Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:38 PM GMT

PDB ID	:	4CQL
Title	:	Crystal structure of heterotetrameric human ketoacyl reductase complexed with NAD
Authors	:	Venkatesan, R.; Sah-Teli, S.K.; Awoniyi, L.O.; Jiang, G.; Prus, P.; Kastaniotis, A.J.; Hiltunen, J.K.; Wierenga, R.K.; Chen, Z.
Deposited on	:	2014-02-19
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

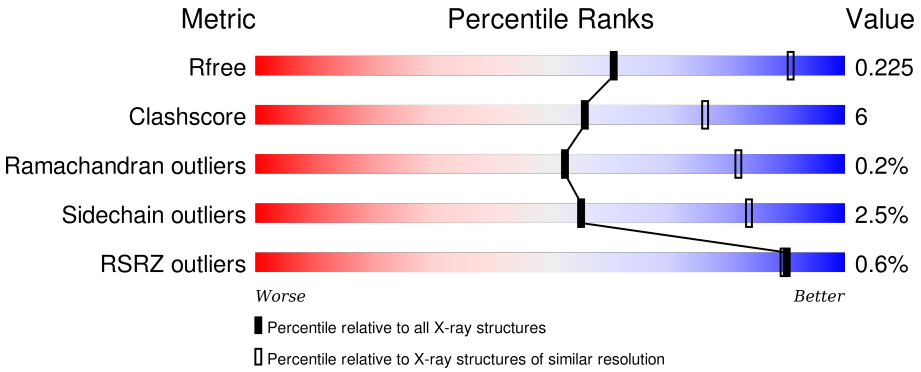
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.



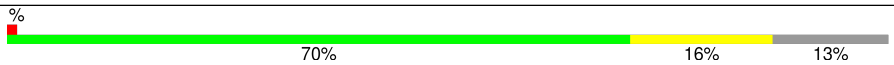
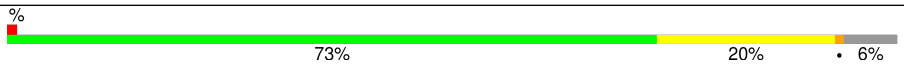
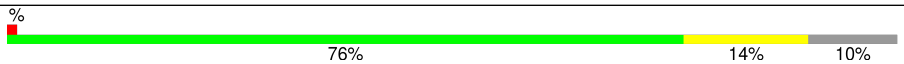
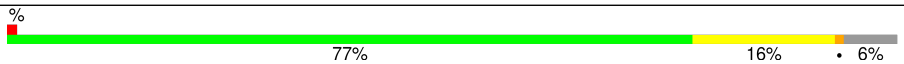
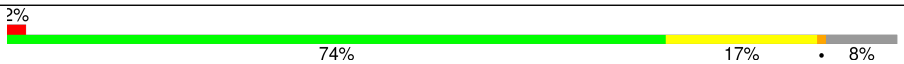
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	% 82% 13% 6%
1	D	261	% 84% 10% 6%
1	E	261	80% 13% 7%
1	H	261	82% 10% 7%
1	I	261	84% 12% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	261	
1	M	261	
1	P	261	
2	B	244	
2	C	244	
2	F	244	
2	G	244	
2	J	244	
2	K	244	
2	N	244	
2	O	244	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26833 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 ESTRADIOL 17-BETA-DEHYDROGENASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1756	1090	313	342	11			
1	D	246	Total	C	N	O	S	0	0	0
			1721	1070	302	339	10			
1	E	244	Total	C	N	O	S	0	0	0
			1733	1075	308	339	11			
1	H	242	Total	C	N	O	S	0	0	0
			1710	1059	306	335	10			
1	I	251	Total	C	N	O	S	0	0	0
			1762	1097	309	345	11			
1	L	240	Total	C	N	O	S	0	0	0
			1697	1053	302	331	11			
1	M	245	Total	C	N	O	S	0	0	0
			1755	1089	315	341	10			
1	P	246	Total	C	N	O	S	0	0	0
			1739	1080	308	341	10			

- Molecule 2 is a protein called CARBONYL REDUCTASE FAMILY MEMBER 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1593	1000	293	291	9			
2	C	216	Total	C	N	O	S	0	0	0
			1496	942	266	280	8			
2	F	231	Total	C	N	O	S	0	0	0
			1623	1013	297	304	9			
2	G	212	Total	C	N	O	S	0	0	0
			1452	905	263	276	8			
2	J	229	Total	C	N	O	S	0	0	0
			1609	1010	292	298	9			
2	K	220	Total	C	N	O	S	0	0	0
			1493	934	271	280	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	229	Total	C	N	O	S	0	0	0
			1616	1014	294	299	9			
2	O	224	Total	C	N	O	S	0	0	0
			1508	946	269	285	8			

There are 56 discrepancies between the modelled and reference sequences:

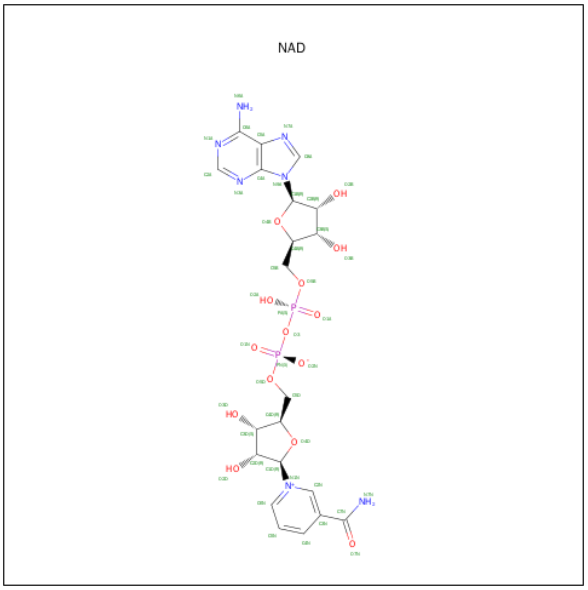
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
B	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
B	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
B	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
B	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
B	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
B	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
C	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
C	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
F	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
F	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
G	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
G	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
J	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
J	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
J	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
J	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
J	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
J	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
K	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
K	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
N	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
N	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	-6	MET	-	EXPRESSION TAG	UNP Q8N4T8
O	-5	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	-4	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	-3	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	-2	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	-1	HIS	-	EXPRESSION TAG	UNP Q8N4T8
O	0	HIS	-	EXPRESSION TAG	UNP Q8N4T8

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	7	Total	O	0	0
			7	7		
4	C	10	Total	O	0	0
			10	10		
4	D	4	Total	O	0	0
			4	4		
4	E	25	Total	O	0	0
			25	25		
4	F	8	Total	O	0	0
			8	8		
4	G	4	Total	O	0	0
			4	4		
4	H	9	Total	O	0	0
			9	9		
4	I	14	Total	O	0	0
			14	14		
4	J	8	Total	O	0	0
			8	8		
4	K	7	Total	O	0	0
			7	7		
4	L	20	Total	O	0	0
			20	20		

Continued on next page...

Continued from previous page...

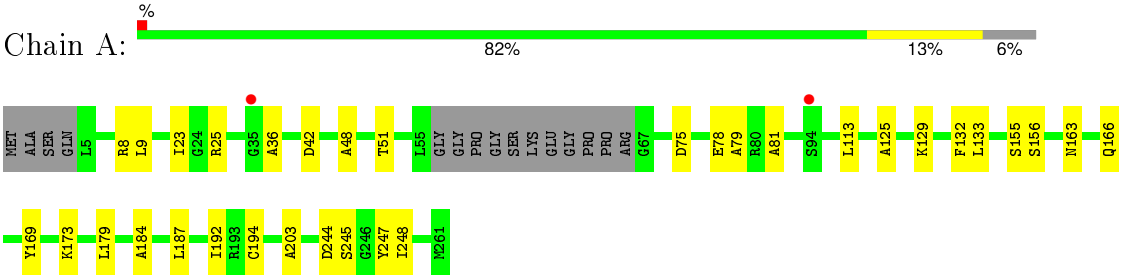
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	38	Total O 38 38	0	0
4	N	24	Total O 24 24	0	0
4	O	6	Total O 6 6	0	0
4	P	10	Total O 10 10	0	0

3 Residue-property plots (i)

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.

