU:HD23	2.34	0.47
1:B:317:TYR:CE1	1:B:346[B]:ARG:HD2	2.49	0.47
1:C:277:PHE:HD2	1:C:278:ILE:HG23	1.80	0.47
1:C:48:LYS:HE3	3:C:419:HOH:O	2.13	0.47
1:D:62:VAL:O	1:D:84:PHE:HA	2.15	0.47
1:E:25:VAL:HG22	1:E:26:PRO:HD2	1.95	0.47
1:A:40:ALA:HB1	1:A:42:MSE:HE2	1.96	0.47
1:C:345:GLU:HA	3:C:436:HOH:O	2.15	0.47
1:G:233:VAL:HA	1:G:237:GLU:OE2	2.15	0.47
1:F:9:MSE:HE2	1:F:65:ALA:CB	2.45	0.47
1:A:-1:ASN:OD1	1:A:-1:ASN:N	2.39	0.47
1:C:305:ASP:OD1	1:C:307:PRO:HD2	2.15	0.47
1:C:6:ASP:OD1	1:C:8:ASN:N	2.43	0.46
1:D:274:TYR:CE2	1:D:278:ILE:HD11	2.50	0.46
1:D:317:TYR:CD1	1:D:346:ARG:HD3	2.50	0.46
1:B:54:LEU:O	1:B:55:SER:C	2.54	0.46
1:G:131:LEU:HD21	1:G:172:THR:HG21	1.97	0.46
1:G:317:TYR:CD1	1:G:346:ARG:CD	2.97	0.46
1:D:57:THR:HB	1:D:58:PRO:HD2	1.98	0.46
1:E:358:ASP:OD1	1:E:360:THR:OG1	2.30	0.46
1:B:18:ARG:O	1:B:19:LEU:HD23	2.16	0.46
1:G:44:ARG:O	1:G:46:VAL:N	2.49	0.46
1:H:43:VAL:CG2	1:H:47:THR:CB	2.86	0.46
1:C:264:ALA:HB2	1:C:290:LEU:HD21	1.98	0.46
1:A:260:LEU:HD13	1:A:345:GLU:HG3	1.96	0.46
1:A:346[A]:ARG:HG3	1:A:347:ARG:N	2.31	0.46
1:C:10:PRO:HB2	1:C:11:TYR:CD2	2.50	0.46
1:G:7:GLU:CG	1:G:7:GLU:O	2.64	0.46
1:C:279:GLY:C	1:C:281:GLU:N	2.70	0.46
1:A:332:ILE:HB	1:A:335:GLU:HG3	1.97	0.46
1:B:207:CYS:SG	1:B:208:ARG:N	2.89	0.45
1:C:61:PHE:CD1	1:C:61:PHE:C	2.89	0.45
1:C:5:VAL:HG12	1:C:42:MSE:HB2	1.98	0.45
1:E:2:LYS:HD2	1:E:37:HIS:O	2.15	0.45
1:G:329:VAL:HA	1:G:332:ILE:HD12	1.98	0.45
1:B:40:ALA:HB1	1:B:42:MSE:HE2	1.98	0.45
1:F:240:LEU:HD12	1:F:240:LEU:C	2.37	0.45
1:G:40:ALA:HB1	1:G:42:MSE:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:VAL:HG21	1:H:144:LEU:HB3	1.98	0.45
1:H:245:LEU:HD23	1:H:330:ALA:CB	2.46	0.45
1:E:207:CYS:HB2	2:E:379:NAD:H4D	1.99	0.45
1:G:280:ARG:O	1:G:281:GLU:C	2.55	0.45
1:H:66:THR:HG21	1:H:71:HIS:HE1	1.82	0.45
1:H:324:ALA:HB3	1:H:325:PRO:HD3	1.98	0.45
1:B:1:MSE:HE3	3:B:457:HOH:O	2.15	0.44
1:E:119:ILE:O	1:E:142:THR:HA	2.17	0.44
1:F:297:ARG:NH1	3:F:386:HOH:O	2.50	0.44
1:G:147:PRO:HD2	2:G:379:NAD:C2A	2.48	0.44
1:G:191:GLU:O	1:G:195:ARG:HB3	2.16	0.44
1:A:41:LEU:HD23	1:A:42:MSE:N	2.33	0.44
1:B:117:ARG:NH1	3:B:385:HOH:O	2.28	0.44
1:B:275:SER:O	1:B:280:ARG:N	2.51	0.44
1:E:132:GLN:O	1:E:136:GLU:HG3	2.17	0.44
1:F:119:ILE:O	1:F:142:THR:HA	2.17	0.44
1:E:207:CYS:SG	1:E:208:ARG:N	2.89	0.44
1:A:43:VAL:CG2	1:A:47:THR:CB	2.94	0.44
1:F:355:MSE:HE1	3:F:386:HOH:O	2.18	0.44
1:H:280:ARG:O	1:H:281:GLU:C	2.55	0.44
1:D:118:THR:HG23	1:D:141:ARG:HG2	2.00	0.44
1:F:4:LEU:HD11	1:F:34:GLU:CB	2.47	0.44
1:B:317:TYR:CG	1:B:346[A]:ARG:HD3	2.52	0.43
1:D:10:PRO:O	1:D:11:TYR:HB2	2.18	0.43
1:F:214:ASN:ND2	1:F:235:GLU:H	2.16	0.43
1:C:51:GLU:CG	1:C:76:TRP:CE2	3.01	0.43
1:D:174:HIS:HA	1:D:207:CYS:HB3	1.99	0.43
1:B:92:ALA:HA	1:B:127:VAL:HG22	2.00	0.43
1:C:214:ASN:ND2	1:C:235:GLU:H	2.17	0.43
1:G:304:LEU:HD23	1:G:364:LEU:HD23	2.00	0.43
1:C:268:THR:O	1:C:272:GLU:HG3	2.19	0.43
1:C:317:TYR:CD1	1:C:346:ARG:HD2	2.53	0.43
1:D:325:PRO:O	1:D:329:VAL:HG22	2.19	0.43
1:G:193:LEU:HD23	1:G:193:LEU:C	2.39	0.43
1:F:234:TRP:HB2	1:F:237:GLU:HG3	2.00	0.43
1:A:265:ARG:HA	1:A:268:THR:HB	2.01	0.43
1:B:214:ASN:HB2	1:B:235:GLU:OE1	2.19	0.43
1:B:256:ALA:O	1:B:346[B]:ARG:NH1	2.45	0.43
1:D:9:MSE:HA	1:D:10:PRO:HD3	1.85	0.43
1:D:190:ASP:HB2	3:D:419:HOH:O	2.19	0.43
1:E:321:ARG:HD2	1:E:322:ASP:OD1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:GLU:CD	1:F:26:PRO:HA	2.39	0.43
1:A:66:THR:HG22	1:A:68:GLY:N	2.27	0.43
1:D:353:TYR:HA	1:D:371:ASN:O	2.19	0.43
1:E:15:LEU:HA	1:E:15:LEU:HD23	1.89	0.43
1:G:240:LEU:CD1	1:G:240:LEU:C	2.86	0.43
1:H:245:LEU:CD2	1:H:330:ALA:CB	2.97	0.42
1:A:192:THR:O	1:A:196:ARG:HG3	2.19	0.42
1:C:155:GLU:OE1	1:H:341:LYS:NZ	2.52	0.42
1:F:279:GLY:C	1:F:280:ARG:HG3	2.38	0.42
1:G:114:LEU:HB3	1:G:140:ILE:HD11	2.00	0.42
1:C:0:ALA:C	1:C:1:MSE:HE2	2.40	0.42
1:F:54:LEU:HD12	1:F:77:LEU:HD21	2.01	0.42
1:G:175:THR:HG22	2:G:379:NAD:C4A	2.49	0.42
1:G:7:GLU:O	1:G:7:GLU:HG3	2.20	0.42
1:B:234:TRP:HB2	1:B:237:GLU:HG3	2.01	0.42
1:G:158:PHE:HB3	3:G:498:HOH:O	2.19	0.42
1:G:317:TYR:CG	1:G:346:ARG:HD2	2.54	0.42
1:B:30:ILE:HG21	1:B:35:LEU:HD21	2.01	0.42
1:E:9:MSE:HA	1:E:10:PRO:HD3	1.94	0.42
1:A:33:GLU:HA	1:A:33:GLU:OE1	2.19	0.42
1:C:274:TYR:O	1:C:278:ILE:HG12	2.19	0.42
1:F:207:CYS:HB2	2:F:379:NAD:H4D	2.02	0.42
1:H:194:ILE:CG2	1:H:220:ARG:HG3	2.49	0.42
1:A:280:ARG:O	1:A:282:GLN:HG3	2.20	0.42
1:B:193:LEU:HD23	1:B:193:LEU:C	2.40	0.42
1:E:207:CYS:HA	2:E:379:NAD:H1D	2.01	0.42
1:G:180:ASP:HB2	1:G:181:GLY:H	1.73	0.42
1:A:173:PHE:HE1	1:A:203:LEU:HD11	1.85	0.42
1:G:179:LYS:O	1:G:184:LYS:HG3	2.20	0.42
1:G:305:ASP:CG	1:G:307:PRO:HD2	2.40	0.42