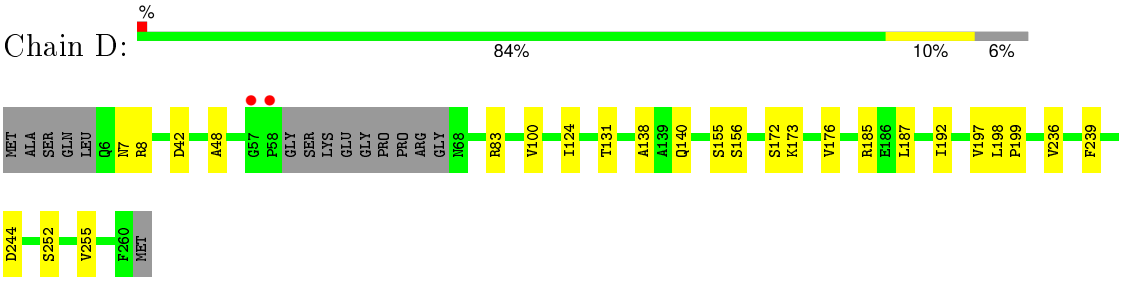
- Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain A:



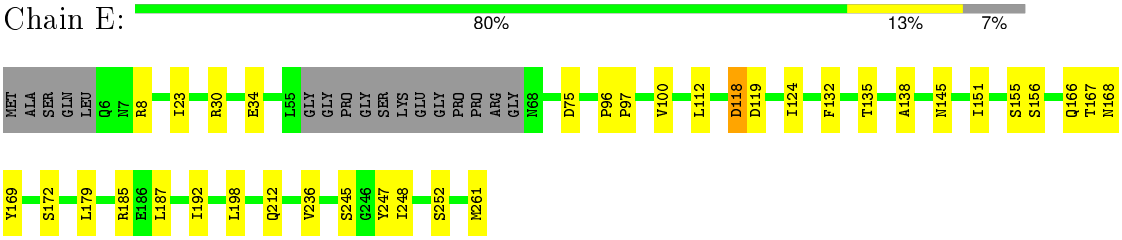
- Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain D:



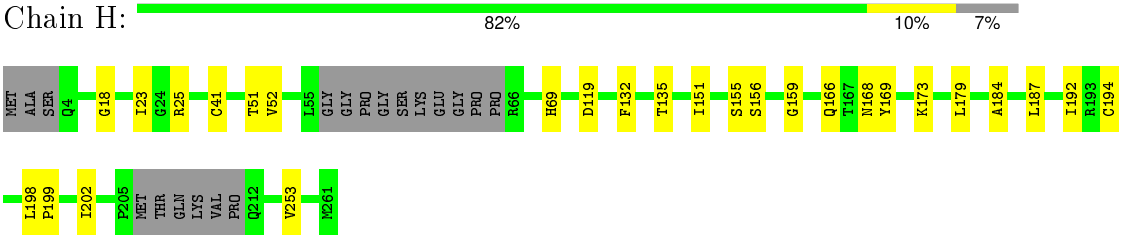
- Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain E:



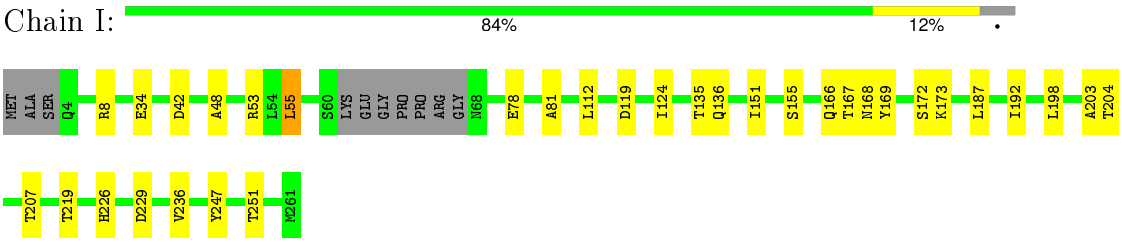
- Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain H:



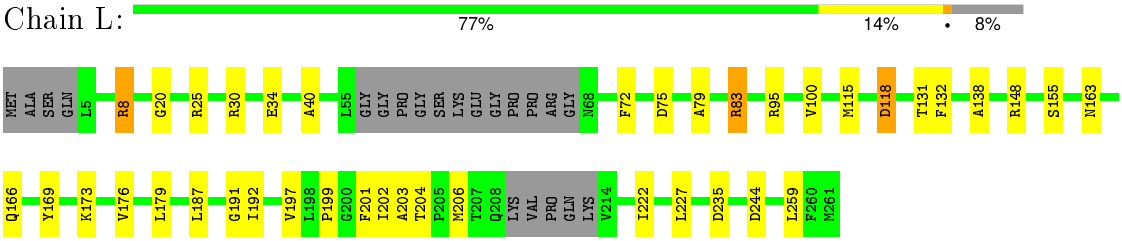
• Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain I:



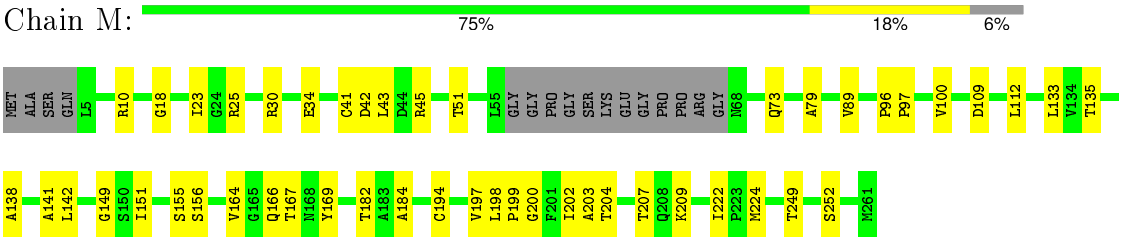
• Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain L:



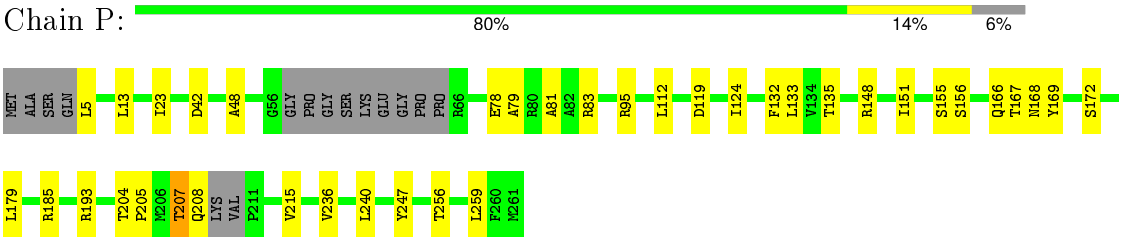
• Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain M:



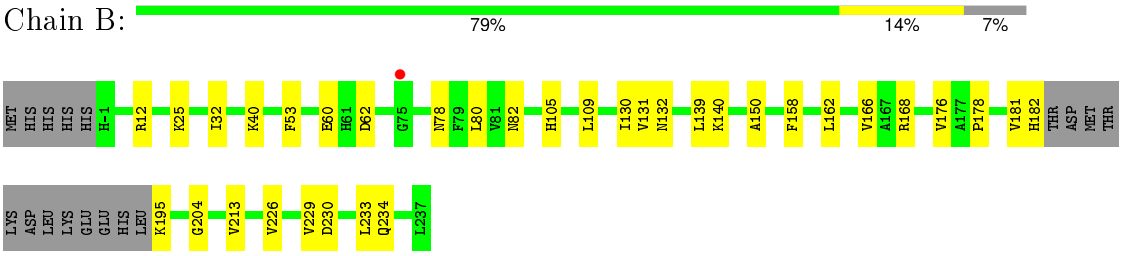
• Molecule 1: ESTRADIOL 17-BETA-DEHYDROGENASE 8

Chain P:



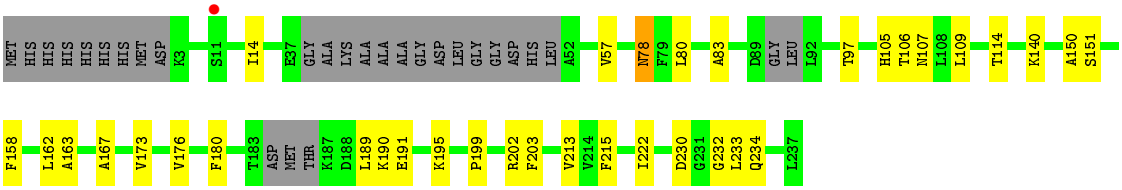
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

Chain B:



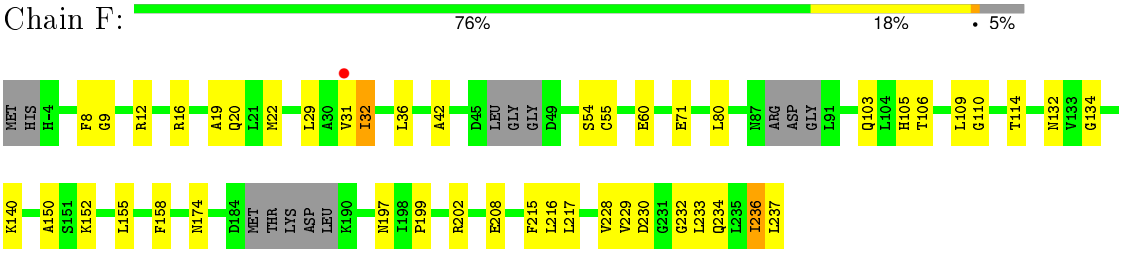
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

Chain C:



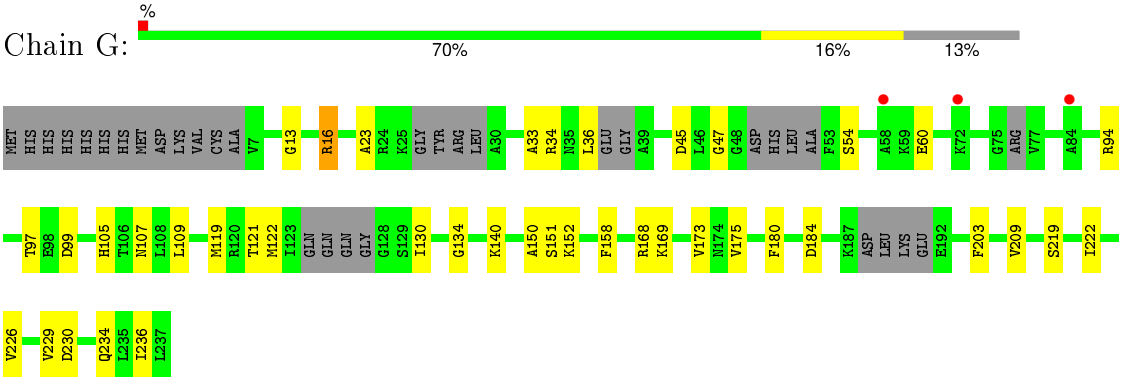
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

Chain F:



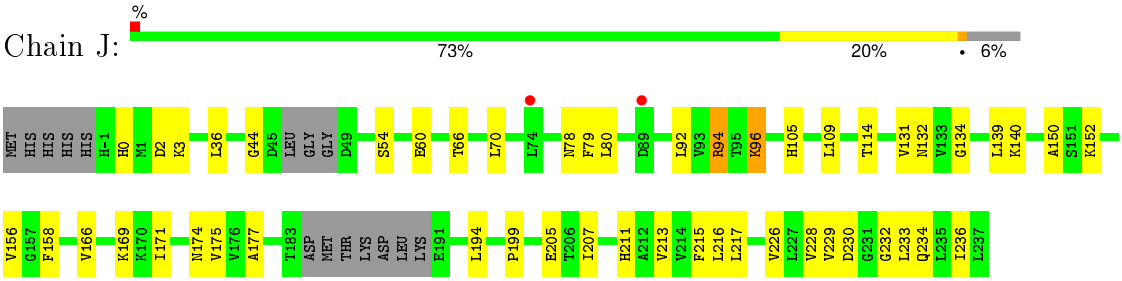
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

Chain G:



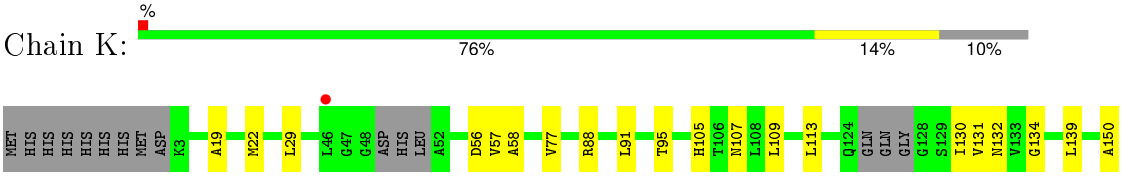
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

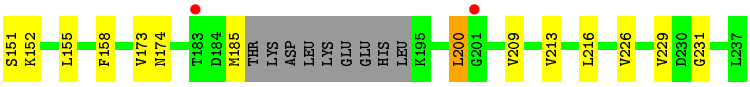
Chain J:



• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

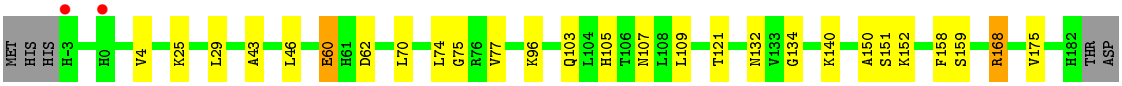
Chain K:





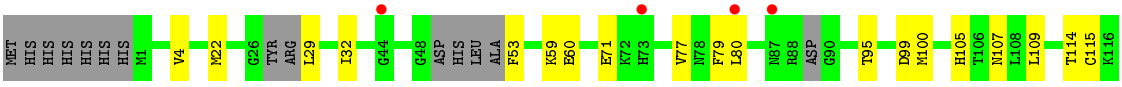
• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

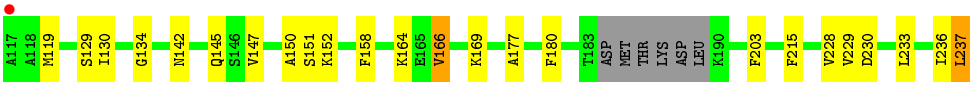
Chain N:



• Molecule 2: CARBONYL REDUCTASE FAMILY MEMBER 4

Chain O:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.15Å 237.11Å 87.35Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	49.78 – 2.85 49.78 – 2.85	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.78-2.85) 87.2 (49.78-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.236 0.182 , 0.225	Depositor DCC
R_{free} test set	3525 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.3	EDS
Estimated twinning fraction	0.320 for L,-K,H 0.308 for l,-k,h	Xtriage
Reported twinning fraction	0.320 for L,-K,H	Depositor
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 75312 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26833	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.20	0/1776	0.36	0/2412
1	D	0.20	0/1742	0.35	0/2373
1	E	0.20	0/1753	0.36	0/2383
1	H	0.19	0/1728	0.35	0/2346
1	I	0.20	0/1783	0.37	0/2427
1	L	0.20	0/1715	0.36	0/2330
1	M	0.20	0/1775	0.36	0/2412
1	P	0.20	0/1758	0.37	0/2387
2	B	0.20	0/1614	0.35	0/2183
2	C	0.20	0/1511	0.34	0/2045
2	F	0.20	0/1639	0.35	0/2216
2	G	0.20	0/1461	0.35	0/1971
2	J	0.20	0/1626	0.36	0/2198
2	K	0.20	0/1507	0.36	0/2040
2	N	0.20	0/1633	0.35	0/2207
2	O	0.20	0/1520	0.34	0/2057
All	All	0.20	0/26541	0.35	0/35987