1:F:159:ARG:HB3	1:F:159:ARG:HE	1.73	0.41
1:A:259:THR:HG22	1:A:346[B]:ARG:HG2	2.03	0.41
1:F:9:MSE:HA	1:F:10:PRO:HD3	1.90	0.41
1:H:214:ASN:ND2	1:H:235:GLU:H	2.18	0.41
1:H:51:GLU:O	1:H:55:SER:HB2	2.20	0.41
1:E:148:PRO:HG3	1:E:183:TYR:CG	2.55	0.41
1:F:141:ARG:NH2	1:F:167:GLU:OE1	2.47	0.41
1:A:40:ALA:HB1	1:A:42:MSE:CE	2.50	0.41
1:B:6:ASP:HB3	1:B:9:MSE:HE3	2.00	0.41
1:G:321:ARG:NH1	1:G:322:ASP:OD1	2.53	0.41
1:G:336:PHE:CD2	1:G:336:PHE:C	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:359:GLU:HB2	1:H:374:HIS:CE1	2.56	0.41
1:B:36:ASN:HA	1:B:57:THR:HG22	2.01	0.41
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.93	0.41
1:C:61:PHE:HB3	1:C:274:TYR:CE1	2.53	0.41
1:E:91:ASN:OD1	2:E:379:NAD:H5N	2.21	0.41
1:A:193:LEU:C	1:A:193:LEU:HD23	2.40	0.41
1:F:124:VAL:HA	1:F:128:GLY:HA3	2.02	0.41
1:A:317:TYR:CG	1:A:346[A]:ARG:CD	3.04	0.41
1:C:25:VAL:HG12	1:C:26:PRO:O	2.21	0.41
1:H:15:LEU:HD12	1:H:15:LEU:HA	1.86	0.41
1:H:176:PRO:HD3	2:H:379:NAD:H52A	2.03	0.41
1:C:353:TYR:HE2	1:C:355:MSE:SE	2.53	0.41
1:C:50:ASN:O	1:C:51:GLU:C	2.57	0.41
1:F:132:GLN:NE2	1:F:144:LEU:HD11	2.36	0.40
1:F:221:LEU:HD11	1:F:229:VAL:HG21	2.02	0.40
1:A:305:ASP:OD1	1:A:307:PRO:HD2	2.21	0.40
1:C:264:ALA:CB	1:C:290:LEU:HD21	2.52	0.40
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.92	0.40
1:G:171:LEU:HA	1:G:171:LEU:HD12	1.91	0.40
1:G:234:TRP:CD2	1:G:240:LEU:HD22	2.56	0.40
1:H:245:LEU:CD2	1:H:330:ALA:HB2	2.51	0.40
1:C:147:PRO:HD2	2:C:379:NAD:C2A	2.52	0.40
1:D:179:LYS:NZ	3:D:409:HOH:O	2.54	0.40
1:G:64:THR:HG23	1:G:86:ALA:HA	2.03	0.40
1:H:231:LEU:O	1:H:251:GLY:HA2	2.20	0.40
1:C:61:PHE:CD1	1:C:62:VAL:N	2.90	0.40
1:D:202:ILE:HG12	1:D:228:SER:HB2	2.02	0.40
1:D:353:TYR:CE2	1:D:355:MSE:HG2	2.56	0.40
1:E:272:GLU:OE2	1:E:283:ARG:HG3	2.20	0.40
1:H:28:ARG:HA	1:H:29:PRO:HA	1.85	0.40
1:B:240:LEU:O	1:B:240:LEU:HD12	2.21	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	372/381 (98%)	360 (97%)	12 (3%)	0	100	100
1	B	372/381 (98%)	352 (95%)	20 (5%)	0	100	100
1	C	365/381 (96%)	341 (93%)	21 (6%)	3 (1%)	22	24
1	D	369/381 (97%)	352 (95%)	17 (5%)	0	100	100
1	E	373/381 (98%)	358 (96%)	15 (4%)	0	100	100
1	F	355/381 (93%)	339 (96%)	16 (4%)	0	100	100
1	G	366/381 (96%)	341 (93%)	22 (6%)	3 (1%)	22	24
1	H	376/381 (99%)	354 (94%)	22 (6%)	0	100	100