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	1756	0	1741	21	0
1	D	1721	0	1673	16	0
1	E	1733	0	1707	22	0
1	H	1710	0	1669	15	0
1	I	1762	0	1721	20	0
1	L	1697	0	1662	23	0
1	M	1755	0	1739	29	0
1	P	1739	0	1706	20	0
2	B	1593	0	1549	22	0
2	C	1496	0	1427	22	0
2	F	1623	0	1562	28	0
2	G	1452	0	1375	21	0
2	J	1609	0	1568	32	0
2	K	1493	0	1410	18	0
2	N	1616	0	1591	25	0
2	O	1508	0	1429	23	0
3	A	44	0	26	3	0
3	D	44	0	26	0	0
3	E	44	0	26	3	0
3	H	44	0	26	2	0
3	I	44	0	26	1	0
3	L	44	0	26	3	0
3	M	44	0	26	4	0
3	P	44	0	26	1	0
4	A	24	0	0	0	0
4	B	7	0	0	0	0
4	C	10	0	0	0	0
4	D	4	0	0	0	0
4	E	25	0	0	0	0
4	F	8	0	0	0	0
4	G	4	0	0	0	0
4	H	9	0	0	0	0
4	I	14	0	0	0	0
4	J	8	0	0	0	0
4	K	7	0	0	0	0
4	L	20	0	0	1	0
4	M	38	0	0	0	0
4	N	24	0	0	0	0
4	O	6	0	0	0	0
4	P	10	0	0	0	0
All	All	26833	0	25737	325	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 (325) 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)
2:J:158:PHE:HB2	2:K:150:ALA:HB2	1.65	0.77
2:B:158:PHE:HB2	2:C:150:ALA:HB2	1.69	0.72
1:P:132:PHE:HB2	1:P:179:LEU:HD11	1.73	0.71
2:G:130:ILE:HB	2:G:173:VAL:HG12	1.73	0.71
1:L:187:LEU:HB3	1:L:192:ILE:HB	1.73	0.70
2:N:158:PHE:HB2	2:O:150:ALA:HB2	1.74	0.68
2:G:140:LYS:NZ	2:G:234:GLN:O	2.26	0.68
2:B:105:HIS:HA	2:B:109:LEU:HB3	1.76	0.67
2:G:107:ASN:HB2	2:G:151:SER:HB3	1.78	0.66
2:C:195:LYS:HD2	2:C:202:ARG:HA	1.77	0.65
2:N:140:LYS:HD2	2:N:234:GLN:HG3	1.79	0.65
2:F:158:PHE:HB2	2:G:150:ALA:HB2	1.79	0.64
2:B:32:ILE:HG12	2:B:53:PHE:HB2	1.80	0.64
2:J:140:LYS:HE3	2:J:234:GLN:HG3	1.81	0.63
2:N:150:ALA:HB2	2:O:158:PHE:HB2	1.79	0.63
1:E:166:GLN:HB3	1:E:169:TYR:HB3	1.80	0.63
2:J:132:ASN:HB2	2:J:175:VAL:HG22	1.81	0.63
1:I:155:SER:HA	1:I:173:LYS:HD2	1.82	0.62
2:K:134:GLY:HA2	2:K:152:LYS:HD2	1.82	0.62
1:M:42:ASP:OD1	3:M:301:NAD:O2B	2.18	0.62
1:E:187:LEU:HB3	1:E:192:ILE:HB	1.81	0.62
1:M:166:GLN:HB3	1:M:169:TYR:HB3	1.82	0.62
2:J:105:HIS:HA	2:J:109:LEU:HB3	1.81	0.62
1:P:207:THR:OG1	1:P:208:GLN:N	2.33	0.61
2:J:3:LYS:HE3	2:J:79:PHE:HE2	1.65	0.61
2:K:155:LEU:HA	2:K:158:PHE:HB3	1.82	0.61
2:N:134:GLY:HA2	2:N:152:LYS:HD2	1.82	0.61
2:G:105:HIS:HA	2:G:109:LEU:HB3	1.82	0.61
1:A:166:GLN:HB3	1:A:169:TYR:HB3	1.82	0.61
2:O:105:HIS:HA	2:O:109:LEU:HB3	1.83	0.61
1:A:163:ASN:HA	1:D:185:ARG:HH21	1.66	0.61
1:M:45:ARG:HD3	1:M:73:GLN:HB2	1.82	0.60
2:C:140:LYS:NZ	2:C:234:GLN:O	2.33	0.60
2:F:140:LYS:NZ	2:F:234:GLN:O	2.32	0.60
1:D:155:SER:HA	1:D:173:LYS:HD2	1.83	0.60
1:L:148:ARG:HD2	1:L:191:GLY:HA3	1.84	0.60
1:E:132:PHE:HB2	1:E:179:LEU:HD11	1.84	0.60
2:N:140:LYS:NZ	2:N:234:GLN:O	2.36	0.59
1:H:155:SER:HA	1:H:173:LYS:HD2	1.85	0.59
1:I:187:LEU:HB3	1:I:192:ILE:HB	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ARG:NH1	1:E:34:GLU:OE2	2.35	0.59
1:P:119:ASP:O	1:P:168:ASN:ND2	2.31	0.59
1:M:112:LEU:HD13	1:M:167:THR:HG21	1.84	0.58
2:F:134:GLY:HA2	2:F:152:LYS:HD2	1.83	0.58
1:E:185:ARG:HH12	2:F:236:ILE:HD12	1.67	0.58
2:G:184:ASP:HA	2:G:203:PHE:HB2	1.86	0.58
2:B:176:VAL:HG12	2:B:178:PRO:HD3	1.85	0.58
1:I:166:GLN:HB3	1:I:169:TYR:HB3	1.85	0.58
1:L:8:ARG:NH1	1:L:244:ASP:OD2	2.36	0.58
1:I:204:THR:OG1	3:I:301:NAD:N7N	2.36	0.58
2:B:140:LYS:NZ	2:B:234:GLN:O	2.34	0.57
1:A:8:ARG:NH1	1:A:244:ASP:OD2	2.36	0.57
2:F:197:ASN:HB3	2:F:236:ILE:HG12	1.87	0.57
1:E:135:THR:HG23	1:E:151:ILE:HG21	1.86	0.57
1:I:42:ASP:HB3	1:I:48:ALA:HB2	1.86	0.57
1:H:187:LEU:HB3	1:H:192:ILE:HB	1.86	0.57
1:D:187:LEU:HB3	1:D:192:ILE:HB	1.87	0.57
1:L:30:ARG:NH2	1:L:235:ASP:OD1	2.38	0.56
2:J:134:GLY:HA2	2:J:152:LYS:HD2	1.87	0.56
2:G:121:THR:OG1	2:G:122:MET:N	2.37	0.56
2:B:150:ALA:HB2	2:C:158:PHE:HB2	1.87	0.56
2:N:4:VAL:HG11	2:N:74:LEU:HD13	1.87	0.56
1:H:23:ILE:HB	3:H:301:NAD:H51N	1.87	0.56
2:O:230:ASP:HB2	2:O:233:LEU:HB2	1.88	0.56
1:H:132:PHE:HB2	1:H:179:LEU:HD11	1.86	0.56
1:I:112:LEU:HD13	1:I:167:THR:HG21	1.87	0.55
1:P:166:GLN:HB3	1:P:169:TYR:HB3	1.88	0.55
1:P:135:THR:HG23	1:P:151:ILE:HG21	1.89	0.55
1:L:222:ILE:HG12	1:L:259:LEU:HD13	1.89	0.55
1:M:135:THR:HG23	1:M:151:ILE:HG21	1.88	0.55
2:F:150:ALA:HB2	2:G:158:PHE:HB2	1.88	0.55
2:G:168:ARG:HE	2:G:169:LYS:HE3	1.71	0.55
2:F:230:ASP:HB2	2:F:233:LEU:HB3	1.88	0.55
2:J:177:ALA:HB3	2:J:228:VAL:HG12	1.87	0.55
1:M:184:ALA:HB2	1:M:194:CYS:HB2	1.89	0.55
2:K:174:ASN:HB3	2:K:216:LEU:HD13	1.89	0.55
2:K:19:ALA:HA	2:K:29:LEU:HD22	1.88	0.54
2:O:177:ALA:HB3	2:O:228:VAL:HG12	1.89	0.54
1:A:23:ILE:HB	3:A:301:NAD:H51N	1.89	0.54
1:E:119:ASP:O	1:E:168:ASN:ND2	2.37	0.54
1:H:135:THR:HG23	1:H:151:ILE:HG21	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3:LYS:HA	2:J:78:ASN:HD21	1.73	0.54
2:C:14:ILE:HG23	2:C:83:ALA:HB1	1.89	0.54
1:L:79:ALA:O	1:L:83:ARG:NE	2.38	0.54
2:O:134:GLY:HA2	2:O:152:LYS:HD2	1.89	0.54
1:E:100:VAL:HG21	1:E:138:ALA:HB1	1.90	0.54
2:B:80:LEU:HB3	2:B:130:ILE:HG12	1.90	0.54
2:N:197:ASN:HB3	2:N:236:ILE:HD13	1.90	0.53
2:B:82:ASN:ND2	2:B:132:ASN:OD1	2.38	0.53
2:F:105:HIS:HA	2:F:109:LEU:HB3	1.90	0.53
2:N:105:HIS:HA	2:N:109:LEU:HB3	1.91	0.53
2:J:207:ILE:O	2:J:211:HIS:ND1	2.30	0.53
2:N:140:LYS:O	2:O:164:LYS:NZ	2.40	0.53
2:K:209:VAL:HG22	2:K:229:VAL:HG11	1.90	0.52
2:N:107:ASN:HB2	2:N:151:SER:HB2	1.90	0.52
2:F:174:ASN:HB3	2:F:216:LEU:HD13	1.90	0.52
2:J:2:ASP:OD1	1:M:209:LYS:NZ	2.42	0.52
2:N:132:ASN:ND2	2:N:159:SER:OG	2.38	0.52
2:C:78:ASN:OD1	2:C:78:ASN:N	2.43	0.51
2:F:8:PHE:HA	2:F:32:ILE:HG23	1.92	0.51
2:K:131:VAL:HG11	2:K:213:VAL:HG13	1.93	0.51
1:D:100:VAL:HG21	1:D:138:ALA:HB1	1.93	0.51
2:J:230:ASP:HB2	2:J:233:LEU:HB3	1.93	0.51
2:F:132:ASN:HB3	2:F:155:LEU:HD21	1.91	0.51
2:O:79:PHE:HD1	2:O:129:SER:HB3	1.75	0.51
1:A:247:TYR:HD2	2:B:229:VAL:HG12	1.76	0.51
1:M:23:ILE:HD12	3:M:301:NAD:H51N	1.92	0.51
2:J:79:PHE:HD1	2:J:217:LEU:HD22	1.76	0.51
1:L:75:ASP:OD1	3:L:301:NAD:N6A	2.44	0.51
1:I:119:ASP:O	1:I:168:ASN:ND2	2.44	0.51
2:J:80:LEU:HD21	2:J:114:THR:HG22	1.93	0.50
1:D:156:SER:HA	1:D:199:PRO:HD2	1.91	0.50
2:N:70:LEU:O	2:N:75:GLY:N	2.42	0.50
2:O:107:ASN:HB2	2:O:151:SER:HB2	1.92	0.50
1:A:125:ALA:HA	1:A:129:LYS:HB3	1.93	0.50
1:M:100:VAL:HG21	1:M:138:ALA:HB1	1.92	0.50
2:O:32:ILE:HG12	2:O:53:PHE:HB2	1.92	0.50
2:F:16:ARG:HH12	2:F:20:GLN:HB2	1.76	0.50
2:C:230:ASP:HB2	2:C:233:LEU:HB3	1.94	0.50
2:K:200:LEU:HD22	2:K:231:GLY:HA2	1.93	0.50
1:D:8:ARG:HH22	1:D:239:PHE:HD1	1.60	0.50
2:N:199:PRO:HG2	2:N:232:GLY:HA3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:ARG:NH2	2:F:208:GLU:OE2	2.44	0.49
2:G:209:VAL:HG22	2:G:229:VAL:HG11	1.93	0.49
1:M:42:ASP:OD1	1:M:43:LEU:N	2.45	0.49
1:M:198:LEU:HD13	1:M:252:SER:HB2	1.92	0.49
2:G:134:GLY:HA2	2:G:152:LYS:HD2	1.94	0.49
2:O:166:VAL:HG12	2:O:169:LYS:HB2	1.95	0.49
2:J:96:LYS:HE2	2:J:96:LYS:H	1.77	0.49
2:F:230:ASP:OD2	2:F:234:GLN:N	2.43	0.49
2:G:23:ALA:HB1	2:G:47:GLY:H	1.78	0.49
1:P:193:ARG:NH2	1:P:240:LEU:O	2.44	0.49
2:J:174:ASN:HB3	2:J:216:LEU:HD13	1.95	0.49
2:K:209:VAL:HG13	2:K:229:VAL:HG21	1.93	0.49
2:O:95:THR:OG1	2:O:99:ASP:OD2	2.30	0.49
1:E:236:VAL:HG22	2:F:215:PHE:HZ	1.78	0.49
1:L:30:ARG:NH1	1:L:34:GLU:OE2	2.46	0.49
1:I:135:THR:HG23	1:I:151:ILE:HG21	1.94	0.49
2:C:180:PHE:HB3	2:C:203:PHE:CE2	2.48	0.49
2:C:215:PHE:HZ	1:D:236:VAL:HG22	1.78	0.49
2:B:181:VAL:O	2:B:182:HIS:ND1	2.46	0.48
2:C:107:ASN:HB2	2:C:151:SER:HB2	1.95	0.48
1:H:18:GLY:N	1:H:41:CYS:O	2.47	0.48
1:L:132:PHE:HB2	1:L:179:LEU:HD11	1.94	0.48
2:B:140:LYS:HD2	2:B:234:GLN:HG3	1.95	0.48
2:F:19:ALA:HA	2:F:29:LEU:HD22	1.96	0.48
2:K:22:MET:HB2	2:K:29:LEU:HD21	1.95	0.48
1:P:124:ILE:HD13	1:P:172:SER:HB3	1.95	0.48
2:B:60:GLU:HG3	2:C:97:THR:HG21	1.96	0.48
1:A:187:LEU:HB3	1:A:192:ILE:HB	1.95	0.48
2:K:91:LEU:O	2:K:95:THR:OG1	2.22	0.48
2:J:230:ASP:OD2	2:J:234:GLN:N	2.47	0.48
1:M:89:VAL:HG11	1:M:97:PRO:HG3	1.95	0.48
1:A:248:ILE:HD11	2:B:229:VAL:HG22	1.96	0.48
1:H:202:ILE:H	3:H:301:NAD:H71N	1.62	0.48
1:A:75:ASP:OD1	3:A:301:NAD:N6A	2.46	0.48
2:K:130:ILE:HB	2:K:173:VAL:HG12	1.96	0.48
2:O:215:PHE:HZ	1:P:236:VAL:HG22	1.79	0.48
1:A:113:LEU:O	1:D:140:GLN:NE2	2.46	0.48
2:K:105:HIS:HA	2:K:109:LEU:HB3	1.95	0.47
3:L:301:NAD:H2N	3:L:301:NAD:H2D	1.68	0.47
2:N:103:GLN:OE1	2:N:107:ASN:ND2	2.46	0.47
2:G:45:ASP:N	2:G:45:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:LEU:HD21	2:C:114:THR:HG22	1.96	0.47
1:M:25:ARG:HG3	1:M:51:THR:HG23	1.97	0.47
2:F:80:LEU:HD21	2:F:114:THR:HG22	1.97	0.47
2:O:229:VAL:HG12	1:P:247:TYR:HD2	1.79	0.47
2:N:202:ARG:NH2	2:N:208:GLU:OE2	2.48	0.47
2:O:80:LEU:HB3	2:O:130:ILE:HG12	1.97	0.47
1:H:166:GLN:HB3	1:H:169:TYR:HB3	1.97	0.47
1:D:42:ASP:HB3	1:D:48:ALA:HB2	1.95	0.47
1:I:124:ILE:HD13	1:I:172:SER:HB3	1.96	0.47
2:G:13:GLY:O	2:G:16:ARG:NH1	2.48	0.47
1:A:184:ALA:HB2	1:A:194:CYS:HB2	1.97	0.47
2:F:36:LEU:HB2	2:F:54:SER:HB3	1.97	0.47
1:I:55:LEU:HD13	1:I:55:LEU:H	1.80	0.47
2:G:175:VAL:HB	2:G:226:VAL:HG22	1.96	0.47
2:K:107:ASN:HB2	2:K:151:SER:HB3	1.98	0.46
1:A:79:ALA:HA	1:A:133:LEU:HD13	1.97	0.46
1:I:236:VAL:HG22	2:J:215:PHE:HZ	1.80	0.46
1:I:229:ASP:OD2	1:P:83:ARG:NH2	2.49	0.46
1:M:142:LEU:HD13	1:M:149:GLY:HA3	1.97	0.46
2:J:139:LEU:HD11	2:J:226:VAL:HG11	1.98	0.46
2:J:199:PRO:HG2	2:J:232:GLY:HA3	1.96	0.46
2:B:40:LYS:HE2	2:B:40:LYS:HB3	1.71	0.46
2:F:32:ILE:HD11	2:F:55:CYS:HB3	1.97	0.46
2:C:189:LEU:HG	2:C:190:LYS:H	1.81	0.46
1:D:198:LEU:HD13	1:D:252:SER:HB3	1.97	0.46
1:E:112:LEU:HD13	1:E:167:THR:HG21	1.98	0.46
1:I:247:TYR:HD2	2:J:229:VAL:HG12	1.80	0.46
1:P:42:ASP:HB3	1:P:48:ALA:HB2	1.98	0.46
1:M:222:ILE:O	2:N:168:ARG:NH1	2.49	0.46
2:C:191:GLU:O	2:C:195:LYS:HG3	2.16	0.45
1:I:155:SER:O	1:I:198:LEU:HA	2.16	0.45
1:P:79:ALA:HA	1:P:133:LEU:HD13	1.98	0.45
1:L:201:PHE:HB3	1:L:227:LEU:HD22	1.98	0.45
2:F:199:PRO:HG2	2:F:232:GLY:HA3	1.98	0.45
1:P:256:THR:HB	1:P:259:LEU:HB3	1.99	0.45
2:C:222:ILE:HG12	1:D:255:VAL:HA	1.98	0.45
2:J:150:ALA:HB2	2:K:158:PHE:HB2	1.98	0.45
2:N:29:LEU:HD23	2:N:46:LEU:HD13	1.99	0.45
2:N:175:VAL:HB	2:N:226:VAL:HG22	1.98	0.45
2:B:139:LEU:HD11	2:B:226:VAL:HG11	1.99	0.45
1:P:112:LEU:HD13	1:P:167:THR:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:SER:OG	1:M:156:SER:N	2.48	0.45
1:A:245:SER:HB2	1:A:248:ILE:HB	1.99	0.45
2:J:166:VAL:HG22	2:J:169:LYS:HB2	1.99	0.45
1:E:247:TYR:HD2	2:F:229:VAL:HG12	1.82	0.45
1:M:199:PRO:HB2	1:M:202:ILE:HD11	2.00	0.44
1:E:96:PRO:HG3	1:E:145:ASN:HD22	1.82	0.44
2:K:132:ASN:HB3	2:K:155:LEU:HD12	1.99	0.44
1:E:198:LEU:HD13	1:E:252:SER:HB2	2.00	0.44
1:A:132:PHE:HB2	1:A:179:LEU:HD11	1.97	0.44
1:L:131:THR:HG21	1:L:176:VAL:HG13	2.00	0.44
1:L:197:VAL:HG12	1:L:199:PRO:HD3	1.99	0.44
2:C:163:ALA:O	2:C:167:ALA:HB2	2.17	0.44
2:F:31:VAL:HG11	2:F:42:ALA:HB3	1.99	0.44
2:B:12:ARG:NE	2:J:44:GLY:HA3	2.32	0.44
1:L:166:GLN:HB3	1:L:169:TYR:HB3	2.00	0.44
1:H:198:LEU:N	1:H:253:VAL:O	2.38	0.44
2:N:60:GLU:H	2:N:60:GLU:HG3	1.53	0.44
1:D:131:THR:HG21	1:D:176:VAL:HG13	1.98	0.44
2:J:166:VAL:HG13	2:J:171:ILE:HB	1.99	0.44
1:H:184:ALA:HB2	1:H:194:CYS:HB2	1.99	0.44
1:D:124:ILE:HD13	1:D:172:SER:HB3	2.00	0.44
1:A:78:GLU:HB2	1:A:81:ALA:HB3	2.00	0.44
2:J:92:LEU:HB3	2:J:94:ARG:HG3	1.99	0.44
2:F:103:GLN:HA	2:F:106:THR:HG22	1.99	0.44
2:N:25:LYS:HE2	2:N:25:LYS:HB3	1.90	0.44
1:L:118:ASP:N	1:L:118:ASP:OD1	2.50	0.44
2:C:230:ASP:OD2	2:C:234:GLN:N	2.43	0.44
1:M:96:PRO:HA	1:M:97:PRO:HD3	1.90	0.44
2:N:207:ILE:O	2:N:211:HIS:ND1	2.40	0.44
2:O:80:LEU:HD21	2:O:114:THR:HG22	2.00	0.43
1:M:79:ALA:HA	1:M:133:LEU:HD13	1.99	0.43
1:H:52:VAL:HG13	1:H:69:HIS:HB2	1.99	0.43
1:E:261:MET:O	2:G:140:LYS:HE2	2.18	0.43
1:I:136:GLN:NE2	1:L:115:MET:O	2.48	0.43
2:B:230:ASP:HB3	2:B:233:LEU:H	1.83	0.43
1:L:40:ALA:O	1:L:72:PHE:N	2.44	0.43
1:E:155:SER:O	3:E:301:NAD:H6N	2.19	0.43
2:O:115:CYS:O	2:O:119:MET:HG2	2.18	0.43
1:H:25:ARG:HG3	1:H:51:THR:HG23	1.99	0.43
1:H:156:SER:HA	1:H:199:PRO:HD2	2.00	0.43
1:M:18:GLY:N	1:M:41:CYS:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LYS:HA	1:D:173:LYS:HD3	1.86	0.43
1:I:204:THR:H	1:I:207:THR:HG1	1.67	0.43
1:A:42:ASP:HB3	1:A:48:ALA:HB2	2.01	0.43
2:O:100:MET:HA	2:O:147:VAL:HG21	2.00	0.43
2:C:199:PRO:HG2	2:C:232:GLY:HA3	2.00	0.43
2:K:139:LEU:HD11	2:K:226:VAL:HG11	2.01	0.43
2:O:180:PHE:HB3	2:O:203:PHE:CE2	2.53	0.43
2:O:4:VAL:HB	2:O:77:VAL:HA	1.99	0.43
2:G:219:SER:HB3	2:G:222:ILE:HD12	2.00	0.43
1:A:173:LYS:HD3	1:A:173:LYS:HA	1.83	0.42
3:M:301:NAD:H2D	3:M:301:NAD:H2N	1.85	0.42
1:E:118:ASP:N	1:E:118:ASP:OD1	2.52	0.42
1:M:222:ILE:HG22	1:M:224:MET:H	1.83	0.42
2:O:22:MET:HB2	2:O:29:LEU:HD21	2.01	0.42
2:O:233:LEU:O	2:O:237:LEU:HB2	2.20	0.42
2:F:9:GLY:HA2	2:F:12:ARG:HH11	1.84	0.42
2:J:139:LEU:HD21	2:J:156:VAL:HG21	2.01	0.42
2:J:199:PRO:HD3	2:J:236:ILE:HD11	2.01	0.42
1:P:23:ILE:HB	3:P:301:NAD:H51N	2.02	0.42
2:B:78:ASN:N	2:B:78:ASN:OD1	2.53	0.42
1:L:163:ASN:ND2	4:L:2017:HOH:O	2.46	0.42
1:I:8:ARG:NH2	1:I:34:GLU:OE2	2.52	0.42
1:E:75:ASP:OD1	3:E:301:NAD:N6A	2.53	0.42
1:A:25:ARG:HG3	1:A:51:THR:HG23	2.01	0.42
1:A:9:LEU:HB3	1:A:36:ALA:HB2	2.02	0.42
1:L:20:GLY:O	1:L:25:ARG:NH2	2.53	0.42
2:F:9:GLY:N	2:F:32:ILE:O	2.46	0.42
1:P:155:SER:OG	1:P:156:SER:N	2.45	0.42
2:J:66:THR:O	2:J:70:LEU:N	2.49	0.42
2:B:182:HIS:N	2:B:204:GLY:O	2.53	0.41
1:M:202:ILE:O	1:M:204:THR:N	2.53	0.41
1:L:155:SER:O	3:L:301:NAD:H6N	2.20	0.41
2:C:106:THR:HG23	2:C:107:ASN:OD1	2.20	0.41
2:N:207:ILE:HG13	2:N:211:HIS:CE1	2.55	0.41
1:E:124:ILE:HD13	1:E:172:SER:HB3	2.02	0.41
1:P:78:GLU:HB2	1:P:81:ALA:HB3	2.02	0.41
2:O:142:ASN:ND2	2:O:145:GLN:OE1	2.45	0.41
1:M:249:THR:HG21	2:N:200:LEU:HD13	2.02	0.41
1:L:202:ILE:HG22	1:L:204:THR:HG23	2.02	0.41
2:C:162:LEU:HG	2:C:173:VAL:HG21	2.02	0.41
1:D:197:VAL:O	1:D:199:PRO:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:33:ALA:O	2:G:54:SER:HA	2.19	0.41
1:L:173:LYS:HA	1:L:173:LYS:HD3	1.79	0.41
1:A:155:SER:OG	1:A:156:SER:N	2.50	0.41
2:F:22:MET:HB2	2:F:29:LEU:HD11	2.02	0.41
1:E:155:SER:OG	1:E:156:SER:N	2.54	0.41
1:M:164:VAL:HG23	1:P:185:ARG:NH1	2.35	0.41
1:H:119:ASP:O	1:H:168:ASN:ND2	2.53	0.41
1:I:251:THR:HG23	2:J:228:VAL:HG22	2.02	0.41
1:M:182:THR:HG21	1:P:167:THR:HA	2.03	0.41
2:C:105:HIS:HA	2:C:109:LEU:HB3	2.03	0.41
2:B:131:VAL:HG11	2:B:213:VAL:HG13	2.02	0.41
2:B:162:LEU:O	2:B:166:VAL:HG22	2.21	0.41
2:B:168:ARG:HD3	2:B:168:ARG:HA	1.91	0.41
1:M:200:GLY:O	3:M:301:NAD:H4N	2.21	0.41
2:J:94:ARG:H	2:J:94:ARG:HG3	1.76	0.41
2:K:56:ASP:C	2:K:58:ALA:H	2.24	0.41
1:M:30:ARG:NH1	1:M:34:GLU:OE2	2.53	0.41
1:P:13:LEU:HB2	1:P:95:ARG:NH1	2.36	0.41
2:C:176:VAL:HG21	2:C:213:VAL:HG22	2.02	0.41
1:E:245:SER:HB2	1:E:248:ILE:HB	2.02	0.41
2:N:43:ALA:HA	2:N:46:LEU:HD12	2.01	0.41
1:M:197:VAL:O	1:M:199:PRO:HD3	2.21	0.41
2:F:60:GLU:HG3	2:G:97:THR:OG1	2.21	0.41
1:I:78:GLU:HB2	1:I:81:ALA:HB3	2.02	0.41
2:G:230:ASP:OD1	2:G:234:GLN:N	2.46	0.40
1:M:96:PRO:HB3	1:M:141:ALA:HB1	2.03	0.40
1:E:23:ILE:HD12	3:E:301:NAD:H51N	2.04	0.40
2:N:219:SER:HA	2:N:220:PRO:HD3	1.93	0.40
2:G:180:PHE:HB3	2:G:203:PHE:CE2	2.56	0.40
2:F:105:HIS:O	2:F:110:GLY:N	2.55	0.40
2:J:131:VAL:HG11	2:J:213:VAL:HG13	2.03	0.40
1:L:100:VAL:HG21	1:L:138:ALA:HB1	2.02	0.40
1:D:8:ARG:HH21	1:D:244:ASP:HB2	1.86	0.40
1:E:96:PRO:HA	1:E:97:PRO:HD3	1.91	0.40
1:L:95:ARG:HD3	1:L:95:ARG:HA	1.93	0.40
1:H:159:GLY:HA3	1:H:173:LYS:HB2	2.03	0.40
1:A:156:SER:HB2	3:A:301:NAD:H6N	2.04	0.40
2:J:36:LEU:HB2	2:J:54:SER:HB2	2.03	0.40
1:I:219:THR:HG23	1:I:226:HIS:HA	2.03	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	242/261 (93%)	228 (94%)	13 (5%)	1 (0%)	39	71
1	D	242/261 (93%)	232 (96%)	10 (4%)	0	100	100
1	E	240/261 (92%)	232 (97%)	8 (3%)	0	100	100
1	H	236/261 (90%)	224 (95%)	12 (5%)	0	100	100
1	I	247/261 (95%)	233 (94%)	13 (5%)	1 (0%)	39	71
1	L	234/261 (90%)	224 (96%)	9 (4%)	1 (0%)	39	71
1	M	241/261 (92%)	230 (95%)	10 (4%)	1 (0%)	39	71
1	P	240/261 (92%)	225 (94%)	14 (6%)	1 (0%)	39	71
2	B	223/244 (91%)	215 (96%)	8 (4%)	0	100	100
2	C	208/244 (85%)	197 (95%)	11 (5%)	0	100	100
2	F	223/244 (91%)	208 (93%)	15 (7%)	0	100	100
2	G	198/244 (81%)	181 (91%)	17 (9%)	0	100	100
2	J	223/244 (91%)	211 (95%)	12 (5%)	0	100	100
2	K	212/244 (87%)	200 (94%)	11 (5%)	1 (0%)	34	67
2	N	225/244 (92%)	215 (96%)	10 (4%)	0	100	100
2	O	214/244 (88%)	207 (97%)	7 (3%)	0	100	100
All	All	3648/4040 (90%)	3462 (95%)	180 (5%)	6 (0%)	52	82