All	All	2948/3048 (97%)	2797 (95%)	145 (5%)	6 (0%)	51	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	45	SER
1	C	70[A]	ASP
1	C	70[B]	ASP
1	G	52	SER
1	G	281	GLU
1	C	43	VAL

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	303/303 (100%)	294 (97%)	9 (3%)	46	58
1	B	303/303 (100%)	290 (96%)	13 (4%)	33	42
1	C	299/303 (99%)	285 (95%)	14 (5%)	30	38
1	D	299/303 (99%)	292 (98%)	7 (2%)	56	68
1	E	303/303 (100%)	299 (99%)	4 (1%)	73	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	291/303 (96%)	285 (98%)	6 (2%)	59	72
1	G	298/303 (98%)	287 (96%)	11 (4%)	39	50
1	H	303/303 (100%)	292 (96%)	11 (4%)	40	51
All	All	2399/2424 (99%)	2324 (97%)	75 (3%)	46	56

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	43	VAL
1	A	105	MSE
1	A	155	GLU
1	A	180	ASP
1	A	281	GLU
1	A	321	ARG
1	A	346[A]	ARG
1	A	346[B]	ARG
1	B	7	GLU
1	B	33	GLU
1	B	105	MSE
1	B	113	SER
1	B	119	ILE
1	B	214	ASN
1	B	240	LEU
1	B	260	LEU
1	B	268	THR
1	B	280	ARG
1	B	286	LEU
1	B	321	ARG
1	B	345	GLU
1	C	-1	ASN
1	C	6	ASP
1	C	8	ASN
1	C	19	LEU
1	C	69[A]	THR
1	C	69[B]	THR
1	C	78	LYS
1	C	85	SER
1	C	105	MSE
1	C	167	GLU
1	C	208	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	268	THR
1	C	321	ARG
1	C	323	ASP
1	D	19	LEU
1	D	34	GLU
1	D	179	LYS
1	D	240	LEU
1	D	268	THR
1	D	321	ARG
1	D	346	ARG
1	E	52	SER
1	E	113	SER
1	E	268	THR
1	E	280	ARG
1	F	25	VAL
1	F	47	THR
1	F	52	SER
1	F	268	THR
1	F	289	LEU
1	F	321	ARG
1	G	46	VAL
1	G	47	THR
1	G	50	ASN
1	G	105	MSE
1	G	113	SER
1	G	195	ARG
1	G	231	LEU
1	G	268	THR
1	G	280	ARG
1	G	321	ARG
1	G	346	ARG
1	H	21	GLU
1	H	66	THR
1	H	115	ARG
1	H	119	ILE
1	H	162	ASP
1	H	191	GLU
1	H	192	THR
1	H	288	THR
1	H	321	ARG
1	H	360	THR
1	H	375	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	B	166	GLN
1	C	269	GLN
1	D	269	GLN
1	E	375	HIS
1	F	214	ASN
1	G	50	ASN
1	G	166	GLN
1	G	214	ASN
1	H	166	GLN
1	H	214	ASN
1	H	374	HIS

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](#)

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	NAD	A	379	-	41,48,48	1.71	3 (7%)	43,73,73	1.58	3 (6%)
2	NAD	B	379	-	41,48,48	1.65	3 (7%)	43,73,73	1.89	3 (6%)
2	NAD	C	379	-	41,48,48	1.73	3 (7%)	43,73,73	1.79	6 (13%)
2	NAD	D	379	-	41,48,48	1.67	3 (7%)	43,73,73	1.74	3 (6%)
2	NAD	E	379	-	41,48,48	1.68	3 (7%)	43,73,73	1.91	4 (9%)