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ALA
1	M	203	ALA
1	P	205	PRO
2	K	57	VAL
1	L	203	ALA
1	I	203	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/198 (90%)	179 (100%)	0	100	100
1	D	171/198 (86%)	169 (99%)	2 (1%)	78	93
1	E	176/198 (89%)	173 (98%)	3 (2%)	68	89
1	H	170/198 (86%)	170 (100%)	0	100	100
1	I	175/198 (88%)	173 (99%)	2 (1%)	80	94
1	L	170/198 (86%)	166 (98%)	4 (2%)	57	84
1	M	179/198 (90%)	176 (98%)	3 (2%)	68	89
1	P	174/198 (88%)	169 (97%)	5 (3%)	50	81
2	B	151/193 (78%)	148 (98%)	3 (2%)	63	87
2	C	140/193 (72%)	138 (99%)	2 (1%)	74	91
2	F	154/193 (80%)	148 (96%)	6 (4%)	39	73
2	G	134/193 (69%)	126 (94%)	8 (6%)	24	53
2	J	153/193 (79%)	147 (96%)	6 (4%)	39	73
2	K	134/193 (69%)	129 (96%)	5 (4%)	41	74
2	N	155/193 (80%)	146 (94%)	9 (6%)	25	55
2	O	136/193 (70%)	130 (96%)	6 (4%)	35	68
All	All	2551/3128 (82%)	2487 (98%)	64 (2%)	55	84

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	25	LYS
2	B	62	ASP
2	B	195	LYS
2	C	57	VAL
2	C	78	ASN
1	D	7	ASN
1	D	83	ARG
1	E	8	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	118	ASP
1	E	212	GLN
2	F	32	ILE
2	F	71	GLU
2	F	217	LEU
2	F	228	VAL
2	F	236	ILE
2	F	237	LEU
2	G	16	ARG
2	G	34	ARG
2	G	36	LEU
2	G	60	GLU
2	G	94	ARG
2	G	99	ASP
2	G	119	MET
2	G	236	ILE
1	I	53	ARG
1	I	55	LEU
2	J	0	HIS
2	J	60	GLU
2	J	94	ARG
2	J	96	LYS
2	J	194	LEU
2	J	205	GLU
2	K	77	VAL
2	K	88	ARG
2	K	113	LEU
2	K	185	MET
2	K	200	LEU
1	L	8	ARG
1	L	83	ARG
1	L	118	ASP
1	L	206	MET
1	M	10	ARG
1	M	109	ASP
1	M	207	THR
2	N	60	GLU
2	N	62	ASP
2	N	77	VAL
2	N	96	LYS
2	N	121	THR
2	N	168	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	200	LEU
2	N	230	ASP
2	N	237	LEU
2	O	59	LYS
2	O	60	GLU
2	O	71	GLU
2	O	166	VAL
2	O	236	ILE
2	O	237	LEU
1	P	5	LEU
1	P	148	ARG
1	P	204	THR
1	P	207	THR
1	P	215	VAL