2	NAD	F	379	-	41,48,48	1.60	3 (7%)	43,73,73	2.12	7 (16%)
2	NAD	G	379	-	41,48,48	1.81	3 (7%)	43,73,73	1.92	3 (6%)
2	NAD	H	379	-	41,48,48	1.69	3 (7%)	43,73,73	1.70	2 (4%)

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	NAD	A	379	-	-	0/22/62/62	0/5/5/5
2	NAD	B	379	-	-	0/22/62/62	0/5/5/5
2	NAD	C	379	-	-	0/22/62/62	0/5/5/5
2	NAD	D	379	-	-	0/22/62/62	0/5/5/5
2	NAD	E	379	-	-	0/22/62/62	0/5/5/5
2	NAD	F	379	-	-	0/22/62/62	0/5/5/5
2	NAD	G	379	-	-	0/22/62/62	0/5/5/5
2	NAD	H	379	-	-	0/22/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	379	NAD	C2A-N1A	2.18	1.38	1.33
2	H	379	NAD	C2A-N1A	2.32	1.38	1.33
2	E	379	NAD	C2A-N1A	2.42	1.38	1.33
2	D	379	NAD	C2A-N1A	2.48	1.38	1.33
2	F	379	NAD	C2A-N1A	2.55	1.38	1.33
2	G	379	NAD	C2A-N1A	2.59	1.38	1.33
2	C	379	NAD	C2A-N1A	2.63	1.38	1.33
2	B	379	NAD	C2A-N1A	2.70	1.39	1.33
2	E	379	NAD	C2A-N3A	3.49	1.38	1.32
2	B	379	NAD	C2A-N3A	3.57	1.38	1.32
2	D	379	NAD	C2A-N3A	3.58	1.38	1.32
2	C	379	NAD	C2A-N3A	3.70	1.38	1.32
2	F	379	NAD	C2A-N3A	3.75	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	379	NAD	C2A-N3A	3.86	1.38	1.32
2	A	379	NAD	C2A-N3A	3.87	1.38	1.32
2	H	379	NAD	C2A-N3A	4.25	1.39	1.32
2	F	379	NAD	O7N-C7N	7.77	1.40	1.24
2	D	379	NAD	O7N-C7N	8.04	1.40	1.24
2	B	379	NAD	O7N-C7N	8.26	1.41	1.24
2	H	379	NAD	O7N-C7N	8.36	1.41	1.24
2	A	379	NAD	O7N-C7N	8.49	1.41	1.24
2	E	379	NAD	O7N-C7N	8.53	1.41	1.24
2	C	379	NAD	O7N-C7N	8.62	1.42	1.24
2	G	379	NAD	O7N-C7N	9.32	1.43	1.24

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	379	NAD	N3A-C2A-N1A	-10.70	119.54	128.86
2	B	379	NAD	N3A-C2A-N1A	-10.48	119.73	128.86
2	F	379	NAD	N3A-C2A-N1A	-10.44	119.77	128.86
2	E	379	NAD	N3A-C2A-N1A	-10.29	119.89	128.86
2	H	379	NAD	N3A-C2A-N1A	-9.56	120.53	128.86
2	D	379	NAD	N3A-C2A-N1A	-9.31	120.75	128.86
2	C	379	NAD	N3A-C2A-N1A	-9.15	120.89	128.86
2	A	379	NAD	N3A-C2A-N1A	-8.66	121.32	128.86
2	F	379	NAD	O7N-C7N-C3N	-3.68	115.33	119.62
2	E	379	NAD	O7N-C7N-C3N	-3.12	115.98	119.62
2	D	379	NAD	C4A-C5A-N7A	-3.03	106.48	109.41
2	F	379	NAD	O3D-C3D-C4D	-2.89	102.63	111.09
2	C	379	NAD	C4A-C5A-N7A	-2.88	106.63	109.41
2	G	379	NAD	C1B-N9A-C4A	-2.71	121.94	126.64
2	H	379	NAD	C4A-C5A-N7A	-2.67	106.83	109.41
2	G	379	NAD	O3D-C3D-C4D	-2.57	103.59	111.09
2	F	379	NAD	C4B-O4B-C1B	-2.50	107.11	109.77