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	A	301	-	38,48,48	0.83	1 (2%)	47,73,73	1.57	5 (10%)
3	NAD	D	301	-	38,48,48	0.82	1 (2%)	47,73,73	1.55	4 (8%)
3	NAD	E	301	-	38,48,48	0.84	1 (2%)	47,73,73	1.58	5 (10%)
3	NAD	H	301	-	38,48,48	0.84	1 (2%)	47,73,73	1.58	5 (10%)
3	NAD	I	301	-	38,48,48	0.87	2 (5%)	47,73,73	1.66	6 (12%)
3	NAD	L	301	-	38,48,48	0.84	1 (2%)	47,73,73	1.58	5 (10%)
3	NAD	M	301	-	38,48,48	0.84	1 (2%)	47,73,73	1.57	4 (8%)
3	NAD	P	301	-	38,48,48	0.84	1 (2%)	47,73,73	1.57	5 (10%)

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
3	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	NAD	D	301	-	-	0/22/62/62	0/5/5/5
3	NAD	E	301	-	-	0/22/62/62	0/5/5/5
3	NAD	H	301	-	-	0/22/62/62	0/5/5/5
3	NAD	I	301	-	-	0/22/62/62	0/5/5/5
3	NAD	L	301	-	-	0/22/62/62	0/5/5/5
3	NAD	M	301	-	-	0/22/62/62	0/5/5/5
3	NAD	P	301	-	-	0/22/62/62	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	NAD	O4B-C1B	2.42	1.44	1.41
3	D	301	NAD	C5A-C4A	3.09	1.47	1.40
3	I	301	NAD	C5A-C4A	3.09	1.47	1.40
3	P	301	NAD	C5A-C4A	3.09	1.47	1.40
3	L	301	NAD	C5A-C4A	3.11	1.47	1.40
3	E	301	NAD	C5A-C4A	3.12	1.47	1.40
3	M	301	NAD	C5A-C4A	3.13	1.47	1.40
3	H	301	NAD	C5A-C4A	3.14	1.47	1.40
3	A	301	NAD	C5A-C4A	3.15	1.47	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	301	NAD	N3A-C2A-N1A	-6.90	123.61	128.89
3	M	301	NAD	N3A-C2A-N1A	-6.87	123.63	128.89
3	A	301	NAD	N3A-C2A-N1A	-6.85	123.65	128.89
3	D	301	NAD	N3A-C2A-N1A	-6.85	123.65	128.89
3	P	301	NAD	N3A-C2A-N1A	-6.81	123.68	128.89
3	H	301	NAD	N3A-C2A-N1A	-6.81	123.68	128.89
3	L	301	NAD	N3A-C2A-N1A	-6.74	123.73	128.89
3	I	301	NAD	N3A-C2A-N1A	-6.63	123.82	128.89
3	P	301	NAD	PN-O3-PA	-4.20	120.94	132.73
3	I	301	NAD	PN-O3-PA	-4.19	120.96	132.73
3	H	301	NAD	PN-O3-PA	-4.16	121.05	132.73
3	L	301	NAD	PN-O3-PA	-4.11	121.19	132.73
3	A	301	NAD	PN-O3-PA	-4.10	121.20	132.73
3	M	301	NAD	PN-O3-PA	-4.01	121.45	132.73
3	E	301	NAD	PN-O3-PA	-3.86	121.90	132.73
3	I	301	NAD	C2B-C1B-N9A	-3.76	108.54	114.29
3	D	301	NAD	PN-O3-PA	-3.72	122.30	132.73
3	I	301	NAD	C4A-C5A-N7A	-3.29	106.45	109.48
3	L	301	NAD	C4A-C5A-N7A	-3.26	106.48	109.48
3	E	301	NAD	C4A-C5A-N7A	-3.20	106.53	109.48
3	M	301	NAD	C4A-C5A-N7A	-3.20	106.54	109.48
3	H	301	NAD	C4A-C5A-N7A	-3.19	106.55	109.48
3	D	301	NAD	C4A-C5A-N7A	-3.17	106.56	109.48
3	P	301	NAD	C4A-C5A-N7A	-3.15	106.58	109.48
3	P	301	NAD	C2B-C1B-N9A	-3.09	109.57	114.29
3	A	301	NAD	C4A-C5A-N7A	-3.04	106.68	109.48
3	E	301	NAD	C2B-C1B-N9A	-3.03	109.66	114.29
3	H	301	NAD	C2B-C1B-N9A	-2.97	109.75	114.29
3	L	301	NAD	C2B-C1B-N9A	-2.91	109.85	114.29
3	A	301	NAD	C2B-C1B-N9A	-2.83	109.97	114.29
3	M	301	NAD	C2B-C1B-N9A	-2.83	109.97	114.29
3	D	301	NAD	C2B-C1B-N9A	-2.70	110.16	114.29
3	E	301	NAD	O4B-C1B-N9A	2.02	112.34	108.10
3	H	301	NAD	O4B-C1B-N9A	2.04	112.37	108.10
3	P	301	NAD	O4B-C1B-N9A	2.07	112.43	108.10
3	L	301	NAD	O4B-C1B-N9A	2.13	112.55	108.10
3	I	301	NAD	C2B-C3B-C4B	2.26	107.26	102.61
3	A	301	NAD	O4D-C1D-N1N	2.32	110.68	108.13
3	I	301	NAD	O4B-C1B-N9A	2.58	113.50	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAD	3	0
3	E	301	NAD	3	0
3	H	301	NAD	2	0
3	I	301	NAD	1	0
3	L	301	NAD	3	0
3	M	301	NAD	4	0
3	P	301	NAD	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	246/261 (94%)	-0.40	2 (0%) 87 86	24, 49, 80, 123	0
1	D	246/261 (94%)	-0.40	2 (0%) 87 86	26, 49, 79, 137	0
1	E	244/261 (93%)	-0.51	0 100 100	23, 45, 70, 120	0
1	H	242/261 (92%)	-0.35	0 100 100	32, 55, 86, 123	0
1	I	251/261 (96%)	-0.44	0 100 100	28, 47, 85, 158	0
1	L	240/261 (91%)	-0.41	0 100 100	28, 49, 88, 156	0
1	M	245/261 (93%)	-0.53	0 100 100	22, 43, 67, 94	0
1	P	246/261 (94%)	-0.40	0 100 100	25, 53, 89, 128	0
2	B	227/244 (93%)	-0.35	1 (0%) 93 92	22, 53, 89, 114	0
2	C	216/244 (88%)	-0.26	1 (0%) 91 90	29, 55, 101, 145	0
2	F	231/244 (94%)	-0.27	1 (0%) 93 92	29, 54, 94, 180	0
2	G	212/244 (86%)	-0.16	3 (1%) 78 75	35, 62, 100, 153	0
2	J	229/244 (93%)	-0.31	2 (0%) 85 84	27, 55, 96, 136	0
2	K	220/244 (90%)	-0.14	3 (1%) 78 75	32, 59, 99, 138	0
2	N	229/244 (93%)	-0.36	2 (0%) 85 84	28, 51, 87, 141	0
2	O	224/244 (91%)	-0.09	5 (2%) 65 61	32, 65, 95, 138	0
All	All	3748/4040 (92%)	-0.34	22 (0%) 90 89	22, 52, 91, 180	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	183	THR	4.9
2	N	0	HIS	4.4
1	D	58	PRO	4.1
2	F	31	VAL	4.0
2	J	89	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	74	LEU	3.7
2	O	44	GLY	3.6
1	D	57	GLY	3.3
2	C	11	SER	3.2
2	N	-3	HIS	2.8
2	K	46	LEU	2.6
2	G	84	ALA	2.6
2	G	72	LYS	2.6
2	O	80	LEU	2.5
2	O	73	HIS	2.4
2	O	87	ASN	2.3
2	B	75	GLY	2.2
1	A	35	GLY	2.2
2	K	201	GLY	2.2
2	G	58	ALA	2.2
2	O	117	ALA	2.1
1	A	94	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAD	L	301	44/44	0.84	0.25	1.46	76,100,128,220	0
3	NAD	H	301	44/44	0.89	0.22	1.18	45,73,108,151	0
3	NAD	P	301	44/44	0.92	0.20	0.92	42,74,93,113	0
3	NAD	A	301	44/44	0.96	0.16	0.27	29,57,80,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAD	E	301	44/44	0.97	0.14	-0.33	5,39,58,68	0
3	NAD	D	301	44/44	0.95	0.14	-0.38	19,49,82,93	0
3	NAD	M	301	44/44	0.96	0.14	-0.43	1,45,58,69	0
3	NAD	I	301	44/44	0.95	0.13	-0.87	7,42,61,87	0

6.5 Other polymers

There are no such residues in this entry.