2	E	379	NAD	C1B-N9A-C4A	-2.39	122.50	126.64
2	F	379	NAD	C4N-C3N-C7N	-2.35	114.82	121.07
2	C	379	NAD	O7N-C7N-C3N	-2.23	117.02	119.62
2	A	379	NAD	C4A-C5A-N7A	-2.13	107.35	109.41
2	B	379	NAD	O3D-C3D-C4D	-2.12	104.89	111.09
2	F	379	NAD	C1B-N9A-C4A	-2.10	123.01	126.64
2	B	379	NAD	C4B-O4B-C1B	-2.07	107.56	109.77
2	C	379	NAD	C1B-N9A-C4A	-2.06	123.08	126.64
2	C	379	NAD	O2N-PN-O1N	2.02	122.74	112.28
2	A	379	NAD	C3N-C7N-N7N	2.28	120.38	117.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	379	NAD	C3N-C7N-N7N	2.76	120.93	117.77
2	D	379	NAD	C3N-C7N-N7N	3.00	121.20	117.77
2	E	379	NAD	C3N-C7N-N7N	3.00	121.20	117.77
2	F	379	NAD	C3N-C7N-N7N	4.08	122.43	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	379	NAD	1	0
2	E	379	NAD	3	0
2	F	379	NAD	1	0
2	G	379	NAD	2	0
2	H	379	NAD	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	370/381 (97%)	0.02	9 (2%) 59 69	26, 41, 83, 116	0
1	B	372/381 (97%)	0.17	15 (4%) 39 51	22, 37, 86, 118	0
1	C	367/381 (96%)	0.31	36 (9%) 8 12	22, 37, 84, 99	0
1	D	370/381 (97%)	0.04	17 (4%) 33 45	23, 37, 91, 121	0
1	E	370/381 (97%)	-0.00	6 (1%) 72 81	23, 38, 59, 73	0
1	F	360/381 (94%)	0.38	33 (9%) 10 15	23, 39, 79, 112	0
1	G	365/381 (95%)	0.33	14 (3%) 41 53	29, 50, 76, 98	0
1	H	373/381 (97%)	0.23	25 (6%) 19 26	28, 51, 76, 95	0
All	All	2947/3048 (96%)	0.19	155 (5%) 27 39	22, 42, 80, 121	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	6.7
1	C	32	VAL	5.2
1	F	37	HIS	5.2
1	C	49	VAL	5.0
1	C	81	GLY	5.0
1	F	15	LEU	5.0
1	A	33	GLU	4.7
1	F	279	GLY	4.7
1	B	84	PHE	4.6
1	B	37	HIS	4.4
1	F	287	GLU	4.4
1	G	80	ALA	4.2
1	F	288	THR	4.2
1	G	49	VAL	4.2
1	A	36	ASN	4.2
1	F	36	ASN	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	33	GLU	4.1
1	F	77	LEU	4.1
1	G	30	ILE	4.0
1	C	79	GLN	4.0
1	H	333	PRO	4.0
1	D	287	GLU	3.9
1	D	279	GLY	3.9
1	F	60	ASN	3.8
1	C	35	LEU	3.7
1	C	48	LYS	3.6
1	B	281	GLU	3.6
1	C	57	THR	3.6
1	F	58	PRO	3.6
1	D	53	LEU	3.6
1	F	35	LEU	3.6
1	F	46	VAL	3.5
1	C	75	ALA	3.5
1	G	183	TYR	3.5
1	C	50	ASN	3.4
1	F	50	ASN	3.3
1	C	80	ALA	3.3
1	C	52	SER	3.2
1	C	61	PHE	3.2
1	F	268	THR	3.2
1	A	345	GLU	3.1
1	G	330	ALA	3.1
1	F	33	GLU	3.1
1	C	82	ILE	3.0
1	E	204	ILE	3.0
1	F	53	LEU	3.0
1	H	150	ALA	3.0
1	A	32	VAL	3.0
1	C	281	GLU	3.0
1	D	33	GLU	3.0
1	C	72	VAL	3.0
1	D	283	ARG	3.0
1	H	334	GLY	2.9
1	B	33	GLU	2.9
1	F	286	LEU	2.9
1	F	48	LYS	2.9
1	G	224	GLY	2.9
1	D	331	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	5	VAL	2.9
1	G	81	GLY	2.8
1	F	277	PHE	2.8
1	D	36	ASN	2.8
1	H	331	GLY	2.8
1	B	345	GLU	2.8
1	C	28	ARG	2.8
1	C	155	GLU	2.8
1	B	79	GLN	2.8
1	C	71[A]	HIS	2.8
1	B	46	VAL	2.7
1	B	77	LEU	2.7
1	D	54	LEU	2.7
1	H	183	TYR	2.7
1	H	157	ASP	2.7
1	B	53	LEU	2.7
1	G	7	GLU	2.6
1	C	46	VAL	2.6
1	C	84	PHE	2.6
1	A	37	HIS	2.6
1	C	74	GLU	2.6
1	G	284	VAL	2.6
1	F	52	SER	2.6
1	H	178	TYR	2.6
1	H	288	THR	2.5
1	C	122	VAL	2.5
1	F	18	ARG	2.5
1	H	153	GLY	2.5
1	H	158	PHE	2.5
1	B	95	VAL	2.5
1	B	99	VAL	2.4
1	F	63	GLY	2.4
1	D	281	GLU	2.4
1	C	99	VAL	2.4
1	C	204	ILE	2.4
1	E	155	GLU	2.4
1	H	204	ILE	2.4
1	H	151	ALA	2.4
1	A	26	PRO	2.4
1	D	377	ALA	2.4
1	B	280	ARG	2.3
1	F	69	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	180	ASP	2.3
1	C	68	GLY	2.3
1	D	34	GLU	2.3
1	D	276	ALA	2.3
1	G	33	GLU	2.3
1	H	172	THR	2.3
1	F	272	GLU	2.3
1	C	77	LEU	2.3
1	D	260	LEU	2.3
1	D	11	TYR	2.3
1	C	78	LYS	2.3
1	F	32	VAL	2.2
1	H	95	VAL	2.2
1	H	155	GLU	2.2
1	G	48	LYS	2.2
1	G	281	GLU	2.2
1	F	27	GLY	2.2
1	B	34	GLU	2.2
1	F	22	VAL	2.2
1	A	35	LEU	2.2
1	H	152	ARG	2.2
1	G	182	PRO	2.2
1	B	96	VAL	2.2
1	F	49	VAL	2.2
1	F	273	ALA	2.2
1	A	283	ARG	2.2
1	H	283	ARG	2.2
1	F	204	ILE	2.2
1	C	19	LEU	2.2
1	H	342	ASN	2.1
1	E	284	VAL	2.1
1	H	284	VAL	2.1
1	H	330	ALA	2.1
1	G	280	ARG	2.1
1	F	183	TYR	2.1
1	F	80	ALA	2.1
1	H	182	PRO	2.1
1	C	287	GLU	2.1
1	D	37	HIS	2.1
1	E	56	GLY	2.1
1	E	153	GLY	2.1
1	C	58	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	ILE	2.1
1	D	19	LEU	2.1
1	D	99	VAL	2.1
1	H	99	VAL	2.1
1	C	277	PHE	2.1
1	H	332	ILE	2.0
1	C	172	THR	2.0
1	C	330	ALA	2.0
1	A	281	GLU	2.0
1	F	275	SER	2.0
1	H	11	TYR	2.0
1	C	47	THR	2.0
1	E	152	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	NAD	D	379	44/44	0.98	0.13	0.04	29,37,47,47	0
2	NAD	E	379	44/44	0.93	0.14	-0.10	40,52,68,69	0
2	NAD	F	379	44/44	0.96	0.11	-0.46	38,43,50,55	0
2	NAD	C	379	44/44	0.97	0.12	-0.50	32,41,46,48	0
2	NAD	A	379	44/44	0.98	0.10	-0.54	33,39,45,47	0
2	NAD	B	379	44/44	0.98	0.11	-0.61	36,39,51,51	0
2	NAD	G	379	44/44	0.95	0.11	-0.70	42,49,55,57	0
2	NAD	H	379	44/44	0.95	0.11	-0.71	49,52,61,64	0

6.5 Other polymers

There are no such residues in this entry.